USER GUIDE

1 How do I get set up? 3
2 How to read the documentation 5
3 Help - I looked at the documentation, but I don’t understand how …? 7
4 I found a bug 9
5 Citing TeNPy 11
6 Acknowledgment 13
7 License 15
  7.1 Installation instructions 15
  7.2 Release Notes 34
  7.3 Introductions 50
  7.4 Examples 93
  7.5 Literature and References 143
  7.6 Papers using TeNPy 144
  7.7 Contributing 147
  7.8 Tenpy main module 152
  7.9 algorithms 153
  7.10 linalg 218
  7.11 models 300
  7.12 networks 527
  7.13 tools 609
  7.14 version 657
8 Indices and tables 659

Bibliography 661

Python Module Index 665

Config Index 667

Config Option Index 669

Index 703
TeNPy (short for ‘Tensor Network Python’) is a Python library for the simulation of strongly correlated quantum systems with tensor networks.

The philosophy of this library is to get a new balance of a good readability and usability for new-comers, and at the same time powerful algorithms and fast development of new algorithms for experts. For good readability, we include an extensive documentation next to the code, both in Python doc strings and separately as user guides, as well as simple example codes and even toy codes, which just demonstrate various algorithms (like TEBD and DMRG) in ~100 lines per file.
CHAPTER ONE

HOW DO I GET SET UP?

If you have the conda package manager, you can install the latest released version of TeNPy with:

```
conda install --channel=conda-forge physics-tenpy
```

Further details and alternative methods can be found the file doc/INSTALL.rst. The latest version of the source code can be obtained from https://github.com/tenpy/tenpy.
CHAPTER TWO

HOW TO READ THE DOCUMENTATION

The documentation is available online at https://tenpy.readthedocs.io/. The documentation is roughly split in two parts: on one hand the full “reference” containing the documentation of all functions, classes, methods, etc., and on the other hand the “user guide” containing some introductions and additional explanations.

The documentation is based on Python’s docstrings, and some additional *.rst files located in the folder doc/ of the repository. All documentation is formatted as reStructuredText, which means it is quite readable in the source plain text, but can also be converted to other formats. If you like it simple, you can just use interactive python help(), Python IDEs of your choice or jupyter notebooks, or just read the source. Moreover, the documentation gets converted into HTML using Sphinx, and is made available online at https://tenpy.readthedocs.io/. The big advantages of the (online) HTML documentation are a lot of cross-links between different functions, and even a search function. If you prefer yet another format, you can try to build the documentation yourself, as described in doc/contr/build_doc.rst.
HELP - I LOOKED AT THE DOCUMENTATION, BUT I DON’T UNDERSTAND HOW …?

We have set up a community forum at https://tenpy.johannes-hauschild.de/, where you can post questions and hopefully find answers. Once you got some experience with TeNPy, you might also be able to contribute to the community and answer some questions yourself ;-) We also use this forum for official announcements, for example when we release a new version.
Chapter 3. Help - I looked at the documentation, but I don’t understand how ...?
I FOUND A BUG

You might want to check the github issues, if someone else already reported the same problem. To report a new bug, just open a new issue on github. If you already know how to fix it, you can just create a pull request :) If you are not sure whether your problem is a bug or a feature, you can also ask for help in the TeNPy forum.
Chapter 4. I found a bug
CITING TENPY

When you use TeNPy for a work published in an academic journal, you can cite this paper to acknowledge the work put into the development of TeNPy. (The license of TeNPy does not force you, however.) For example, you could add the sentence "Calculations were performed using the TeNPy Library (version X.X.X) \cite{tenpy}." in the acknowledgements or in the main text.

The corresponding BibTeX Entry would be the following (the \url{...} requires \usepackage{hyperref} in the LaTeX preamble):

```latex
@Article{tenpy,
  title={Efficient numerical simulations with Tensor Networks: Tensor Network \textarrow{\rightarrow} Python (TeNPy)},
  author={Johannes Hauschild and Frank Pollmann},
  pages={5},
  year={2018},
  publisher={SciPost},
  doi={10.21468/SciPostPhysLectNotes.5},
  url={https://scipost.org/10.21468/SciPostPhysLectNotes.5},
  archiveprefix={arXiv},
  eprint={1805.00055},
  note={Code available from \url{https://github.com/tenpy/tenpy}},
}
```

To keep us motivated, you can also include your work into the list of papers using TeNPy.
ACKNOWLEDGMENT

This work was funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05-CH11231 through the Scientific Discovery through Advanced Computing (SciDAC) program (KC23DAC Topological and Correlated Matter via Tensor Networks and Quantum Monte Carlo).
The code is licensed under GPL-v3.0 given in the file LICENSE of the repository, in the online documentation readable at https://tenpy.readthedocs.io/en/latest/install/license.html.

# 7.1 Installation instructions

With the [conda] package manager you can install python with:

```bash
conda install --channel=conda-forge physics-tenpy
```

More details and tricks in *Installation with conda from conda-forge*.

If you don’t have conda, but you have [pip], you can:

```bash
pip install physics-tenpy
```

More details for this method can be found in *Installation from PyPi with pip*.

We also have a bunch of optional *Extra requirements*, which you don’t have to install to use TeNPy, but you might want to.

The method with the minimal requirements is to just download the source and adjust the `PYTHONPATH`, as described in *Installation from source*. This is also the recommended way if you plan to modify parts of the source.

## 7.1.1 Installation with conda from conda-forge

We provide a package for the [conda] package manager in the conda-forge channel, so you can install TeNPy as:

```bash
conda install --channel=conda-forge physics-tenpy
```

Following the recommendation of conda-forge, you can also make conda-forge the default channel as follows:

```bash
conda config --add channels conda-forge
conda config --set channel_priority strict
```

If you have done this, you don’t need to specify the `--channel=conda-forge` explicitly.

Moreover, it is actually recommended to create a separate environment. To create a conda environment with the name `tenpy`, where the TeNPy package (called `physics-tenpy`) is installed:

```bash
conda create --name tenpy --channel=conda-forge physics-tenpy
```

In that case, you need to activate the environment each time you want to use the package with:
conda activate tenpy

The big advantage of this approach is that it allows multiple version of software to be installed in parallel, e.g., if one of your projects requires python>=3.8 and another one requires an old library which doesn’t support that. Further info can be found in the conda documentation.

### 7.1.2 Installation from PyPi with pip

**Preparation: install requirements**

If you have the [conda] package manager from anaconda, you can just download the environment.yml file out of the repository and create a new environment (called tenpy, if you don’t specify another name) for TeNPy with all the required packages:

```
conda env create -f environment.yml
conda activate tenpy
```

Further information on conda environments can be found in the conda documentation. Note that installing conda also installs a version of [pip].

Alternatively, if you only have [pip] (and not [conda]), install the required packages with the following command (after downloading the requirements.txt file from the repository):

```
pip install -r requirements.txt
```

**Note:** Make sure that the pip you call corresponds to the python version you want to use. (One way to ensure this is to use `python -m pip` instead of a simple `pip`.) Also, you might need to use the argument `--user` to install the packages to your home directory, if you don’t have `sudo` rights. (Using `--user` with conda’s pip is discouraged, though.)

**Warning:** It might just be a temporary problem, but I found that the pip version of numpy is incompatible with the python distribution of anaconda. If you have installed the intelpython or anaconda distribution, use the conda packagemanager instead of pip for updating the packages whenever possible!

### Installing the latest stable TeNPy package

Now we are ready to install TeNPy. It should be as easy as (note the different package name - ‘tenpy’ was taken!)

```
pip install physics-tenpy
```

**Note:** If the installation fails, don’t give up yet. In the minimal version, tenpy requires only pure Python with somewhat up-to-date NumPy and SciPy. See *Installation from source*.
Installation of the latest version from Github

To get the latest development version from the github main branch, you can use:

```
pip install git+git://github.com/tenpy/tenpy.git
```

This should already have the lastest features described in [latest]. Disclaimer: this might sometimes be broken, although we do our best to keep to keep it stable as well.

Installation from the downloaded source folder

Finally, if you downloaded the source and want to modify parts of the source, You can also install TeNPy with in development version with `--editable`:

```
cd $HOME/tenpy # after downloading the source, got to the repository
pip install --editable .
```

Uninstalling a pip-installed version

In all of the above cases, you can uninstall tenpy with:

```
pip uninstall physics-tenpy
```

### 7.1.3 Updating to a new version

**Before** you update, take a look at the Release Notes, which lists the changes, fixes, and new stuff. Most importantly, it has a section on backwards incompatible changes (i.e., changes which may break your existing code) along with information how to fix it. Of course, we try to avoid introducing such incompatible changes, but sometimes, there’s no way around them. If you skip some intermediate version(s) for the update, read also the release notes of those!

How to update depends a little bit on the way you installed TeNPy. Of course, you have always the option to just remove the TeNPy files (possibly with a pip uninstall physics-tenpy or conda uninstall physics-tenpy), and to start over with downloading and installing the newest version.

**When installed with conda**

When you installed TeNPy with [conda], you just need to activate the corresponding environment (e.g. conda activate tenpy) and do a:

```
conda update physics-tenpy
```

**When installed with pip**

When you installed TeNPy with [pip], you just need to do a:

```
pip install --upgrade physics-tenpy
```
When installed from source

If you used `git clone` ... to download the repository, you can update to the newest version using [git]. First, briefly check that you didn’t change anything you need to keep with `git status`. Then, do a `git pull` to download (and possibly merge) the newest commit from the repository.

**Note:** If some Cython file (ending in `.pyx`) got renamed/removed (e.g., when updating from v0.3.0 to v0.4.0), you first need to remove the corresponding binary files. You can do so with the command `bash cleanup.sh`.

Furthermore, whenever one of the cython files (ending in `.pyx`) changed, you need to re-compile it. To do that, simply call the command `bash ./compile.sh` again. If you are unsure whether a cython file changed, compiling again doesn’t hurt.

To summarize, you need to execute the following bash commands in the repository:

```
# 0) make a backup of the whole folder
git status  # check the output whether you modified some files
git pull
bash ./cleanup.sh  # (confirm with 'y')
bash ./compile.sh
```

7.1.4 Installation from source

Minimal Requirements

This code works with a minimal requirement of pure Python>=3.6 and somewhat recent versions of NumPy and SciPy.

Getting the source

The following instructions are for (some kind of) Linux, and tested on Ubuntu. However, the code itself should work on other operating systems as well (in particular MacOS and Windows).

The official repository is at [https://github.com/tenpy/tenpy.git](https://github.com/tenpy/tenpy.git). To get the latest version of the code, you can clone it with [git] using the following commands:

```
git clone https://github.com/tenpy/tenpy.git $HOME/TeNPy
cd $HOME/TeNPy
```

**Note:** Adjust `$HOME/TeNPy` to the path wherever you want to save the library.

Optionally, if you don’t want to contribute, you can checkout the latest stable release:

```
git tag  # this prints the available version tags
git checkout v0.3.0  # or whatever is the lastest stable version
```

**Note:** In case you don’t have [git] installed, you can download the repository as a ZIP archive. You can find it under releases, or the latest development version.
**Minimal installation: Including tenpy into PYTHONPATH**

The python source is in the directory `tenpy/` of the repository. This folder `tenpy/` should be placed in (one of the folders of) the environment variable `PYTHONPATH`. On Linux, you can simply do this with the following line in the terminal:

```
export PYTHONPATH=$HOME/TeNPy
```

(If you have already a path in this variable, separate the paths with a colon :) However, if you enter this in the terminal, it will only be temporary for the terminal session where you entered it. To make it permanently, you can add the above line to the file `$HOME/.bashrc`. You might need to restart the terminal session or need to relogin to force a reload of the `$HOME/.bashrc`.

Whenever the path is set, you should be able to use the library from within python:

```
>>> import tenpy
   warnings.warn("Couldn't load compiled cython code. Code will run a bit slower.")
>>> tenpy.show_config()
tenpy 0.4.0.dev0+7706003 (not compiled),
git revision 77060034a9fa64d2c7c16b4211e130cf5b6f5272 using
python 3.7.3 (default, Mar 27 2019, 22:11:17)
   [GCC 7.3.0]
numpy 1.16.3, scipy 1.2.1
```

`tenpy.show_config()` prints the current version of the used TeNPy library as well as the versions of the used python, numpy and scipy libraries, which might be different on your computer. It is a good idea to save this data (given as string in `tenpy.version.version_summary` along with your data to allow to reproduce your results exactly.

If you got a similar output as above: congratulations! You can now run the codes :)

**Compilation of np_conserved**

At the heart of the TeNPy library is the module `tenpy.linalg.np_conserved`, which provides an Array class to exploit the conservation of abelian charges. The data model of python is not ideal for the required book-keeping, thus we have implemented the same `np_conserved` module in Cython. This allows to compile (and thereby optimize) the corresponding python module, thereby speeding up the execution of the code. While this might give a significant speed-up for code with small matrix dimensions, don’t expect the same speed-up in cases where most of the CPU-time is already spent in matrix multiplications (i.e. if the bond dimension of your MPS is huge).

To compile the code, you first need to install Cython

```
conda install cython  # when using anaconda, or
pip install --upgrade Cython  # when using pip
```

Moreover, you need a C++ compiler. For example, on Ubuntu you can install `sudo apt-get install build_essential`, or on Windows you can download MS Visual Studio 2015. If you use anaconda, you can also use `conda install -c conda-forge cxx-compiler`.

After that, go to the root directory of TeNPy (`$HOME/TeNPy`) and simply run

```
bash ./compile.sh
```
Note: There is no need to compile if you installed TeNPy directly with conda or pip. (You can verify this with `tenpy.show_config()` as illustrated below.)

Note that it is not required to separately download (and install) Intel MKL: the compilation just obtains the includes from numpy. In other words, if your current numpy version uses MKL (as the one provided by anaconda), the compiled TeNPy code will also use it.

After a successful compilation, the warning that TeNPy was not compiled should go away:

```python
>>> import tenpy
>>> tenpy.show_config()
tenpy 0.4.0.dev0+b60bad3 (compiled from git rev. b60bad3243b7e54f549f4f7c1f074dc55bb54ba3),
git revision b60bad3243b7e54f549f4f7c1f074dc55bb54ba3 using
python 3.7.3 (default, Mar 27 2019, 22:11:17)
[GCC 7.3.0]
numpy 1.16.3, scipy 1.2.1
```

Note: For further optimization options, look at `tenpy.tools.optimization`.

### 7.1.5 Extra requirements

We have some extra requirements that you don’t need to install to use TeNPy, but that you might find useful to work with. TeNPy does not import the following libraries (at least not globally), but some functions might expect arguments behaving like objects from these libraries.

Note: If you created a [conda] environment with `conda env create -f environment.yml`, all the extra requirements below should already be installed :) (However, a `pip install -r requirements.txt` does not install them.)

**Matplotlib**

The first extra requirement is the [matplotlib] plotting library. Some functions expect a `matplotlib.axes.Axes` instance as argument to plot some data for visualization.

**Intel’s Math Kernel Library (MKL)**

If you want to run larger simulations, we recommend the use of Intel’s MKL. It ships with a Lapack library, and uses optimization for Intel CPUs. Moreover, it uses parallelization of the LAPACK/BLAS routines, which makes execution much faster. As of now, the library itself supports no other way of parallelization.

If you don’t have a python version which is built against MKL, we recommend using [conda] or directly `intelpython`. Conda has the advantage that it allows to use different environments for different projects. Both are available for Linux, Mac and Windows; note that you don’t even need administrator rights to install it on linux. Simply follow the (straight-forward) instructions of the web page for the installation. After a successful installation, if you run `python` interactively, the first output line should state the python version and contain Anaconda or Intel Corporation, respectively.

If you have a working conda package manager, you can install the numpy build against mkl with:
conda install mkl numpy scipy

Note: MKL uses different threads to parallelize various BLAS and LAPACK routines. If you run the code on a cluster, make sure that you specify the number of used cores/threads correctly. By default, MKL uses all the available CPUs, which might be in stark contrast than what you required from the cluster. The easiest way to set the used threads is using the environment variable `MKL_NUM_THREADS` (or `OMP_NUM_THREADS`). For a dynamic change of the used threads, you might want to look at `process`.

HDF5 file format support

We support exporting data to files in the [HDF5] format through the python interface of the `h5py` <https://docs.h5py.org/en/stable/> package, see Saving to disk: input/output for more information. However, that requires the installation of the HDF5 library and h5py.

YAML parameter files

The `tenpy.tools.params.Config` class supports reading and writing YAML files, which requires the package `pyyaml`; `pip install pyyaml`.

Tests

To run the tests, you need to install `pytest`, which you can for example do with `pip install pytest`. For information how to run the tests, see Checking the installation.

7.1.6 Checking the installation

The first check of whether tenpy is installed successfully, is to try to import it from within python:

```python
>>> import tenpy
```

Note: If this raises a warning Couldn't load compiled cython code. Code will run a bit slower., something went wrong with the compilation of the Cython parts (or you didn’t compile at all). While the code might run slower, the results should still be the same.

The function `tenpy.show_config()` prints information about the used versions of tenpy, numpy and scipy, as well on the fact whether the Cython parts were compiled and could be imported.

As a further check of the installation you can try to run (one of) the python files in the `examples/` subfolder; hopefully all of them should run without error.

You can also run the automated testsuite with `pytest` to make sure everything works fine. If you have `pytest` installed, you can go to the `tests` folder of the repository, and run the tests with:

```bash
cd tests
pytest
```

In case of errors or failures it gives a detailed traceback and possibly some output of the test. At least the stable releases should run these tests without any failures.
If you can run the examples but not the tests, check whether pytest actually uses the correct python version. The test suite is also run automatically by github actions and with travis-ci, results can be inspected here.

### 7.1.7 TeNPy developer team

The following people are part of the TeNPy developer team. The full list of contributors can be obtained from the git repository with `git --shortlog -sn`.

- Johannes Hauschild  
  tenpy@johannes-hauschild.de
- Frank Pollmann
- Michael P. Zaletel
- Maximilian Schulz
- Leon Schoonderwoerd
- Kévin Hémery
- Samuel Scalet
- Markus Drescher
- Wilhelm Kadow
- Gunnar Moeller
- Jakob Unfried
- Yu-Chin Tzeng

Further, the code is based on an earlier version of the library, mainly developed by Frank Pollmann, Michael P. Zaletel and Roger S. K. Mong.

### 7.1.8 License

The source code documented here is published under a GPL v3 license, which we include below.

---

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*Version 3, 29 June 2007*

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(continues on next page)
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7.1. Installation instructions
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7.2 Release Notes

The project adheres semantic versioning.

All notable changes to the project should be documented in the changelog. The most important things should be
summarized in the release notes.

The changes in [latest] are implemented in the latest development version on github, but not yet released.

Changes compared to previous TeNPy highlights the most important changes compared to the other, previously devel-
oped (closed source) TeNPy version.

7.2.1 [latest]

Release Notes

The default (stable) git branch was renamed from master to main.

Changelog

Backwards incompatible changes

- Drop official support for Python 3.5
- tenpy.linalg.np_conserved.from_ndarray(): raise ValueError instead of just a warning in case
  of the wrong non-zero blocks. This behaviour can be switched back with the new argument raise_wrong_sector.
- Argument \(v0\) of tenpy.networks.mps.MPS.TransferMatrix.eigenvectors() is renamed to
  \(v0\_npc\); \(v0\) now serves for non-\(np\_conserved\) guess.
Added

- `entanglement_entropy_segment2()`

- `tenpy.tools.misc.group_by_degeneracy()`

- `tenpy.tools.fit.entropy_profile_from_CFT()` and `central_charge_from_S_profile()`

- `tenpy.networks.site.Site.multiply_operators()` as a variant of `multiply_op_names()` accepting both string and npc arrays.

- `tenpy.tools.events.EventHandler()` to simplify call-backs e.g. for measurement codes during an algorithms.

- `tenpy.models.lattice.Lattice.Lu` as a class attribute.

Changed

- For finite DMRG, `DMRGEngine.N_sweeps_check` now defaults to 1 instead of 10 (which is still the default for infinite MPS).

- Merge
  ```python
  tenpy.linalg.sparse.FlatLinearOperator.npc_to_flat_all_sectors()
  ```
  into
  ```python
  npc_to_flat()
  ```
  merge
  ```python
  tenpy.linalg.sparse.FlatLinearOperator.flat_to_npc_all_sectors()
  ```
  into
  ```python
  flat_to_npc()
  ```

- Change the `chinfo.names` of the specific `Site` classes to be more consistent and clear.

- Add the more powerful `tenpy.networks.site.set_common_charges()` to replace `tenpy.networks.site.multi_sites_combine_charges()`.

Fixed

- The form of the eigenvectors returned by `tenpy.networks.mps.TransferMatrix.eigenvectors()` was dependent on the `charge_sector` given in the initialization; we try to avoid this now (if possible).

- The charge conserved by `SpinHalfFermionSite(cons_Sz='parity')` was wired.

- Allow to pass npc Arrays as Arguments to `expectation_value_multi_sites()` and other correlation functions (issue #116).

- `tenpy.tools.hdf5_io` did not work with h5py version >= (3,0) due to a change in string encoding (issue #117).
7.2.2 [0.7.2] - 2020-10-09

Release Notes

We’ve added a list of all papers using (and citing) TeNPy, see Papers using TeNPy. Feel free to include your own works!

And a slight simplicifation, which might affect your code: using the MultiCouplingModel is no longer necessary, just use the tenpy.models.model.CouplingModel directly.

Changelog

Backwards incompatible changes

- Deprecated the tenpy.models.model.MultiCouplingModel. The functionality is fully merged into the CouplingModel, no need to subclass the MultiCouplingModel anymore.
- The Kagome lattice did not include all next_next_nearest_neighbors. (It had only the ones across the hexagon, missing those maiking up a bow-tie.)
- Combined arguments onsite_terms and coupling_terms of tenpy.networks.mpo.MPOGraph. from_terms() into a single argument terms.

Added

- Allow to include jupyter notebooks into the documentation; collect example notebooks in [TeNPyNotebooks].
- term_correlation_function_right() and term_correlation_function_left() for correlation functions with more than one operator on each end.
- tenpy.networks.terms.ExponentiallyDecayingTerms for constructing MPOs with exponential decay. and tenpy.networks.model.CouplingModel.add_exponentially_decaying_coupling() for using it. This closes issue #78.

Fixed

- The IrregularLattice used the 'default' order of the regular lattice instead of whatever the order of the regular lattice was.
- charge_variance() did not work for more than 1 charge.

7.2.3 [0.7.1] - 2020-09-04

Release Notes

This is just a minor fix to allow building the conda package
7.2.4 [0.7.0] - 2020-09-04

Release Notes

The big new feature is the implementation of the $W_I$ and $W_{II}$ method for approximating exponentials of an MPO with an MPO, and MPS compression / MPO application to an MPS, to allow time evolution with $\text{ExpMPOEvolution}()$.

Changelog

Backwards incompatible changes

- Remove argument $\text{leg0}$ from $\text{build\_MPO}$.
- Remove argument $\text{leg0}$ from $\text{from\_grids}$, instead optionally give all legs as argument.
- Moved/renamed the module $\text{tenpy\_algorithms\_mps\_sweeps}$ to $\text{tenpy\_algorithms\_mps\_common}$. The old $\text{mps\_sweeps}$ still exists for compatibility, but raises a warning upon import.
- Moved/renamed the module $\text{tenpy\_algorithms\_purification\_tebd}$ to $\text{tenpy\_algorithms\_purification}$ (for the $\text{PurificationTEBD}$ and $\text{PurificationTEBD2}$) and $\text{tenpy\_algorithms\_disentangler}$ (for the disentanglers).

Added

- $\text{VariationalCompression}$ and $\text{VariationalApplyMPO}$ for variational compression
- $\text{PurificationApplyMPO}$ and $\text{PurificationTwoSiteU}$ for variational compression with purifications.
- Argument $\text{insert\_all\_id}$ for $\text{tenpy\_networks\_mpo\_MPOGraph\_from\_terms()}$ and $\text{from\_term\_list()}$
- implemented the $\text{IrregularLattice}$.
- extended user guide on lattices, $\text{Details on the lattice geometry}$.
- Function to approximate a decaying function by a sum of exponentials.
- $\text{spatial\_inversion()}$ to perform an explicit spatial inversion of the MPS.

Changed

- By default, for an usual MPO define $\text{IdL}$ and $\text{IdR}$ on all bonds. This can generate “dead ends” in the MPO graph of finite systems, but it is useful for the $\text{make\_WI/make\_WII}$ for MPO-exponentiation.
- $\text{tenpy\_models\_lattice\_Lattice\_plot\_basis()}$ now allows to shade the unit cell and shift the origin of the plotted basis.
- Don’t use $\text{bc\_shift}$ in $\text{tenpy\_models\_lattice\_Lattice\_plot\_couplings()}$ any more - it lead to confusing figures. Instead, the new keyword $\text{wrap=True}$ allows to directly connect all sites. This is done to avoid confusing in combination with $\text{plot\_bc\_identified()}$.
- Error handling of non-zero qtotal for $\text{TransferMatrix}$. 
Fixed

- Removed double counting of chemical potential terms in the `BosonicHaldaneModel` and `FermionicHaldaneModel`.
- Wrong results of `tenpy.networks.mps.MPS.get_total_charge()` with `only_physical_legs=True`.
- `tenpy.models.lattice.Lattice.plot_bc_identified()` had a sign error for the `bc_shift`.
- `calc_H_MPO_from_bond()` didn’t work for charges with blocks > 1.
- `tenpy.models.lattice.Lattice.plot_bc_identified()` had a sign error for the `bc_shift`.
- `order` model parameter was read out but not used in `tenpy.models.model.CouplingMPOModel`.

7.2.5 [0.6.1] - 2020-05-18

Release Notes

This only is a follow-up release to [0.6.0] - 2020-05-16. It fixes a small bug in the `examples/c_tebd.py` and some roundoff problems in the tests.

It is now possible to install TeNPy with the conda package manager:

```
conda install --channel=conda-forge physics-tenpy
```

7.2.6 [0.6.0] - 2020-05-16

Release Notes

This release contains a major update of the documentation, which is now hosted by “Read the Docs” at https://tenpy.readthedocs.io/. Update your bookmark :-)

Apart from that, this release introduces a format how to save and load data (in particular TeNPy classes) to HDF5 files. See Saving to disk: input/output for more details. To use that feature, you need to install the h5py package (and therefore some version of the HDF5 library). This is easy with anaconda, conda install h5py, but might be cumbersome on your local computing cluster. (However, many university computing clusters have some version of HDF5 installed already. Check with your local sysadmin.)

Moreover, we changed how we read out parameter dictionaries - instead of the `get_parameter()` function, we have now a `Config` class which behaves like a dictionary, you can simply use `options.get(key, default)` for model parameters - as you would do for a python dictionary.
Changelog

Backwards incompatible changes

- Created a class `Config` to replace Python-native parameter dictionaries and add some useful functionality. Old code using `tenpy.tools.params.get_parameter()` and `tenpy.tools.params.unused_parameters()` still works as before, but raises a warning, and should be replaced. For example, if you defined your own models, you should replace calls `get_parameter(model_params, "key", "default_value", "ModelName")` with `model_params.get("key", "default_value")`, the latter syntax being what you would use for a normal python dictionary as well.

- Renamed the following class parameter dictionaries to simply `options` for more consistency. Old code using the class attributes should still work (since we provide property aliases), but raises warnings. Note that this affects also derived classes (for example the `TwoSiteDMRGEngine`).
  - `tenpy.algorithms.dmrg.DMRGEngine.DMRG_params` (was already renamed to `engine_params` in versin 0.5.0)
  - `tenpy.algorithms.mps_common.Sweep.engine_params`
  - `tenpy.algorithms.tebd.Engine.TEBD_params`
  - `tenpy.algorithms.tdvp.Engine.TDVP_params`
  - `tenpy.linalg.lanczos.Lanczos`

- Changed the arguments of `tenpy.models.model.MultiCouplingModel()`: We replaced the three arguments `u0, op0` and `other_op` with `other_ops=[(u1, op1, dx1), (op2, u2, dx2), ...]` by single, equivalent argument `ops` which should now read `ops=[(op0, dx0, u0), (op1, dx1, u1), (op2, dx2, u2), ...]`, where `dx0 = [0]*lat.dim`. Note the changed order inside the tuple! Old code (which specifies `opstr` and `category` as keyword argument, if at all) still works as before, but raises a warning, and should be replaced. Since `tenpy.lattice.Lattice.possible_multi_couplings()` used similar arguments, they were changed as well.

- Don’t save `H_MPO_graph` as model attribute anymore - this also wasn’t documented.

- Renamed the truncation parameter `symmetry_tol` to `degeneracy_tol` and make the criterion more reasonable by not checking \( \log(S_i/S_j) < \log(symmetry_{tol}) \), but simply \( \log(S_i/S_j) < degeneracy_{tol} \). The latter makes more sense, as it is equivalent to \( (S_i - S_j)/S_j < \exp(degeneracy_{tol}) - 1 = degeneracy_{tol} + O(degeneracy_{tol}^2) \).

- Deprecated `tenpy.networks.mps.MPS.increase_L()` in favor of the newly added `tenpy.networks.mps.MPS.enlarge_mps_unit_cell()` (taking `factor` instead of `new_L=factor*L` as argument).

- `tenpy.networks.mps.MPS.correlation_function()` now auto-determines whether a Jordan-Wigner string is necessary. If any of the given operators is directly an npc Array, it will now raise an error; set `autoJW=False` in that case.

- Instead of “monkey-patching” `matvec` of the `tenpy.algorithms.mps_common.EffectiveH` for the case that `ortho_to_ens` is not empty, we defined a proper class `NpcLinearOperatorWrapper`, which serves as baseclass for `OrthogonalNpcLinearOperator`. The argument `ortho_to_ens` has been removed from `EffectiveH`.

- Switch order of the sites in the unit cell for the `DualSquare`, and redefine what the "default" order means. This is a huge optimization of DMRG, reducing the necessary MPS bond dimension for the ground state to the optimal \( 2^{L-1} \) on each bond.

- Deprecated the Lanczos function/class argument `orthogonal_to` of in `LanczosGroundState`. Instead, one can use the `OrthogonalNpcLinearOperator`.

7.2. Release Notes
• Deprecation warning for changing the default argument of shift_ket for non-zero shift_bra of the TransferMatrix.

Added

• `tenpy.networks.mpo.MPO.variance()` to calculate the variance of an MPO against a finite MPS.
• Classmethod `tenpy.networks.MPS.from_lat_product_state()` to initialize an MPS from a product state given in lattice coordinates (independent of the order of the lattice).
• argument `plus_hc` for `tenpy.models.model.CouplingModel.add_onsite()`, `tenpy.models.model.CouplingModel.add_coupling()`, and `tenpy.models.model.MultiCouplingModel.add_multi_coupling()` to simplify adding the hermitian conjugate terms.
• parameter `explicit_plus_hc` for `MPOModel`, `CouplingModel` and MPO, to reduce MPO bond dimension by not storing Hermitian conjugate terms, but computing them at runtime.
• `tenpy.models.model.CouplingModel.add_local_term()` for adding a single term to the lattice, and still handling Jordan-Wigner strings etc.
• `tenpy.networks.site.Site.get_hc_opname()` and `hc_ops` to allow getting the hermitian conjugate operator (name) of the onsite operators.
• `tenpy.tools.hdf5_io` with convenience functions for import and output with pickle, as well as an implementation allowing to save and load objects to HDF5 files in the format specified in Saving to disk: input/output.
• human-readable `boundary_conditions` property in `Lattice`.
• `save_hdf5` and `load_hdf5` methods to support saving/loading to HDF5 for the following classes (and their subclasses): ChargeInfo - LegCharge - LegPipe - Array - MPS - MPO - Lattice
• `tenpy.networks.mps.MPSEnvironment.get_initialization_data()` for a convenient way of saving the necessary parts of the environment after an DMRG run.
• Method `enlarge_mps_unit_cell` for the following classes: MPS - MPO - Lattice - Model, MPOModel, NearestNeighborModel
• `tenpy.tools.misc.to_iterable_of_len()` for convenience of handling arguments.
• `tenpy.models.lattice.Lattice.mps2lat_values_masked()` as generalization of `tenpy.models.lattice.Lattice.mps2lat_values()`.
• `tenpy.linalg.sparse.OrthogonalNpcLinearOperator` to orthogonalize against vectors.
• `tenpy.linalg.sparse.ShiftNpcLinearOperator` to add a constant.
• `tenpy.linalg.sparse.SumNpcLinearOperator` which serves e.g. to add the h.c. during the matvec (in combination with the new `tenpy.linalg.sparse.NpcLinearOperator.adjoint()`).
• `tenpy.algorithms.mps_common.make_eff_H()` to simplify implementations of prepare_update().
• attribute `options` for the Model.
• `tenpy.networks.mps.MPS.roll_mps_unit_cell()`.
Changed

- **DEFAULT DMRG parameter 'diag_method'** from 'lanczos' to 'default', which is the same for large bond dimensions, but performs a full exact diagonalization if the effective Hamiltonian has small dimensions. The threshold introduced is the new DMRG parameter 'max_N_for_ED'.

- **DEFAULT parameter charge_sector=None instead of charge_sector=0** in tenpy.networks.mps.MPS.overlap() to look for eigenvalues of the transfer matrix in all charge sectors, and not assume that it's the 0 sector.

- Derive the following classes (and their subclasses) from the new Hdf5Exportable to support saving to HDF5: Site - Terms - OnsiteTerms - CouplingTerms - Model, i.e., all model classes.

- Instead of just defining to_matrix and adjoint for EffectiveH, define the interface directly for NpcLinearOperator.

- Try to keep the charge block structure as far as possible for add_charge() and drop_charge()?

Fixed

- Adjust the default DMRG parameter min_sweeps if chi_list is set.

- Avoid some unnecessary transpositions in MPO environments for MPS sweeps (e.g. in DMRG).

- sort(bunch=True) could return un-bunched Array, but still set the bunched flag.

- **LegPipe** did not initialize self.bunched correctly.

- **issue #98**: Error of calling psi.canonical_form() directly after disabling the DMRG mixer.

- **svd()** with full_matrices=True gave wrong charges.

- tenpy.linalg.np_conserved.Array.drop_charge() and tenpy.lina.np_conserved.Array.drop_charge() did not copy over labels.

- wrong pairs for the fifth_nearest_neighbors of the Honeycomb.

- Continue in tenpy.algorithms.dmrg.full_diag_effH() with a warning instead of raising an Error, if the effective Hamiltonian is zero.

- **correlation_length():** check for hermitian Flag might have raised and Error with new numpy warnings

- correlation_function did not respect argument str_on_first=False.

- tenpy.networks.mps.MPS.get_op() worked unexpected for infinite bc with incomensurate self.L and len(op_list).

- tenpy.networks.mps.MPS.permute_sites() did modify the given perm.

- **issue #105** Unintended side-effects using lanczos_params.verbose in combination with orthogonal_to

- **issue #108** tenpy.linalg.sparse.FlatLinearOperator._matvec() changes self._charge_sector
7.2.7 [0.5.0] - 2019-12-18

Backwards incompatible changes

- **Major** rewriting of the DMRG Engines, see issue #39 and issue #85 for details. The EngineCombine and EngineFracture have been combined into a single TwoSiteDMRGEngine with an The run function works as before. In case you have directly used the EngineCombine or EngineFracture, you should update your code and use the TwoSiteEngine instead.

- Moved init_LP and init_RP method from MPS into MPSEnvironment and MPOEnvironment.

Changed

- Addition/subtraction of Array: check whether the both arrays have the same labels in Different order, and in that case raise a warning that we will transpose in the future.


- groundstate() now returns a tuple (E0, psi0) instead of just psi0. Moreover, the argument charge_sector was added.

- Simplification in the Lattice: Instead of having separate arguments/attributes/functions for 'nearest_neighbors', 'next_nearest_neighbors', 'next_next_nearest_neighbors' and possibly (Honeycomb) even 'fourth_nearest_neighbors', 'fifth_nearest_neighbors', collect them in a dictionary called pairs. Old call structures still allowed, but deprecated.

- issue #94: Array addition and inner() should reflect the order of the labels, if they coincided. Will change the default behaviour in the future, raising FutureWarning for now.

- Default parameter for DMRG params: increased precision by setting P_tol_min down to the maximum of 1.e-30, lanczos_params['svd_min']**2 * P_tol_to_trunc, lanczos_params['trunc_cut']**2 * P_tol_to_trunc by default.

Added

- tenpy.algorithms.mps_common with the Sweep class and EffectiveH to be a OneSiteH or TwoSiteH.

- Single-Site DMRG with the SingleSiteDMRG.

- Example function in examples/c_tebd.py how to run TEBD with a model originally having next-nearest neighbors.

- increase_L() to allow increasing the unit cell of an MPS.

- Additional option order='folded' for the Chain.

- tenpy.algorithms.exact_diag.ExactDiag.from_H_mpo() wrapper as replacement for tenpy.networks.mpo.MPO.get_full_hamiltonian() and tenpy.networks.mpo.MPO.get_grouped_mpo(). The latter are now deprecated.

- Argument max_size to limit the matrix dimension in ExactDiag.

- tenpy.linalg.sparse.FlatLinearOperator.from_guess_with_pipe() to allow quickly converting matvec functions acting on multi-dimensional arrays to a FlatLinearOperator by combining the legs into a LegPipe.
• `tenpy.tools.math.speigsh()` for hermitian variant of `speigs()`

• Allow for arguments 'LA', 'SA' in `argsort()`.

• `tenpy.linalg.lanczos.lanczos_arpack()` as possible replacement of the self-implemented `lanczos` function.

• `tenpy.algorithms.dmrg.full_diag_effH()` as another replacement of `lanczos()`.

• The new DMRG parameter 'diag_method' allows to select a method for the diagonalization of the effective Hamiltonian. See `tenpy.algorithms.dmrgr.DMRGEngine.diag()` for details.

• `dtype` attribute in `EffectiveH`.

• `tenpy.linalg.charges.LegCharge.get_qindex_of_charges()` to allow selecting a block of an Array from the charges.

• `tenpy.algorithms.mps_common.EffectiveH.to_matrix` to allow contracting an `EffectiveH` to a matrix, as well as metadata `tenpy.linalg.sparse.NpcLinearOperator.acts_on` and `tenpy.algorithms.mps_common.EffectiveH.N`.

• Argument `only_physical_legs` in `tenpy.networks.mps.MPS.get_total_charge()`

Fixed

• MPO `expectation_value()` did not work for finite systems.

• Calling `compute_K()` repeatedly with default parameters but on states with different `chi` would use the `chi` of the very first call for the truncation parameters.

• Allow MPSEnvironment and MPOEnvironment to have MPS/MPO with different length.

• `group_sites()` didn't work correctly in some situations.

• `matvec_to_array()` returned the transposed of A.

• `tenpy.networks.mps.MPS.from_full()` messed up the form of the first array.

• Issue #95: blowup of errors in DMRG with `update_env > 0`. Turns out to be a problem in the precision of the truncation error: `TruncationError.eps` was set to 0 if it would be smaller than machine precision. To fix it, I added `from_S()`.

7.2.8 [0.4.1] - 2019-08-14

Backwards incompatible changes

• Switch the sign of the BoseHubbardModel and FermiHubbardModel to hopping and chemical potential having negative prefactors. Of course, the same adjustment happens in the BoseHubbardChain and FermiHubbardChain.

• Moved BoseHubbardModel and BoseHubbardChain as well as FermiHubbardModel and FermiHubbardChain into the new module `tenpy.models.hubbard`.

• Change arguments of `coupling_term_handle_JW()` and `multi_coupling_term_handle_JW()` to use `strength` and `sites` instead of `op_needs_JW`.

• Only accept valid identifiers as operator names in `add_op()`.
Changed

- `grid_concat()` allows for `None` entries (representing zero blocks).
- `from_full()` allows for ‘segment’ boundary conditions.
- `apply_local_op()` allows for n-site operators.

Added

- `max_range` attribute in MPO and `MPOGraph`.
- `is_hermitian()`
- Nearest-neighbor interaction in `BoseHubbardModel`
- `multiply_op_names()` to replace `' '.join(op_names)` and allow explicit compression/multiplication.
- `order_combine_term()` to group operators together.
- `dagger()` of MPO’s (and to implement that also `flip_charges_qconj()`).
- `has_label()` to check if a label exists
- `qr_li()` and `rq_li()`
- Addition of MPOs
- 3 additional examples for chern insulators in `examples/chern_insulators/`
- `FermionicHaldaneModel` and `BosonicHaldaneModel`.
- `from_MPOModel()` for initializing nearest-neighbor models after grouping sites.

Fixed

- Issue #36: long-range couplings could give `IndexError`.
- Issue #42: Onsite-terms in `FermiHubbardModel` were wrong for lattices with non-trivial unit cell.
- Missing a factor 0.5 in `GUE()`.
- Allow `TermList` to have terms with multiple operators acting on the same site.
- Allow MPS indices outside unit cell in `mps2lat_idx()` and `lat2mps_idx()`.
- `expectation_value()` did not work for n-site operators.

7.2.9 [0.4.0] - 2019-04-28

Backwards incompatible changes

- The argument order of `tenpy.models.lattice.Lattice` could be a tuple `(priority, snake_winding)` before. This is no longer valid and needs to be replaced by ("standard", snake_winding, priority).
- Moved the boundary conditions `bc_coupling` from the `tenpy.models.model.CouplingModel` into the `tenpy.models.lattice.Lattice` (as `bc`). Using the parameter `bc_coupling` will raise a FutureWarning, one should set the boundary conditions directly in the lattice.
• Added parameter `permute` (True by default) in `tenpy.networks.mps.MPS.from_product_state()` and `tenpy.networks.mps.MPS.from_Bflat()`. The resulting state will therefore be independent of the "conserve" parameter of the Sites - unlike before, where the meaning of the `p_state` argument might have changed.

• Generalize and rename `tenpy.networks.site.DoubleSite` to `tenpy.networks.site.GroupedSite`, to allow for an arbitrary number of sites to be grouped. Arguments `site0`, `sitel`, `label0`, `label1` of the `__init__` can be replaced with `[site0, sitel], [label0, label1]` and `op0`, `op1` of the `kronecker_product` with `[op0, op1]`; this will recover the functionality of the `DoubleSite`.

• Restructured callstructure of Mixer in DMRG, allowing an implementation of other mixers. To enable the mixer, set the DMRG parameter "mixer" to True or 'DensityMatrixMixer' instead of just 'Mixer'.

• The interaction parameter in the `tenpy.models.bose_hubbard_chain.BoseHubbardModel` (and `tenpy.models.bose_hubbard_chain.BoseHubbardChain`) did not correspond to $\frac{U}{2}N(\frac{N}{2} - 1)$ as claimed in the Hamiltonian, but to $UN^2$. The correcting factor 1/2 and change in the chemical potential have been fixed.

• Major restructuring of `tenpy.linalg.np_conserved` and `tenpy.linalg.charges`. This should not break backwards-compatibility, but if you compiled the cython files, you need to remove the old binaries in the source directory. Using bash `cleanup.sh` might be helpful to do that, but also remove other files within the repository, so be careful and make a backup beforehand to be on the save side. Afterwards recompile with bash `compile.sh`.

• Changed structure of `tenpy.models.model.CouplingModel.onsite_terms` and `tenpy.models.model.CouplingModel.coupling_terms`: Each of them is now a dictionary with category strings as keys and the newly introduced `tenpy.networks.terms.OnsiteTerms` and `tenpy.networks.terms.CouplingTerms` as values.

• `tenpy.models.model.CouplingModel.calc_H_onsite()` is deprecated in favor of new methods.

• Argument `raise_op2_left` of `tenpy.models.model.CouplingModel.add_coupling()` is deprecated.

**Added**

• `tenpy.networks.mps.MPS.canonical_form_infinite()`.

• `tenpy.networks.mps.MPS.expectation_value_term()`, `tenpy.networks.mps.MPS.expectation_value_terms_sum()` and `tenpy.networks.mps.MPS.expectation_value_multi_sites()` for expectation values of terms.

• `tenpy.networks.mpo.MPO.expectation_value()` for an MPO.

• `tenpy.linalg.np_conserved.Array.extend()` and `tenpy.linalg.charges.LegCharge.extend()`, allowing to extend an Array with zeros.

• DMRG parameter 'orthogonal_to' allows to calculate excited states for finite systems.

• possibility to change the number of charges after creating LegCharges/Arrays.

• more general way to specify the order of sites in a `tenpy.models.lattice.Lattice`.

• new `tenpy.models.lattice.Triangular`, `tenpy.models.lattice.Honeycomb` and `tenpy.models.lattice.Kagome` lattice

• a way to specify nearest neighbor couplings in a `Lattice`, along with methods to count the number of nearest neighbors for sites in the bulk, and a way to plot them (plot_coupling() and friends)

• `tenpy.networks.mpo.MPO.from_grids()` to generate the MPO from a grid.

• `tenpy.models.model.MultiCouplingModel` for couplings involving more than 2 sites.
• request #8: Allow shift in boundary conditions of `CouplingModel`.
• Allow to use state labels in `tenpy.networks.mps.MPS.from_product_state()`.
• `tenpy.models.model.CouplingMPOModel` structuring the default initialization of most models.
• Allow to force periodic boundary conditions for finite MPS in the `CouplingMPOModel`. This is not recommended, though.
• `tenpy.models.model.NearestNeighborModel.calc_H_MPO_from_bond()` and `tenpy.models.model.MPOModel.calc_H_bond_from_MPO()` for conversion of $H_{\text{bond}}$ into $H_{\text{MPO}}$ and vice versa.
• `tenpy.algorithms.tebd.RandomUnitaryEvolution` for random unitary circuits
• `tenpy.models.model.CouplingModel.coupling_strength_add_ext_flux()` for adding hoppings with external flux.
• `tenpy.models.model.CouplingModel.plot_coupling_terms()` to visualize the added coupling terms.
• `tenpy.networks.terms.OnsiteTerms`, `tenpy.networks.terms.CouplingTerms`, `tenpy.networks.terms.MultiCouplingTerm` containing the of terms for the `CouplingModel` and `MultiCouplingModel`. This allowed to add the `category` argument to `add_onsite`, `add_coupling` and `add_multi_coupling`.
• `tenpy.networks.terms.TermList` as another (more human readable) representation of terms with conversion from and to the other `*Term` classes.
• `tenpy.networks.mps.MPS.init_LP()` and `tenpy.networks.mps.MPS.init_RP()` to initialize left and right parts of an Environment.
• `tenpy.networks.mpo.MPOGraph.from_terms()` and `tenpy.networks.mpo.MPOGraph.from_term_list()`.
• argument `charge_sector` in `tenpy.networks.mps.MPS.correlation_length()`.

**Changed**

• moved toycodes from the folder `examples/` to a new folder `toycodes/` to separate them clearly.
• major remodelling of the internals of `tenpy.linalg.np_conserv` and `tenpy.linalg.charges`.
  – Introduced the new module `tenpy/linalg/_npc_helper.pyx` which contains all the Cython code, and gets imported by
  – `Array` now rejects addition/subtraction with other types
  – `Array` now rejects multiplication/division with non-scalar types
  – By default, make deep copies of npc Arrays.
• Restructured lanczos into a class, added time evolution calculating $\exp(A dt)|\psi_0>$
• Warning for poorly conditioned Lanczos; to overcome this enable the new parameter `reortho`.
• Simplified call structure of `extend()`, and `extend()`.
• Restructured `tenpy.algorithms.dmrg`:
- run() is now just a wrapper around the new run().run(psi, model, pars) is roughly equivalent to eng = EngineCombine(psi, model, pars); eng.run().
- Added init_env() and reset_stats() to allow a simple restart of DMRG with slightly different parameters, e.g. for tuning Hamiltonian parameters.
- Call canonical_form() for infinite systems if the final state is not in canonical form.

- Changed default values for some parameters:
  - set trunc_params['chi_max'] = 100. Not setting a chi_max at all will lead to memory problems. Disable DMRG_params['chi_list'] = None by default to avoid conflicting settings.
  - reduce to mixer_params['amplitude'] = 1.e-5. A too strong mixer screws DMRG up pretty bad.
  - increase Lanczos_params['N_cache'] = N_max (i.e., keep all states)
  - set DMRG_params['P_tol_to_trunc'] = 0.05 and provide reasonable ..._min and ..._max values.
  - increased (default) DMRG accuracy by setting DMRG_params['max_E_err'] = 1.e-8 and DMRG_params['max_S_err'] = 1.e-5.
  - don’t check the (absolute) energy for convergence in Lanczos.
  - set DMRG_params['norm_tol'] = 1.e-5 to check whether the final state is in canonical form.

- Verbosity of get_parameter() reduced: Print parameters only for verbosity >=1. and default values only for verbosity >= 2.

- Don’t print the energy during real-time TEBD evolution - it’s preserved up to truncation errors.
- Renamed the SquareLattice class to tenpy.models.lattice.Square for better consistency.
- auto-determine whether Jordan-Wigner strings are necessary in add_coupling().
- The way the labels of npc Arrays are stored internally changed to a simple list with None entries. There is a deprecated propery setter yielding a dictionary with the labels.
- renamed first_LP and last_RP arguments of MPSEnvironment and MPOEnvironment to init_LP and init_RP.
- Testing: insetad of the (outdated) nose, we now use pytest <https://pytest.org> for testing.

Fixed

- issue #22: Serious bug in tenpy.linalg.np_conserved.inner(): if do_conj=True is used with non-zero qtotal, it returned 0. instead of non-zero values.
- avoid error in tenpy.networks.mps.MPS.apply_local_op()
- Don’t carry around total charge when using DMRG with a mixer
- Corrected couplings of the FermionicHubbardChain
- issue #2: memory leak in cython parts when using intelpython/anaconda
- issue #4: incompatible data types.
- issue #6: the CouplingModel generated wrong Couplings in some cases
- issue #19: Convergence of energy was slow for infinite systems with N_sweeps_check=1
- more reasonable traceback in case of wrong labels
• wrong dtype of npc.Array when adding/subtracting/... arrays of different data types
• could get wrong H_bond for completely decoupled chains.
• SVD could return outer indices with different axes
• tenpy.networks.mps.MPS.overlap() works now for MPS with different total charge (e.g. after psi.
  apply_local_op(i, 'Sp')).
• skip existing graph edges in MPOGraph.add() when building up terms without the strength part.

Removed

• Attribute chinfo of Lattice.

7.2.10 [0.3.0] - 2018-02-19

This is the first version published on github.

Added

• Cython modules for np_conserved and charges, which can optionally be compiled for speed-ups
• tools.optimization for dynamical optimization
• Various models.
• More predefined lattice sites.
• Example toy-codes.
• Network contractor for general networks

Changed

• Switch to python3

Removed

• Python 2 support.

7.2.11 [0.2.0] - 2017-02-24

• Compatible with python2 and python3 (using the 2to3 tool).
• Development version.
• Includes TEBD and DMRG.
7.2.12 Changes compared to previous TeNPy

This library is based on a previous (closed source) version developed mainly by Frank Pollmann, Michael P. Zaletel and Roger S. K. Mong. While almost all files are completely rewritten and not backwards compatible, the overall structure is similar. In the following, we list only the most important changes.

Global Changes

- syntax style based on PEP8. Use $>yapf -r -i ./ to ensure consistent formatting over the whole project. Special comments # yapf: disable and # yapf: enable can be used for manual formatting of some regions in code.

- Following PEP8, we distinguish between ‘private’ functions, indicated by names starting with an underscore and to be used only within the library, and the public API. The public API should be backwards-compatible with different releases, while private functions might change at any time.

- all modules are in the folder tenpy to avoid name conflicts with other libraries.

- within the library, relative imports are used, e.g., from ..tools.math import (toiterable, tonparray) Exception: the files in tests/ and examples/ run as __main__ and can’t use relative imports

- Introduced the class LegPipe to replace the old leg_pipe. It is derived from LegCharge and used as a leg in the array class. Thus any inherited array (after tensordot etc still has all the necessary information to split the legs. (The legs are shared between different arrays, so it’s saved only once in memory)

- Enhanced indexing of the array class to support slices and 1D index arrays along certain axes

- Introduced TruncationError for easy handling of total truncation error.

- some truncation parameters are renamed and may have a different meaning, e.g. svd_max -> svd_min has no ‘log’ in the definition.
DMRG

- separate Lanczos module in `tenpy/linalg/`. Strangely, the old version orthogonalized against the complex conjugates of `orthogonal_to` (contrary to it’s doc string!) (and thus calculated ‘theta_o’ as bra, not ket).

- cleaned up, provide prototypes for DMRG engine and mixer.

Tools

- added `tenpy.tools.misc`, which contains ‘random stuff’ from old `tools.math` like `to_iterable` and `to_array` (renamed to follow PEP8, documented)

- moved stuff for fitting to `tenpy.tools.fit`

- enhanced `tenpy.tools.string.vert_join()` for nice formatting

- moved (parts of) old `cluster/omp.py` to `tenpy.tools.process`

- added `tenpy.tools.params` for a simplified handling of parameter/arguments for models and/or algorithms. Similar as the old `models.model.set_var`, but use it also for algorithms. Also, it may modify the given dictionary.

7.3 Introductions

The following documents are meant as introductions to various topics relevant to TeNPy.

If you are new to TeNPy, read the **Overview**.

7.3.1 Overview

Repository

The root directory of the git repository contains the following folders:

- **tenpy** The actual source code of the library. Every subfolder contains an `__init__.py` file with a summary what the modules in it are good for. (This file is also necessary to mark the folder as part of the python package. Consequently, other subfolders of the git repo should not include a `__init__.py` file.)

- **toycodes** Simple toy codes completely independet of the remaining library (i.e., codes in `tenpy/`). These codes should be quite readable and intend to give a flavor of how (some of) the algorithms work.

- **examples** Some example files demonstrating the usage and interface of the library.

- **doc** A folder containing the documentation: the user guide is contained in the `*.rst` files. The online documentation is autogenerated from these files and the docstrings of the library. This folder contains a make file for building the documentation, run `make help` for the different options. The necessary files for the reference in `doc/reference` can be auto-generated/updated with `make src2html`.

- **tests** Contains files with test routines, to be used with `pytest`. If you are set up correctly and have `pytest` installed, you can run the test suite with `pytest` from within the `tests/` folder.

- **build** This folder is not distributed with the code, but is generated by `setup.py` (or `compile.sh`, respectively). It contains compiled versions of the Cython files, and can be ignored (and even removed without loosing functionality).


**Code structure: getting started**

There are several layers of abstraction in TeNPy. While there is a certain hierarchy of how the concepts build up on each other, the user can decide to utilize only some of them. A maximal flexibility is provided by an object oriented style based on classes, which can be inherited and adjusted to individual demands.

The following figure gives an overview of the most important modules, classes and functions in TeNPy. Gray backgrounds indicate (sub)modules, yellow backgrounds indicate classes. Red arrows indicate inheritance relations, dashed black arrows indicate a direct use. (The individual models might be derived from the `NearestNeighborModel` depending on the geometry of the lattice.) There is a clear hierarchy from high-level algorithms in the `tenpy.algorithms` module down to basic operations from linear algebra in the `tenpy.linalg` module.
Most basic level: linear algebra

Note: See Charge conservation with np_conserved for more information on defining charges for arrays.

The most basic layer is given by the \texttt{linalg} module, which provides basic features of linear algebra. In particular, the \texttt{np_conserved} submodule implements an \texttt{Array} class which is used to represent the tensors. The basic interface of \texttt{np_conserved} is very similar to that of the NumPy and SciPy libraries. However, the \texttt{Array} class implements abelian charge conservation. If no charges are to be used, one can use ‘trivial’ arrays, as shown in the following example code.

```python
"""Basic use of the `Array` class with trivial arrays."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3
import tenpy.linalg.np_conserved as npc

M = npc.Array.from_ndarray_trivial([[0., 1.], [1., 0.]])
v = npc.Array.from_ndarray_trivial([2., 4. + 1.j])
v[0] = 3.  # set individual entries like in numpy
print("|v> =", v.to_ndarray())
# |v> = [ 3.+0.j 4.+1.j]
M_v = npc.tensordot(M, v, axes=[1, 0])
print("M|v> =", M_v.to_ndarray())
# M|v> = [ 4.+1.j 3.+0.j]
print("<v|M|v> =", npc.inner(v.conj(), M_v, axes='range'))
# <v|M|v> = (24+0j)
```

The number and types of symmetries are specified in a \texttt{ChargeInfo} class. An \texttt{Array} instance represents a tensor satisfying a charge rule specifying which blocks of it are nonzero. Internally, it stores only the non-zero blocks of the tensor, along with one \texttt{LegCharge} instance for each leg, which contains the charges and sign \texttt{qconj} for each leg. We can combine multiple legs into a single larger \texttt{LegPipe}, which is derived from the \texttt{LegCharge} and stores all the information necessary to later split the pipe.

The following code explicitly defines the spin-1/2 $\mathbf{S}^+$, $\mathbf{S}^-$, $\mathbf{S}^z$ operators and uses them to generate and diagonalize the two-site Hamiltonian $\hat{H} = \mathbf{S} \cdot \mathbf{S}$. It prints the charge values (by default sorted ascending) and the eigenvalues of $\hat{H}$.

```python
"""Explicit definition of charges and spin-1/2 operators."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3
import tenpy.linalg.np_conserved asnpc

# consider spin-1/2 with Sz-conservation
chinfo = npc.ChargeInfo([1])  # just a U(1) charge
# charges for up, down state
p_leg = npc.LegCharge.from_qflat(chinfo, [[1], [-1]])
Sz = npc.Array.from_ndarray([[0.5, 0.], [0., -0.5]), [p_leg, p_leg.conj()]])
Sp = npc.Array.from_ndarray([[0., 1.], [0., 0.]), [p_leg, p_leg.conj()]])
Sm = npc.Array.from_ndarray([[0., 0.], [1., 0.]), [p_leg, p_leg.conj()]])
Hxy = 0.5 * (npc.outer(Sp, Sm) + npc.outer(Sm, Sp))
Hz = npc.outer(Sz, Sz)
H = Hxy + Hz
# here, H has 4 legs
H.iset_leg_labels(["s1", "t1", "s2", "t2"])
H = H.combine_legs(["s1", "s2"], ["t1", "t2"], qconj=[+1, -1])
```

(continues on next page)
# here, $H$ has 2 legs
print(H.legs[0].to_qflat().flatten())
# prints [-2 0 0 2]
E, U = npc.eigh(H)  # diagonalize blocks individually
print(E)
# [0.25 -0.75 0.25 0.25]

Sites for the local Hilbert space and tensor networks

The next basic concept is that of a local Hilbert space, which is represented by a *Site* in TeNPy. This class does not only label the local states and define the charges, but also provides onsite operators. For example, the *SpinHalfSite* provides the $S^+$, $S^-$, $S^z$ operators under the names 'Sp', 'Sm', 'Sz', defined as *Array* instances similarly as in the code above. Since the most common sites like for example the *SpinSite* (for general spin $S=0.5, 1, 1.5,\ldots$), *BosonSite* and *FermionSite* are predefined, a user of TeNPy usually does not need to define the local charges and operators explicitly. The total Hilbert space, i.e, the tensor product of the local Hilbert spaces, is then just given by a list of *Site* instances. If desired, different kinds of *Site* can be combined in that list. This list is then given to classes representing tensor networks like the *MPS* and *MPO*. The tensor network classes also use *Array* instances for the tensors of the represented network.

The following example illustrates the initialization of a spin-1/2 site, an *MPS* representing the Neel state, and an *MPO* representing the Heisenberg model by explicitly defining the $W$ tensor.

```python
from tenpy.networks.site import SpinHalfSite
from tenpy.networks.mps import MPS
from tenpy.networks.mpo import MPO

spin = SpinHalfSite(conserve="Sz")
print(spin.Sz.to_ndarray())
# [[0.5 0. ]
# [0. -0.5]]

N = 6  # number of sites
sites = [spin] * N  # repeat entry of list N times
pstate = ["up", "down"] * (N // 2)  # Neel state
psi = MPS.from_product_state(sites, pstate, bc="finite")
print("<Sz> =", psi.expectation_value("Sz"))
# <Sz> = [0.5 -0.5 0.5 -0.5]
print("<Sp_i Sm_j> =", psi.correlation_function("Sp", "Sm"), sep="\n")
# <Sp_i Sm_j> =
# [[1. 0. 0. 0. 0. 0.]
# [0. 0. 0. 0. 0. 0.]
# [0. 0. 1. 0. 0. 0.]
# [0. 0. 0. 0. 0. 0.]
# [0. 0. 0. 0. 1. 0.]
# [0. 0. 0. 0. 0. 0.]]

# define an MPO
Id, Sp, Sm, Sz = spin.Id, spin.Sp, spin.Sm, spin.Sz
J, Delta, hz = 1., 1., 0.2
W_bulk = [[Id, Sp, Sm, Sz, -hz * Sz], [None, None, None, None, 0.5 * J * Sm],
          [None, None, None, None, 0.5 * J * Sp], [None, None, None, None, J * Delta],
          [None, None, None, None, -hz * Sz]],
```
Models

Note: See *Models* for more information on sites and how to define and extend models on your own.

Technically, the explicit definition of an MPO is already enough to call an algorithm like DMRG in *dmrg*. However, writing down the $W$ tensors is cumbersome especially for more complicated models. Hence, TeNPy provides another layer of abstraction for the definition of models, which we discuss first. Different kinds of algorithms require different representations of the Hamiltonian. Therefore, the library offers to specify the model abstractly by the individual onsite terms and coupling terms of the Hamiltonian. The following example illustrates this, again for the Heisenberg model.

```python
"""Definition of a model: the XXZ chain."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3
from tenpy.networks.site import SpinSite
from tenpy.models.lattice import Chain
from tenpy.models.model import CouplingModel, NearestNeighborModel, MPOModel
class XXZChain(CouplingModel, NearestNeighborModel, MPOModel):
    def __init__(self, L=2, S=0.5, J=1., Delta=1., hz=0.):
        spin = SpinSite(S=S, conserve="Sz")
        # the lattice defines the geometry
        lattice = Chain(L, spin, bc="open", bc_MPS="finite")
        CouplingModel.__init__(self, lattice)
        # add terms of the Hamiltonian
        self.add_coupling(J * 0.5, 0, "Sp", 0, "Sm", 1)  # $Sp_i Sm_{i+1}$
        self.add_coupling(J * 0.5, 0, "Sp", 0, "Sm", -1)  # $Sp_i Sm_{i-1}$
        self.add_coupling(J * Delta, 0, "Sz", 0, "Sz", 1)
        # (for site dependent prefactors, the strength can be an array)
        self.add_onsite(-hz, 0, "Sz")
        # finish initialization
        # generate MPO for DMRG
        MPOModel.__init__(self, lat, self.calc_H_MPO())
        # generate $H_{\text{bond}}$ for TEBD
        NearestNeighborModel.__init__(self, lat, self.calc_H_bond())
```

While this generates the same MPO as in the previous code, this example can easily be adjusted and generalized, for example to a higher dimensional lattice by just specifying a different lattice. Internally, the MPO is generated using a finite state machine picture. This allows not only to translate more complicated Hamiltonians into their corresponding MPOs, but also to automate the mapping from a higher dimensional lattice to the 1D chain along which the MPS winds. Note that this mapping introduces longer-range couplings, so the model can no longer be defined to be a *NearestNeighborModel* suited for TEBD if another lattice than the *Chain* is to be used. Of course, many
commonly studied models are also predefined. For example, the following code initializes the Heisenberg model on a kagome lattice; the spin liquid nature of the ground state of this model is highly debated in the current literature.

```python
from tenpy.models.spins import SpinModel

model_params = {
    "S": 0.5,  # Spin 1/2
    "lattice": "Kagome",
    "bc_MPS": "infinite",
    "bc_y": "cylinder",
    "Ly": 2,  # defines cylinder circumference
    "conserve": "Sz",  # use Sz conservation
    "Jx": 1.,
    "Jy": 1.,
    "Jz": 1.  # Heisenberg coupling
}
model = SpinModel(model_params)
```

### Algorithms

The highest level in TeNPy is given by algorithms like DMRG and TEBD. Using the previous concepts, setting up a simulation running those algorithms is a matter of just a few lines of code. The following example runs a DMRG simulation, see `dmrg`, exemplary for the transverse field Ising model at the critical point.

```python
from tenpy.networks.mps import MPS
from tenpy.models.tf_ising import TFIChain
from tenpy.algorithms import dmrg

N = 16  # number of sites
model = TFIChain({"L": N, "J": 1., "g": 1., "bc_MPS": "finite"})
sites = model.lat.mps_sites()
psi = MPS.from_product_state(sites, ["up"] * N, "finite")
dmrg_params = {"trunc_params": {"chi_max": 100, "svd_min": 1.e-10}, "mixer": True}
info = dmrg.run(psi, model, dmrg_params)
print("E =", info['E'])
# E = -20.01638790048513
print("max. bond dimension =", max(psi.chi))
# max. bond dimension = 27
```

The switch from DMRG to gls{iDMRG} in TeNPy is simply accomplished by a change of the parameter "bc_MPS" from "finite" to "infinite", both for the model and the state. The returned $E$ is then the energy density per site. Due to the translation invariance, one can also evaluate the correlation length, here slightly away from the critical point.

```python
from tenpy.networks.mps import MPS
from tenpy.models.tf_ising import TFIChain
from tenpy.algorithms import dmrg
```

(continues on next page)
N = 2  # number of sites in unit cell
model = TFIChain({"L": N, "J": 1., "g": 1.1, "bc_MPS": "infinite"})
sites = model.lat.mps_sites()
psi = MPS.from_product_state(sites, ['up'] * N, "infinite")
dmrg_params = {"trunc_params": {"chi_max": 100, "svd_min": 1.e-10}, "mixer": True}
info = dmrg.run(psi, model, dmrg_params)
print("E =", info['E'])
# E = -1.342864022725017
print("max. bond dimension =", max(psi.chi))
# max. bond dimension = 56
print("corr. length =", psi.correlation_length())
# corr. length = 4.915809146764157

Running time evolution with TEBD requires an additional loop, during which the desired observables have to be measured. The following code shows this directly for the infinite version of TEBD.

```python
"""Call of (infinite) TEBD."""
from tenpy.networks.mps import MPS
from tenpy.models.tf_ising import TFIChain
from tenpy.algorithms import tebd

M = TFIChain({"L": 2, "J": 1., "g": 1.5, "bc_MPS": "infinite"})
psi = MPS.from_product_state(M.lat.mps_sites(), [0] * 2, "infinite")
tebd_params = {
    "order": 2,
    "delta_tau_list": [0.1, 0.001, 1.e-5],
    "max_error_E": 1.e-6,
    "trunc_params": {
        "chi_max": 30,
        "svd_min": 1.e-10
    }
}
eng = tebd.Engine(psi, M, tebd_params)
eng.run_GS()  # imaginary time evolution with TEBD
print("E =", sum(psi.expectation_value(M.H_bond)) / psi.L)
print("final bond dimensions =", psi.chi)
```

### 7.3.2 Charge conservation with np_conserved

The basic idea is quickly summarized: By inspecting the Hamiltonian, you can identify symmetries, which correspond to conserved quantities, called charges. These charges divide the tensors into different sectors. This can be used to infer for example a block-diagonal structure of certain matrices, which in turn speeds up SVD or diagonalization a lot. Even for more general (non-square-matrix) tensors, charge conservation imposes restrictions which blocks of a tensor can be non-zero. Only those blocks need to be saved, which ultimately (= for large enough arrays) leads to a speedup of many routines, e.g., tensordot.

This introduction covers our implementation of charges; explaining mathematical details of the underlying symmetry is beyond its scope. We refer you to the corresponding chapter in our [TeNPyNotes] for a more general introduction of the idea (also stating the “charge rule” introduced below). [singh2010] explains why it works form a mathematical point of view, [singh2011] has the focus on a $U(1)$ symmetry and might be easier to read.
Notations

Let’s fix the notation of certain terms for this introduction and the doc-strings in `np_conserved`. This might be helpful if you know the basics from a different context. If you’re new to the subject, keep reading even if you don’t understand each detail, and come back to this section when you encounter the corresponding terms again.

A `Array` is a multi-dimensional array representing a `tensor` with the entries:

\[ T_{a_0, a_1, \ldots a_{\text{rank}-1}} \quad \text{with} \quad a_i \in \{0, \ldots, n_i - 1\} \]

Each leg \( a_i \) corresponds to a vector space of dimension \( n_i \).

An `index` of a leg is a particular value \( a_i \in \{0, \ldots, n_i - 1\} \).

The `rank` is the number of legs, the `shape` is \( (n_0, \ldots, n_{\text{rank}-1}) \).

We restrict ourselves to abelian charges with entries in \( \mathbb{Z} \) or in \( \mathbb{Z}_m \). The nature of a charge is specified by \( m \); we set \( m = 1 \) for charges corresponding to \( \mathbb{Z} \). The number of charges is referred to as `qnumber` as a short hand, and the collection of \( m \) for each charge is called `qmod`. The `qnumber`, `qmod` and possibly descriptive names of the charges are saved in an instance of `ChargeInfo`.

To each index of each leg, a value of the charge(s) is associated. A `charge block` is a contiguous slice corresponding to the same charge(s) of the leg. A `qindex` is an index in the list of charge blocks for a certain leg. A `charge sector` is for given charge(s) is the set of all qindices of that charge(s). A leg is `blocked` if all charge sectors map one-to-one to qindices. Finally, a leg is `sorted`, if the charges are sorted lexiographically. Note that a `sorted` leg is always `blocked`. We can also speak of the complete array to be `blocked by charges` or `legcharge-sorted`, which means that all of its legs are blocked or sorted, respectively. The charge data for a single leg is collected in the class `LegCharge`. A `LegCharge` has also a flag `qconj`, which tells whether the charges point `inward` (+1) or `outward` (-1). What that means, is explained later in `Which entries of the npc Array can be non-zero?`.

For completeness, let us also summarize also the internal structure of an `Array` here: The array saves only non-zero `blocks`, collected as a list of `np.array` in `self._data`. The qindices necessary to map these blocks to the original leg indices are collected in `self._qdata` An array is said to be `qdata-sorted` if its `self._qdata` is lexiographically sorted. More details on this follow `later`. However, note that you usually shouldn’t access `_qdata` and `_data` directly - this is only necessary from within `tensordot`, `svd`, etc. Also, an array has a `total charge`, defining which entries can be non-zero - details in `Which entries of the npc Array can be non-zero?`.

Finally, a `leg pipe` (implemented in `LegPipe`) is used to formally combine multiple legs into one leg. Again, more details follow `later`.

Physical Example

For concreteness, you can think of the Hamiltonian \( H = -t \sum_{<i,j>} (c_i^\dagger c_j + H.c.) + U n_i n_j \) with \( n_i = c_i^\dagger c_i \). This Hamiltonian has the global \( U(1) \) gauge symmetry \( c_i \rightarrow c_i e^{i\theta} \). The corresponding charge is the total number of particles \( N = \sum_i n_i \). You would then introduce one charge with \( m = 1 \).

Note that the total charge is a sum of local terms, living on single sites. Thus, you can infer the charge of a single physical site: it’s just the value \( q_i = n_i \in \mathbb{N} \) for each of the states.

Note that you can only assign integer charges. Consider for example the spin 1/2 Heisenberg chain. Here, you can naturally identify the magnetization \( S^z = \sum_i S^z_i \) as the conserved quantity, with values \( S^z_i = \pm \frac{1}{2} \). Obviously, if \( S^z \) is conserved, then so is \( 2S^z \), so you can use the charges \( q_i = 2S^z_i \in \{-1, +1\} \) for the `down` and `up` states, respectively. Alternatively, you can also use a shift and define \( q_i = S^z_i + \frac{1}{2} \in \{0, 1\} \).

As another example, consider BCS like terms \( \sum_k (c_k^\dagger c_{-k}^\dagger + H.c.) \). These terms break the total particle conservation, but they preserve the total parity, i.e., \( N \).

In the above examples, we had only a single charge conserved at a time, but you might be lucky and have multiple conserved quantities, e.g. if you have two chains coupled only by interactions. TeNPy is designed to handle the general
case of multiple charges. When giving examples, we will restrict to one charge, but everything generalizes to multiple charges.

The different formats for LegCharge

As mentioned above, we assign charges to each index of each leg of a tensor. This can be done in three formats: qflat, as qind and as qdict. Let me explain them with examples, for simplicity considering only a single charge (the most inner array has one entry for each charge).

qflat form: simply a list of charges for each index. An example:

\[
\text{qflat} = \([-2, -1, -1, 0, 0, 0, 0, 3, 3]\)
\]

This tells you that the leg has size 9, the charges for are \([-2, -1, -1, \ldots, 3]\) for the indices 0, 1, 2, 3, \ldots, 8. You can identify four charge blocks slice(0, 1), slice(1, 3), slice(3, 7), slice(7, 9) in this example, which have charges \([-2, -1, 0, 3]\). In other words, the indices 1, 2 (which are in slice(1, 3)) have the same charge value \([-1]\). A qindex would just enumerate these blocks as 0, 1, 2, 3.

qind form: a 1D array slices and a 2D array charges. This is a more compact version than the qflat form: the slices give a partition of the indices and the charges give the charge values. The same example as above would simply be:

\[
\text{slices} = [0, 1, 3, 7, 9] \\
\text{charges} = \([-2, -1, 0, 3]\)
\]

Note that slices includes 0 as first entry and the number of indices (here 9) as last entries. Thus it has len block_number + 1, where block_number (given by block_number) is the number of charge blocks in the leg, i.e. a qindex runs from 0 to block_number-1. On the other hand, the 2D array charges has shape (block_number, qnumber), where qnumber is the number of charges (given by qnumber).

In that way, the qind form maps an qindex, say qi, to the indices slice(slices[qi], slices[qi+1]) and the charge(s) charges[qi].

qdict form: a dictionary in the other direction than qind, taking charge tuples to slices. Again for the same example:

\[
\{(\text{-2,}) : \text{slice(0, 1)}, \\
\text{(-1,)} : \text{slice(1, 3)}, \\
\text{(0,)} : \text{slice(3, 7)}, \\
\text{(3,)} : \text{slice(7, 9)}\}
\]

Since the keys of a dictionary are unique, this form is only possible if the leg is completely blocked.

The LegCharge saves the charge data of a leg internally in qind form, directly in the attribute slices and charges. However, it also provides convenient functions for conversion between from and to the qflat and qdict form.

The above example was nice since all charges were sorted and the charge blocks were ‘as large as possible’. This is however not required.

The following example is also a valid qind form:

\[
\text{slices} = [0, 1, 3, 5, 7, 9] \\
\text{charges} = \([-2, -1, 0, 0, 3]\)
\]

This leads to the same qflat form as the above examples, thus representing the same charges on the leg indices. However, regarding our Arrays, this is quite different, since it divided the leg into 5 (instead of previously 4) charge blocks. We say the latter example is not bunched, while the former one is bunched.
To make the different notions of sorted and bunched clearer, consider the following (valid) examples:

<table>
<thead>
<tr>
<th>charges</th>
<th>bunched</th>
<th>sorted</th>
<th>blocked</th>
</tr>
</thead>
<tbody>
<tr>
<td>([-2], [-1], [0], [1], [3])</td>
<td>True</td>
<td>True</td>
<td>True</td>
</tr>
<tr>
<td>([-2], [-1], [0], [0], [3])</td>
<td>False</td>
<td>True</td>
<td>False</td>
</tr>
<tr>
<td>([-2], [0], [-1], [1], [3])</td>
<td>True</td>
<td>False</td>
<td>True</td>
</tr>
<tr>
<td>([-2], [0], [-1], [0], [3])</td>
<td>True</td>
<td>False</td>
<td>False</td>
</tr>
</tbody>
</table>

If a leg is bunched and sorted, it is automatically blocked (but not vice versa). See also below for further comments on that.

### Which entries of the npc Array can be non-zero?

The reason for the speedup with np_conserved lies in the fact that it saves only the blocks ‘compatible’ with the charges. But how is this ‘compatible’ defined?

Assume you have a tensor, call it \(T\), and the LegCharge for all of its legs, say \(a, b, c, \ldots\).

Remeber that the LegCharge associates to each index of the leg a charge value (for each of the charges, if \(qnumber > 1\)). Let \(a.to_qflat()[ia]\) denote the charge(s) of index \(ia\) for leg \(a\), and similar for other legs.

In addition, the LegCharge has a flag \(qconj\). This flag \(qconj\) is only a sign, saved as +1 or -1, specifying whether the charges point ‘inward’ (+1, default) or ‘outward’ (-1) of the tensor.

Then, the total charge of an entry \(T[ia, ib, ic, \ldots]\) of the tensor is defined as:

\[
qtotal[ia, ib, ic, \ldots] = a.to_qflat()[ia] \ast a.qconj + b.to_qflat()[ib] \ast b.qconj + c.to_qflat()[ic] \ast c.qconj + \ldots \mod qmod
\]

The rule which entries of the Array can be non-zero (i.e., are ‘compatible’ with the charges), is then very simple:

**Rule for non-zero entries**

An entry \(ia, ib, ic, \ldots\) of a Array can only be non-zero, if \(qtotal[ia, ib, ic, \ldots]\) matches the unique \(qtotal\) attribute of the class.

In other words, there is a single total charge \(qtotal\) attribute of a Array. All indices \(ia, ib, ic, \ldots\) for which the above defined \(qtotal[ia, ib, ic, \ldots]\) matches this total charge, are said to be compatible with the charges and can be non-zero. All other indices are incompatible with the charges and must be zero.

In case of multiple charges, \(qnumber > 1\), is a straightforward generalization: an entry can only be non-zero if it is compatible with each of the defined charges.

### The pesky \(qconj\) - contraction as an example

Why did we introduce the \(qconj\) flag? Remember it’s just a sign telling whether the charge points inward or outward. So what’s the reasoning?

The short answer is, that LegCharges actually live on bonds (i.e., legs which are to be contracted) rather than individual tensors. Thus, it is convenient to share the LegCharges between different legs and even tensors, and just adjust the sign of the charges with \(qconj\).

As an example, consider the contraction of two tensors, \(C_{ia,ic} = \sum_{ib} A_{ia,ib} B_{ib,ic}\). For simplicity, say that the total charge of all three tensors is zero. What are the implications of the above rule for non-zero entries? Or rather, how can
we ensure that \( C \) complies with the above rule? An entry \( C[ia,ic] \) will only be non-zero, if there is an \( ib \) such that both \( A[ia,ib] \) and \( B[ib,ic] \) are non-zero, i.e., both of the following equations are fullfilled:

\[
A.qtotal == A.legs[0].to_qflat()[ia] * A.legs[0].qconj + A.legs[1].to_qflat()[ib] * A.legs[1].qconj \mod qmod \\
B.qtotal == B.legs[0].to_qflat()[ib] * B.legs[0].qconj + B.legs[1].to_qflat()[ic] * B.legs[1].qconj \mod qmod
\]

(A.legs[0] is the LegCharge saving the charges of the first leg (with index \( ia \)) of \( A \).)

For the uncontracted legs, we just keep the charges as they are:

\[
C.legs = [A.legs[0], B.legs[1]]
\]

It is then straight-forward to check, that the rule is fullfilled for \( C \), if the following condition is met:

\[
A.qtotal + B.qtotal - C.qtotal == A.legs[1].to_qflat()[ib] A.b.qconj + B.legs[0].to_qflat()[ib] B.b.qconj \mod qmod
\]

The easiest way to meet this condition is (1) to require that \( A.b \) and \( B.b \) share the same charges \( b.to_qflat() \), but have opposite \( qconj \), and (2) to define \( C.qtotal = A.qtotal + B.qtotal \). This justifies the introduction of \( qconj \): when you define the tensors, you have to define the LegCharge for the \( b \) only once, say for \( A.legs[1] \). For \( B.legs[0] \) you simply use \( A.legs[1].conj() \) which creates a copy of the LegCharge with shared slices and charges, but opposite \( qconj \). As a more impressive example, all ‘physical’ legs of an MPS can usually share the same LegCharge (up to different \( qconj \) if the local Hilbert space is the same). This leads to the following convention:

\section*{Convention}

When an npc algorithm makes tensors which share a bond (either with the input tensors, as for tensordot, or amongst the output tensors, as for SVD), the algorithm is free, but not required, to use the same LegCharge for the tensors sharing the bond, \textit{without} making a copy. Thus, if you want to modify a LegCharge, you must make a copy first (e.g. by using methods of LegCharge for what you want to achieve).

\section*{Assigning charges to non-physical legs}

From the above physical examples, it should be clear how you assign charges to physical legs. But what about other legs, e.g. the virtual bond of an MPS (or an MPO)?

The charge of these bonds must be derived by using the ‘rule for non-zero entries’, as far as they are not arbitrary. As a concrete example, consider an MPS on just two spin 1/2 sites:

\[
\begin{array}{c|c|c|c}
| & x->- & A & -y->- & B & -z \\
| & ^ & ^ & ^ & ^ & \\
| & |p & |p \\
\end{array}
\]

The two legs \( p \) are the physical legs and share the same charge, as they both describe the same local Hilbert space. For better distinction, let me label the indices of them by \( \uparrow = 0 \) and \( \downarrow = 1 \). As noted above, we can associate the charges 1 (\( p = \uparrow \)) and -1 (\( p = \downarrow \)), respectively, so we define:

\[
\text{chinfo} = \text{npc.ChargeInfo}([1], ['2*Sz']) \\
p = \text{npc.LegCharge.from_qflat(chinfo, [1, -1], qconj=+1)}
\]
For the qconj signs, we stick to the convention used in our MPS code and indicated by the arrows in above ‘picture’: physical legs are incoming (qconj=+1), and from left to right on the virtual bonds. This is achieved by using [p, x, y.conj()] as legs for A, and [p, y, z.conj()] for B, with the default qconj=+1 for all p, x, y, z; y.conj() has the same charges as y, but opposite qconj=-1.

The legs x and z of an L=2 MPS, are ‘dummy’ legs with just one index 0. The charge on one of them, as well as the total charge of both A and B is arbitrary (i.e., a gauge freedom), so we make a simple choice: total charge 0 on both arrays, as well as for x = 0, x = npc.LegCharge.from_qflat(chinfo, [0], qconj=+1).

The charges on the bonds y and z then depend on the state the MPS represents. Here, we consider a singlet $\psi = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ as a simple example. A possible MPS representation is given by:

\[
\begin{align*}
A[\text{up, :, :}] &= \begin{bmatrix} 1/2.**0.5, 0 \end{bmatrix} \\
B[\text{up, :, :}] &= \begin{bmatrix} 0, [-1] \end{bmatrix} \\
A[\text{down, :, :}] &= \begin{bmatrix} 0, 1/2.**0.5 \end{bmatrix} \\
B[\text{down, :, :}] &= \begin{bmatrix} 1, [0] \end{bmatrix}
\end{align*}
\]

There are two non-zero entries in A, for the indices $(a, x, y) = (\uparrow, 0, 0)$ and $(\downarrow, 0, 1)$. For $(a, x, y) = (\uparrow, 0, 0)$, we want:

\[
\begin{align*}
A.qtotal &= 0 = p.to_qflat()[\text{up}] * p.qconj + x.to_qflat()[0] * x.qconj + y.conj().to_qflat()[0] * y.conj().qconj \\
&= 1 * (+1) + 0 * (+1) + y.conj().to_qflat()[0] * (-1)
\end{align*}
\]

This fixes the charge of $y=0$ to 1. A similar calculation for $(a, x, y) = (\downarrow, 0, 1)$ yields the charge -1 for $y=1$. We have thus all the charges of the leg y and can define $y = npc.LegCharge.form_qflat(chinfo, [1, -1], qconj=+1)$.

Now take a look at the entries of B. For the non-zero entry $(b, y, z) = (\uparrow, 1, 0)$, we want:

\[
\begin{align*}
B.qtotal &= 0 = p.to_qflat()[\text{up}] * p.qconj + y.to_qflat()[1] * y.qconj + z.conj().to_qflat()[0] * z.conj().qconj \\
&= 1 * (+1) + (-1) * (+1) + z.conj().to_qflat()[0] * (-1)
\end{align*}
\]

This implies the charge 0 for $z=0$, thus $z = npc.LegCharge.form_qflat(chinfo, [0], qconj=+1)$. Finally, note that the rule for $(b, y, z) = (\downarrow, 0, 0)$ is automatically fulfilled! This is an implication of the fact that the singlet has a well defined value for $S^z_A + S^z_B$. For other states without fixed magnetization (e.g., $|\uparrow\uparrow\rangle + |\down\down\rangle$) this would not be the case, and we could not use charge conservation.

As an exercise, you can calculate the charge of $z$ in the case that $A.qtotal=5, B.qtotal = -1$ and charge 2 for $x=0$. The result is -2.

**Note:** This section is meant be an pedagogical introduction. In you program, you can use the functions `detect_legcharge()` (which does exactly what’s described above) or `detect_qtotal()` (if you know all `LegCharges`, but not `qtotal`).

### 7.3. Introductions 61
Array creation

Making an new `Array` requires both the tensor entries (data) and charge data.

The default initialization `a = Array(...)` creates an empty Array, where all entries are zero (equivalent to `zeros()`). (Non-zero) data can be provided either as a dense `np.array` to `from_ndarray()`, or by providing a numpy function such as `np.random, np.ones` etc. to `from_func()`.

In both cases, the charge data is provided by one `ChargeInfo`, and a `LegCharge` instance for each of the legs.

Note: The charge data instances are not copied, in order to allow it to be shared between different Arrays. Consequently, you must make copies of the charge data, if you manipulate it directly. (However, methods like `sort()` do that for you.)

Of course, a new `Array` can also created using the charge data from existing Arrays, for examples with `zeros_like()` or creating a (deep or shallow) `copy()`. Further, there are the higher level functions like `tensordot()` or `svd()`, which also return new Arrays.

Further, new Arrays are created by the various functions like `tensordot` or `svd` in `np_conserved`.

Complete blocking of Charges

While the code was designed in such a way that each charge sector has a different charge, the code should still run correctly if multiple charge sectors (for different qindex) correspond to the same charge. In this sense `Array` can act like a sparse array class to selectively store subblocks. Algorithms which need a full blocking should state that explicitly in their doc-strings. (Some functions (like `svd` and `eigh`) require complete blocking internally, but if necessary they just work on a temporary copy returned by `as_completely_blocked()`).

If you expect the tensor to be dense subject to charge constraints (as for MPS), it will be most efficient to fully block by charge, so that work is done on large chunks.

However, if you expect the tensor to be sparser than required by charge (as for an MPO), it may be convenient not to completely block, which forces smaller matrices to be stored, and hence many zeroes to be dropped. Nevertheless, the algorithms were not designed with this in mind, so it is not recommended in general. (If you want to use it, run a benchmark to check whether it is really faster!)

If you haven’t created the array yet, you can call `sort()` (with `bunch=True`) on each `LegCharge` which you want to block. This sorts by charges and thus induces a permutation of the indices, which is also returned as an 1D array perm. For consistency, you have to apply this permutation to your flat data as well.

Alternatively, you can simply call `sort_legcharge()` on an existing `Array`. It calls `sort()` internally on the specified legs and performs the necessary permutations directly to (a copy of) `self`. Yet, you should keep in mind, that the axes are permuted afterwards.

Internal Storage schema of npc Arrays

The actual data of the tensor is stored in `_data`. Rather than keeping a single `np.array` (which would have many zeros in it), we store only the non-zero sub blocks. So `_data` is a python list of `np.array`'s. The order in which they are stored in the list is not physically meaningful, and so not guaranteed (more on this later). So to figure out where the sub block sits in the tensor, we need the `_qdata` structure (on top of the LegCharges in `legs`).

Consider a rank 3 tensor `T`, with the first leg like:

```python
legs[0].slices = np.array([0, 1, 4, ...])
legs[0].charges = np.array([-2, [1], ...])
```
Each row of \textit{charges} gives the charges for a \textit{charge block} of the leg, with the actual indices of the total tensor determined by the \textit{slices}. The \textit{qindex} simply enumerates the charge blocks of a lex. Picking a \textit{qindex} (and thus a \textit{charge block}) from each leg, we have a subblock of the tensor.

For each (non-zero) subblock of the tensor, we put a (numpy) ndarray entry in the \_data list. Since each subblock of the tensor is specified by \textit{rank} \textit{qindices}, we put a corresponding entry in \_qdata, which is a 2D array of shape (\textit{#stored_blocks, rank}). Each row corresponds to a non-zero subblock, and there are rank columns giving the corresponding \textit{qindex} for each leg.

Example: for a rank 3 tensor we might have:

\begin{verbatim}
T._data = [t1, t2, t3, t4, ...]
T._qdata = np.array([[3, 2, 1],
                    [1, 1, 1],
                    [4, 2, 2],
                    [2, 1, 2],
                    ...])
\end{verbatim}

The third subblock has an ndarray \(t3\), and \textit{qindices} [4 2 2] for the three legs.

- To find the position of \(t3\) in the actual tensor you can use \textit{get_slice()}:
  \begin{verbatim}
  T.legs[0].get_slice(4), T.legs[1].get_slice(2), T.legs[2].get_slice(2)
  \end{verbatim}

  The function \textit{leg.get_charges(qi)} simply returns \texttt{slice(leg.slices[qi], leg.slices[qi+1])}

- To find the charges of \(t3\), we an use \textit{get_charge()}:
  \begin{verbatim}
  T.legs[0].get_charge(2), T.legs[1].get_charge(2), T.legs[2].get_charge(2)
  \end{verbatim}

  The function \textit{leg.get_charge(qi)} simply returns \(\text{leg.charges[qi]} \ast \text{leg.qconj}\).

\textbf{Note:} Outside of \textit{np_conserved}, you should use the API to access the entries. If you really need to iterate over all blocks of an Array \textit{T}, try for (block, blockslices, charges, \textit{qindices}) in \textit{T}: \text{do\_something()}.

The order in which the blocks stored in \_data/\_qdata is arbitrary (although of course \_data and \_qdata must be in correspondence). However, for many purposes it is useful to sort them according to some convention. So we include a flag \_qdata\_sorted to the array. So, if sorted (with \textit{isort_qdata()}, the \_qdata example above goes to

\begin{verbatim}
_qdata = np.array([[1, 1, 1],
                  [3, 2, 1],
                  [2, 1, 2],
                  [4, 2, 2],
                  ...])
\end{verbatim}

Note that \textit{np.lexsort} chooses the right-most column to be the dominant key, a convention we follow throughout.

If \_qdata\_sorted == True, \_qdata and \_data are guaranteed to be lexsorted. If \_qdata\_sorted == False, there is no guarantee. If an algorithm modifies \_qdata, it must set \_qdata\_sorted == False (unless it guarantees it is still sorted). The routine \textit{sort_qdata()} brings the data to sorted form.
Indexing of an Array

Although it is usually not necessary to access single entries of an Array, you can of course do that. In the simplest case, this is something like \( A[0, 2, 1] \) for a rank-3 Array \( A \). However, accessing single entries is quite slow and usually not recommended. For small Arrays, it may be convenient to convert them back to flat numpy arrays with \( \text{to_ndarray()} \).

On top of that very basic indexing, Array supports slicing and some kind of advanced indexing, which is however different from the one of numpy arrays (described here). Unlike numpy arrays, our Array class does not broadcast existing index arrays – this would be terribly slow. Also, \( \text{np.newaxis} \) is not supported, since inserting new axes requires additional information for the charges.

Instead, we allow just indexing of the legs independent of each other, of the form \( A[i_0, i_1, \ldots] \). If all indices \( i_0, i_1, \ldots \) are integers, the single corresponding entry (of type dtype) is returned.

However, the individual ‘indices’ \( i_0 \) for the individual legs can also be one of what is described in the following list. In that case, a new Array with less data (specified by the indices) is returned.

The ‘indices’ can be:

• an `int`: fix the index of that axis, return array with one less dimension. See also \( \text{take_slice()} \).

• a `slice(\text{None})` or `::`: keep the complete axis

• an `Ellipsis` or `...`: shorthand for \( \text{slice(\text{None})} \) for missing axes to fix the len

• an 1D bool \( \text{ndarray} \) mask: apply a mask to that axis, see \( \text{iproject()} \). This is also implemented with \( \text{iproject} \).

• an 1D int \( \text{ndarray} \) mask: keep only the indices specified by the array. This is also implemented with \( \text{iproject} \).

For slices and 1D arrays, additional permutations may be performed with the help of \( \text{permute()} \).

If the number of indices is less than \( \text{rank} \), the remaining axes remain free, so for a rank 4 Array \( A \), \( A[i_0, i_1] == A[i_0, i_1, \ldots] == A[i_0, i_1, :, :] \).

Note that indexing always copies the data – even if \( \text{int} \) contains just slices, in which case numpy would return a view. However, assigning with \( A[:, [3, 5], 3] = B \) should work as you would expect.

**Warning:** Due to numpy’s advanced indexing, for 1D integer arrays \( a_0 \) and \( a_1 \) the following holds

\[
A[a_0, a_1].\text{to_ndarray}() == A.\text{to_ndarray}()[\text{np.ix_}(a_0, a_1)] != A.\text{to_ndarray}()[a_0, a_1]
\]

For a combination of slices and arrays, things get more complicated with numpy’s advanced indexing. In that case, a simple \( \text{np.ix_}(\ldots) \) doesn’t help any more to emulate our version of indexing.

Introduction to combine_legs, split_legs and LegPipes

Often, it is necessary to “combine” multiple legs into one: for example to perform a SVD, a tensor needs to be viewed as a matrix. For a flat array, this can be done with \( \text{np.reshape} \), e.g., if \( A \) has shape \((10, 3, 7)\) then \( B = \text{np.reshape}(A, (30, 7)) \) will result in a (view of the) array with one less dimension, but a “larger” first leg. By default \( \text{order}='C' \), this results in

\[
B[i*3 + j, k] == A[i, j, k] \quad \text{for \( i \) in range(10) for \( j \) in range(3) for \( k \) in range(7)}
\]

While for a \( \text{np.array} \), also a reshaping \((10, 3, 7) \rightarrow (2, 21, 5)\) would be allowed, it does not make sense physically. The only sensible “reshape” operation on an Array are
1) to **combine** multiple legs into one **leg pipe** (*LegPipe*) with `combine_legs()`, or
2) to **split** a pipe of previously combined legs with `split_legs()`.

Each leg has a Hilbert space, and a representation of the symmetry on that Hilbert space. Combining legs corresponds to the tensor product operation, and for abelian groups, the corresponding “fusion” of the representation is the simple addition of charge.

Fusion is not a lossless process, so if we ever want to split the combined leg, we need some additional data to tell us how to reverse the tensor product. This data is saved in the class *LegPipe*, derived from the *LegCharge* and used as new leg. Details of the information contained in a *LegPipe* are given in the class doc string.

The rough usage idea is as follows:

1) You can call `combine_legs()` without supplying any *LegPipes*, `combine_legs` will then make them for you. Nevertheless, if you plan to perform the combination over and over again on sets of legs you know to be identical [with same charges etc, up to an overall -1 in $qconj$ on all incoming and outgoing Legs] you might make a *LegPipe* anyway to save on the overhead of computing it each time.

2) In any way, the resulting Array will have a *LegPipe* as a *LegCharge* on the combined leg. Thus, it – and all tensors inheriting the leg (e.g. the results of $svd$, $tensordot$ etc.) – will have the information how to split the *LegPipe* back to the original legs.

3) Once you performed the necessary operations, you can call `split_legs()`. This uses the information saved in the *LegPipe* to split the legs, recovering the original legs.

For a *LegPipe*, $conj()$ changes $qconj$ for the outgoing pipe and the incoming legs. If you need a *LegPipe* with the same incoming $qconj$, use `outer_conj()`.

### Leg labeling

It’s convenient to name the legs of a tensor: for instance, we can name legs 0, 1, 2 to be ‘a’, ‘b’, ‘c’: $T_{i_a,i_b,i_c}$. That way we don’t have to remember the ordering! Under $tensordot$, we can then call

```python
U = npc.tensordot(S, T, axes = [ [..], ['b'] ])
```

without having to remember where exactly ‘b’ is. Obviously $U$ should then inherit the name of its legs from the uncontracted legs of $S$ and $T$. So here is how it works:

- Labels can only be strings. The labels should not include the characters , or ?. Internally, the labels are stored as dict $a.labels = \{\text{label: leg_position, ...}\}$. Not all legs need a label.
- To set the labels, call

```python
A.set_labels(["a", "b", None, "c", ...])
```

which will set up the labeling {"a": 0, "b": 1, "c": 3 ...}.

- (Where implemented) the specification of axes can use either the labels or the index positions. For instance, the call $tensordot(A, B, [["a", 2, "c"], [...]])$ will interpret ‘a’ and ‘c’ as labels (calling `get_leg_indices()` to find their positions using the dict) and 2 as ‘the 2nd leg’. That’s why we require labels to be strings!

- Labels will be intelligently inherited through the various operations of `np_conserved`.
  - Under `transpose`, labels are permuted.
  - Under `tensordot`, labels are inherited from uncontracted legs. If there is a collision, both labels are dropped.
– Under `combine_legs`, labels get concatenated with a . delimiter and surrounded by brackets. Example: let `a.labels = {'a': 1, 'b': 2, 'c': 3}`. Then if `b = a. combine_legs([[0], [1, 2]])`, it will have `b.labels = {'(a.b)': 0, '(c)': 1}`. If some sub-leg of a combined leg isn’t named, then a '?' label is inserted (with # the leg index), e.g., 'a.?0.c'.

– Under `split_legs`, the labels are split using the delimiters (and the '?' are dropped).

– Under `conj, iconj`: take 'a' -> 'a*', 'a*' -> 'a', and '(a.(b*.c))' -> '(a*.b. c*)'

– Under `svd`, the outer labels are inherited, and inner labels can be optionally passed.

– Under `pinv`, the labels are transposed.

**See also**

- The module `tenpy.linalg.np_conserved` should contain all the API needed from the point of view of the algorithms. It contains the fundamental `Array` class and functions for working with them (creating and manipulating).

- The module `tenpy.linalg.charges` contains implementations for the charge structure, for example the classes `ChargeInfo`, `LegCharge`, and `LegPipe`. As noted above, the ‘public’ API is imported to (and accessible from) `np_conserved`.

**A full example code for spin-1/2**

Below follows a full example demonstrating the creation and contraction of Arrays. (It’s the file `a_np_conserved.py` in the examples folder of the tenpy source.)

```python
"""An example code to demonstrate the usage of `Array`

This example includes the following steps:
1) create Arrays for an Neel MPS
2) create an MPO representing the nearest-neighbour AFM Heisenberg Hamiltonian
3) define 'environments' left and right
4) contract MPS and MPO to calculate the energy
5) extract two-site hamiltonian 'H2' from the MPO
6) calculate 'exp(-1.j*dt*H2)' by diagonalization of H2
7) apply 'exp(H2)' to two sites of the MPS and truncate with svd

Note that this example uses only `np_conserved`, but no other modules. Compare it to the example `b_mps.py`, which does the same steps using a few predefined classes like MPS and MPO.
"""

# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

```
import tenpy.linalg.np_conserved as npc
import numpy as np

# model parameters
Jxx, Jz = 1., 1.
L = 20
dt = 0.1
cutoff = 1.e-10
print("Jxx=\{Jxx\}, Jz=\{Jz\}, L=\{L:d\}".format(Jxx=Jxx, Jz=Jz, L=L))
```

(continues on next page)
print("1) create Arrays for an Neel MPS")
# vL --> B --> vR
# |
# ^
# |
# p

# create a ChargeInfo to specify the nature of the charge
chinfo = npc.ChargeInfo([1], ['2*Sz'])  # the second argument is just a descriptive name

# create LegCharges on physical leg and even/odd bonds
p_leg = npc.LegCharge.from_qflat(chinfo, [[1], [-1]])  # charges for up, down
v_leg_even = npc.LegCharge.from_qflat(chinfo, [[0]])
v_leg_odd = npc.LegCharge.from_qflat(chinfo, [[1]])

B_even = npc.zeros([v_leg_even, v_leg_odd.conj(), p_leg], labels=['vL', 'vR', 'p'])
# virtual left/right, physical
B_odd = npc.zeros([v_leg_odd, v_leg_even.conj(), p_leg], labels=['vL', 'vR', 'p'])
B_even[0, 0, 0] = 1.  # up
B_odd[0, 0, 1] = 1.  # down

Bs = [B_even, B_odd] * (L // 2) + [B_even] * (L % 2)  # (right-canonical)
Ss = [np.ones(1)] * L  # Ss[i] are singular values between Bs[i-1] and Bs[i]

# Side remark:
# An MPS is expected to have non-zero entries everywhere compatible with the charges.
# In general, we recommend to use `sort_legcharge` (or `as_completely_blocked`) to ensure complete blocking. (But the code will also work, if you don't do it.)
# The drawback is that this might introduce permutations in the indices of single legs,
# which you have to keep in mind when converting dense numpy arrays to and from npc.Arrays.

print("2) create an MPO representing the AFM Heisenberg Hamiltonian")

# wL --> W --> wR
# |
# ^
# |
# p

# create physical spin-1/2 operators Sz, S+, S-
Sz = npc.Array.from_ndarray([[0.5, 0.], [0., -0.5]], [p_leg, p_leg.conj()], labels=['p', 'p⋆'])
Sp = npc.Array.from_ndarray([[0., 1.], [0., 0.]], [p_leg, p_leg.conj()], labels=['p', 'p⋆'])
Sm = npc.Array.from_ndarray([[0., 0.], [1., 0.]], [p_leg, p_leg.conj()], labels=['p', 'p⋆'])
Id = npc.eye_like(Sz, labels=Sz.get_leg_labels())  # identity

(continues on next page)
mpo_leg = npc.LegCharge.from_qflat(chinfo, [[0], [2], [-2], [0], [0]])

W_grid = [[Id, Sp, Sm, Sz, None],
          [None, None, None, None, 0.5 * Jxx * Sm],
          [None, None, None, None, 0.5 * Jxx * Sp],
          [None, None, None, None, Jz * Sz],
          [None, None, None, None, Id]]  # yapf:disable

W = npc.grid.outer(W_grid, [mpo_leg, mpo_leg.conj()], grid_labels=['wL', 'wR'])

Ws = [W] * L

print("3) define 'environments' left and right")

# .---->- vR vL ----<.
# | |
# envL->- wR wL ->-envR
# | |
# .---->- vR* vL*----<.

envL = npc.zeros([W.get_leg('wL').conj(), Bs[0].get_leg('vL').conj()], labels=['wR', 'vR', 'vR*'])
envL[0, :, :] = npc.diag(1., envL.legs[1])

envR = npc.zeros([W.get_leg('wR').conj(), Bs[-1].get_leg('vR').conj()], labels=['wL', 'vL', 'vL*'])
envR[-1, :, :] = npc.diag(1., envR.legs[1])

print("4) contract MPS and MPO to calculate the energy <psi|H|psi>")

contr = envL

for i in range(L):
    # contr labels: wR, vR, vR*
    contr = npc.tensordot(contr, Bs[i], axes=('vR', 'vL'))
    # wR, vR*, vR, p
    contr = npc.tensordot(contr, Ws[i], axes=( ['p', 'wR'], ['p*', 'wL'] ))
    # vR*, vR, wR, p
    contr = npc.tensordot(contr, Bs[i].conj(), axes=( ['p', 'vR*'], ['p*', 'vL*'] ))
    # vR, wR, vR*
    # note that the order of the legs changed, but that's no problem with labels:
    # the arrays are automatically transposed as necessary
E = npc.inner(contr, envR, axes=( ['vR', 'wR', 'vR*'], ['vL', 'wL', 'vL*'] ))

print("E = ", E)

print("5) calculate two-site hamiltonian \"H2\" from the MPO")

# label left, right physical legs with p, q
W0 = W.replace_labels([['p', 'p*'], ['p0', 'p0*']])
W1 = W.replace_labels([['p', 'p*'], ['p1', 'p1*']])

H2 = npc.tensordot(W0, W1, axes=( ['wR', 'wL'])).itranspose([ ['wL', 'wR', 'p0', 'p1', 'p0*', 'p1*']])

H2 = H2[0, -1]  # (If H has single-site terms, it's not that simple anymore)

print("H2 labels:", H2.get_leg_labels())

print("6) calculate exp(H2) by diagonalization of H2")
# diagonalization requires to view H2 as a matrix
H2 = H2.combine_legs([['p0', 'p1'], ['p0*', 'p1*']], qconj=[+1, -1])

print("labels after combine_legs:", H2.get_leg_labels())
E2, U2 = npc.eigh(H2)
print("Eigenvalues of H2:", E2)
U_expE2 = U2.scale_axis(np.exp(-1.j * dt * E2), axis=1)  # scale_axis ~= apply an
→ diagonal matrix
exp_H2 = npc.tensordot(U_expE2, U2.conj(), axes=(1, 1))
exp_H2.iset_leg_labels(H2.get_leg_labels())
exp_H2 = exp_H2.split_legs()  # by default split all legs which are 'LegPipe'
# (this restores the original labels ['p0', 'p1', 'p0*', 'p1*'] of 'H2' in 'exp_H2')
print("7) apply exp(H2) to even/odd bonds of the MPS and truncate with svd")
# (this implements one time step of first order TEBD)
for even_odd in [0, 1]:
    for i in range(even_odd, L - 1, 2):
        B_L = Bs[i].scale_axis(Ss[i], 'vL').ireplace_label('p', 'p0')
        B_R = Bs[i + 1].replace_label('p', 'p1')
        theta = npc.tensordot(B_L, B_R, axes=('vR', 'vL'))
        theta = npc.tensordot(exp_H2, theta, axes=[['p0*', 'p1*'], ['p0', 'p1']])
        # view as matrix for SVD
        theta = theta.combine_legs([('vL', 'p0'), ('p1', 'vR')], new_axes=[0, 1], qconj=[+1, -1])
        # now theta has labels '(vL,p0)', '(p1,vR)',
        U, S, V = npc.svd(theta, inner_labels=['vR', 'vL'])
        # truncate
        keep = S > cutoff
        S = S[keep]
        invsq = np.linalg.norm(S)
        Ss[i + 1] = S / invsq
        U = U.iscale_axis(S / invsq, 'vR')
        Bs[i] = U.split_legs('(vL,p0)').iscale_axis(Ss[i]**(-1), 'vL').ireplace_label(
→'p0', 'p')
        Bs[i + 1] = V.split_legs('(p1,vR)').ireplace_label('p1', 'p')
print("finished")

7.3.3 Models

What is a model?

Abstractly, a model stands for some physical (quantum) system to be described. For tensor networks algorithms, the
model is usually specified as a Hamiltonian written in terms of second quantization. For example, let us consider a
spin-1/2 Heisenberg model described by the Hamiltonian

\[ H = J \sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z \]

Note that a few things are defined more or less implicitly.

- The local Hilbert space: it consists of Spin-1/2 degrees of freedom with the usual spin-1/2 operators \( S^x, S^y, S^z \).
- The geometric (lattice) structure: above, we spoke of a 1D “chain”.
- The boundary conditions: do we have open or periodic boundary conditions? The “chain” suggests open bound-
daries, which are in most cases preferable for MPS-based methods.
- The range of \( i \): How many sites do we consider (for a 2D system: in each direction)?

Obviously, these things need to be specified in TeNPy in one way or another, if we want to define a model.
Ultimately, our goal is to run some algorithm. However, different algorithm requires the model and Hamiltonian to be specified in different forms. We have one class for each such required form. For example, \texttt{dmrg} requires an \texttt{MPOModel}, which contains the Hamiltonian written as an MPO. So a new model class suitable for DMRG should have this general structure:

```python
class MyNewModel(MPOModel):
    def __init__(self, model_params):
        lattice = somehow_generate_lattice(model_params)
        H_MPO = somehow_generate_MPO(lattice, model_params)
        # initialize MPOModel
        MPOModel.__init__(self, lattice, H_MPO)
```

On the other hand, if we want to evolve a state with \texttt{tebd} we need a \texttt{NearestNeighborModel}, in which the Hamiltonian is written in terms of two-site bond-terms to allow a Suzuki-Trotter decomposition of the time-evolution operator:

```python
class MyNewModel2(NearestNeighborModel):
    def __init__(self, model_params):
        lattice = somehow_generate_lattice(model_params)
        H_bond = somehow_generate_H_bond(lattice, model_params)
        # initialize MPOModel
        NearestNeighborModel.__init__(self, lattice, H_bond)
```

Of course, the difficult part in these examples is to generate the $H_{MPO}$ and $H_{bond}$ in the required form. If you want to write it down by hand, you can of course do that. But it can be quite tedious to write every model multiple times, just because we need different representations of the same Hamiltonian. Luckily, there is a way out in TeNPy: the \texttt{CouplingModel}. Before we describe this class, let’s discuss the background of the \texttt{Site} and \texttt{Site} class.

### The Hilbert space

The local Hilbert space is represented by a \texttt{Site} (read its doc-string!). In particular, the \texttt{Site} contains the local \texttt{LegCharge} and hence the meaning of each basis state needs to be defined. Beside that, the site contains the local operators - those give the real meaning to the local basis. Having the local operators in the site is very convenient, because it makes them available by name for example when you want to calculate expectation values. The most common sites (e.g. for spins, spin-less or spin-full fermions, or bosons) are predefined in the module \texttt{tenpy.networks.site}, but if necessary you can easily extend them by adding further local operators or completely write your own subclasses of \texttt{Site}.

The full Hilbert space is a tensor product of the local Hilbert space on each site.

**Note:** The \texttt{LegCharge} of all involved sites need to have a common \texttt{ChargeInfo} in order to allow the contraction of tensors acting on the various sites. This can be ensured with the function \texttt{multi_sites_combine_charges()}.

An example where \texttt{multi_sites_combine_charges()} is needed would be a coupling of different types of sites, e.g., when a tight binding chain of fermions is coupled to some local spin degrees of freedom. Another use case of this function would be a model with a $U(1)$ symmetry involving only half the sites, say $\sum_{i=0}^{L/2} n_{2i}$.

**Note:** If you don’t know about the charges and \texttt{np\_conserved} yet, but want to get started with models right away, you can set \texttt{conserve=None} in the existing sites or use \texttt{leg = tenpy.linalg.np_conserved.LegCharge.from_trivial(d)} for an implementation of your custom site, where $d$ is the dimension of the local Hilbert space. Alternatively, you can find some introduction to the charges in the \texttt{Charge conservation with np\_conserved}. 

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70 Chapter 7. License
The geometry: lattice class

The geometry is usually given by some kind of lattice structure how the sites are arranged, e.g. implicitly with the sum over nearest neighbours \( \sum_{<i,j>} \). In TeNPy, this is specified by a Lattice class, which contains a unit cell of a few Site which are shifted periodically by its basis vectors to form a regular lattice. Again, we have pre-defined some basic lattices like a Chain, two chains coupled as a Ladder or 2D lattices like the Square, Honeycomb and Kagome lattices; but you are also free to define your own generalizations.

MPS based algorithms like DMRG always work on purely 1D systems. Even if our model “lives” on a 2D lattice, these algorithms require to map it onto a 1D chain (probably at the cost of longer-range interactions). This mapping is also done by the lattice by defining the order(order) of the sites.

Note: Further details on the lattice geometry can be found in Details on the lattice geometry.

The CouplingModel: general structure

The CouplingModel provides a general, quite abstract way to specify a Hamiltonian of couplings on a given lattice. Once initialized, its methods add_onsite() and add_coupling() allow to add onsite and coupling terms repeated over the different unit cells of the lattice. In that way, it basically allows a straight-forward translation of the Hamiltonian given as a math formula \( H = \sum_{i} A_{i}B_{i+d} + \ldots \) with onsite operators \( A, B, \ldots \) into a model class.

The general structure for a new model based on the CouplingModel is then:

```python
class MyNewModel3(CouplingModel, MPOModel, NearestNeighborModel):
    def __init__(self, ...):
        ... # follow the basic steps explained below
```

In the initialization method __init__(self, ...) of this class you can then follow these basic steps:

0. Read out the parameters.
1. Given the parameters, determine the charges to be conserved. Initialize the LegCharge of the local sites accordingly.
2. Define (additional) local operators needed.
3. Initialize the needed Site.

Note: Using pre-defined sites like the SpinHalfSite is recommended and can replace steps 1-3.

4. Initialize the lattice (or if you got the lattice as a parameter, set the sites in the unit cell).
5. Initialize the CouplingModel with CouplingModel.__init__(self, lat).
6. Use add_onsite() and add_coupling() to add all terms of the Hamiltonian. Here, the pairs of the lattice can come in handy, for example:

```python
self.add_onsite(-np.asarray(h), 0, 'Sz')
for ul, u2, dx in self.lat.pairs['nearest_neighbors']:
    self.add_coupling(0.5*J, ul, 'Sp', u2, 'Sm', dx, plus_hc=True)
self.add_coupling(J, ul, 'Sz', u2, 'Sz', dx)
```

Note: The method add_coupling() adds the coupling only in one direction, i.e. not switching \( i \) and \( j \) in \( \sum_{<i,j>} \). If you have terms like \( c_i^\dagger c_j \) or \( S_i^+ S_j^- \) in your Hamiltonian, you need to add it in both directions to get a Hermitian Hamiltonian! The easiest way to do that is to use the plus_hc option of add_onsite() and
**add_coupling()**, as we did for the $J/2(S^+_i S^-_i + h.c.)$ terms of the Heisenberg model above. Alternatively, you can add the hermitian conjugate terms explicitly, see the examples in **add_coupling()** for more details.

Note that the *strength* arguments of these functions can be (numpy) arrays for site-dependent couplings. If you need to add or multiply some parameters of the model for the *strength* of certain terms, it is recommended use `np.asarray` beforehand – in that way lists will also work fine.

7. Finally, if you derived from the `MPOModel`, you can call `calc_H_MPO()` to build the MPO and use it for the initialization as `MPOModel.__init__(self, lat, self.calc_H_MPO())`.

8. Similarly, if you derived from the `NearestNeighborModel`, you can call `calc_H_bond()` to initialize it as `NearestNeighborModel.__init__(self, lat, self.calc_H_bond())`. Calling `self.calc_H_bond()` will fail for models which are not nearest-neighbors (with respect to the MPS ordering), so you should only subclass the `NearestNeighborModel` if the lattice is a simple Chain.

**Note:** The method **add_coupling()** works only for terms involving operators on 2 sites. If you have couplings involving more than two sites, you can use the **add_multi_coupling()** instead. A prototypical example is the exactly solvable ToricCode.

The code of the module `tenpy.models.xxz_chain` is included below as an illustrative example how to implement a Model. The implementation of the XXZChain directly follows the steps outlined above. The XXZChain2 implements the very same model, but based on the CouplingMPOModel explained in the next section.

```python
"""
Prototypical example of a 1D quantum model: the spin-1/2 XXZ chain.

The XXZ chain is contained in the more general :class:`tenpy.models.spins.SpinChain`; the idea of this module is more to serve as a pedagogical example for a model.
"""

# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import numpy as np
from .lattice import Site, Chain
from .model import CouplingModel, NearestNeighborModel, MPOModel, CouplingMPOModel
from ..linalg import np_conserved as npc
from ..tools.params import asConfig
from ..networks.site import SpinHalfSite  # if you want to use the predefined site

__all__ = ['XXZChain', 'XXZChain2']

class XXZChain(CouplingModel, NearestNeighborModel, MPOModel):
    r"""Spin-1/2 XXZ chain with Sz conservation.

    The Hamiltonian reads:

    .. math::
        H = \sum_i \mathtt{Jxx}/2 (S^+_i S^-_{i+1} + S^-_i S^+_{i+1})
        + \mathtt{Jz} S^z_i S^z_{i+1} \\
        - \sum_i \mathtt{hz} S^z_i

    All parameters are collected in a single dictionary `model_params`, which is turned into a :class:`tenpy.tools.params.Config` object.

    Parameters
    """
```
model_params : :class:`tenpy.tools.params.Config`
Parameters for the model. See :cfg:config:`XXZChain` below.

Options
-------
.. cfg:config :: XXZChain
  :include: CouplingMPOModel
  L : int
    Length of the chain.
  Jxx, Jz, hz : float | array
    Coupling as defined for the Hamiltonian above.
  bc_MPS : {'finite' | 'infinite'}
    MPS boundary conditions. Coupling boundary conditions are chosen appropriately.

```python
def __init__(self, model_params):
  # 0) read out/set default parameters
  model_params = asConfig(model_params, "XXZChain")
  L = model_params.get('L', 2)
  Jxx = model_params.get('Jxx', 1.)
  Jz = model_params.get('Jz', 1.)
  hz = model_params.get('hz', 0.)
  bc_MPS = model_params.get('bc_MPS', 'finite')
  # 1-3):
  USE_PREDEFINED_SITE = False
  if not USE_PREDEFINED_SITE:
    # 1) charges of the physical leg. The only time that we actually define charges!
    leg = npc.LegCharge.from_qflat(npc.ChargeInfo([1], ['2*Sz']), [1, -1])
    # 2) onsite operators
    Sp = [[0., 1.], [0., 0.]]
    Sm = [[0., 0.], [1., 0.]]
    Sz = [[0.5, 0.], [0., -0.5]]
    # (Can't define Sx and Sy as onsite operators: they are incompatible with Sz charges.)
    # 3) local physical site
    site = Site(leg, ['up', 'down'], Sp=Sp, Sm=Sm, Sz=Sz)
  else:
    # there is a site for spin-1/2 defined in TeNPy, so just we can just use it
    # replacing steps 1-3)
    site = SpinHalfSite(conserve='Sz')
  # 4) lattice
  bc = 'periodic' if bc_MPS == 'infinite' else 'open'
  lat = Chain(L, site, bc=bc, bc_MPS=bc_MPS)
  # 5) initialize CouplingModel
  CouplingModel.__init__(self, lat)
  # 6) add terms of the Hamiltonian
  # (u is always 0 as we have only one site in the unit cell)
  self.add_onsite(-hz, 0, 'Sz')
  self.add_coupling(Jxx * 0.5, 0, 'Sp', 0, 'Sm', 1, plus_hc=True)
  # instead of plus_hc=True, we could explicitly add the h.c. term with:
  self.add_coupling(Jz, 0, 'Sz', 0, 'Sz', 1)
  # 7) initialize H_MPO
```
MPOModel.__init__(self, lat, self.calc_H_MPO())

# 8) initialize H_bond (the order of 7/8 doesn't matter)
NearestNeighborModel.__init__(self, lat, self.calc_H_bond())

class XXZChain2(CouplingMPOModel, NearestNeighborModel):
    """Another implementation of the Spin-1/2 XXZ chain with Sz conservation.

    This implementation takes the same parameters as the :class:`XXZChain`, but is implemented based on the :class:`~tenpy.models.model.CouplingMPOModel`.

    Parameters
    ----------
    model_params : dict | :class:`~tenpy.tools.params.Config`
        See :cfg:config:`XXZChain`
    """
    def __init__(self, model_params):
        model_params = asConfig(model_params, "XXZChain2")
        model_params.setdefault('lattice', "Chain")
        CouplingMPOModel.__init__(self, model_params)

    def init_sites(self, model_params):
        return SpinHalfSite(conserve='Sz')  # use predefined Site

    def init_terms(self, model_params):
        # read out parameters
        Jxx = model_params.get('Jxx', 1.)
        Jz = model_params.get('Jz', 1.)
        hz = model_params.get('hz', 0.)
        # add terms
        for u in range(len(self.lat.unit_cell)):
            self.add_onsite(-hz, u, 'Sz')
        for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
            self.add_coupling(Jxx * 0.5, u1, 'Sp', u2, 'Sm', dx, plus_hc=True)
            self.add_coupling(Jz, u1, 'Sz', u2, 'Sz', dx)

The easiest way: the CouplingMPOModel

Since many of the basic steps above are always the same, we don’t need to repeat them all the time. So we have yet another class helping to structure the initialization of models: the CouplingMPOModel. The general structure of this class is like this:

class CouplingMPOModel(CouplingModel, MPOModel):
    def __init__(self, model_param):
        # ... follows the basic steps 1-8 using the methods
        lat = self.init_lattice(self, model_param)  # for step 4
        # ...
        self.init_terms(self, model_param)  # for step 6
        # ...

    def init_sites(self, model_param):
        # You should overwrite this

    def init_lattice(self, model_param):
The `XXZChain2` included above illustrates, how it can be used. You need to implement steps 1-3) by overwriting the method `init_sites()` Step 4) is performed in the method `init_lattice()`, which initializes arbitrary 1D or 2D lattices; by default a simple 1D chain. If your model only works for specific lattices, you can overwrite this method in your own class. Step 6) should be done by overwriting the method `init_terms()`. Steps 5,7,8 and calls to the `init_...` methods for the other steps are done automatically if you just call the `CouplingMPOModel.__init__(self, model_param)`.

The `XXZChain` and `XXZChain2` work only with the `Chain` as lattice, since they are derived from the `NearestNeighborModel`. This allows to use them for TEBD in 1D (yeah!), but we can’t get the MPO for DMRG on (for example) a `Square` lattice cylinder - although it’s intuitively clear, what the Hamiltonian there should be: just put the nearest-neighbor coupling on each bond of the 2D lattice.

It’s not possible to generalize a `NearestNeighborModel` to an arbitrary lattice where it’s no longer nearest neighbors in the MPS sense, but we can go the other way around: first write the model on an arbitrary 2D lattice and then restrict it to a 1D chain to make it a `NearestNeighborModel`.

Let me illustrate this with another standard example model: the transverse field Ising model, implemented in the module `tenpy.models.tf_ising` included below. The `TFIModel` works for arbitrary 1D or 2D lattices. The `TFIChain` is then taking the exact same model making a `NearestNeighborModel`, which only works for the 1D chain.

```
"""Prototypical example of a quantum model: the transverse field Ising model.

Like the :class:`~tenpy.models.xxz_chain.XXZChain`, the transverse field ising chain
:class:`TFIChain` is contained in the more general :class:`~tenpy.models.spins.
→SpinChain`;
the idea is more to serve as a pedagogical example for a 'model'.

We choose the field along z to allow to conserve the parity, if desired.
"""

# Copyright 2018–2020 TeNPy Developers, GNU GPLv3

import numpy as np
from .model import CouplingMPOModel, NearestNeighborModel
from ..tools.params import asConfig
from ..networks.site import SpinHalfSite

__all__ = ["TFIModel", 'TFIChain']

class TFIModel(CouplingMPOModel):
    r"""Transverse field Ising model on a general lattice.

    The Hamiltonian reads:
    .. math ::
    \sum_{\langle i,j\rangle, i < j} J \sigma^x_i \sigma^x_j"
```

(continues on next page)
\[ - \sum_{i} \mathbf{g} \sigma^z_i \]

Here, :math:`\langle i,j \rangle, i< j` denotes nearest neighbor pairs, each pair appearing exactly once.

All parameters are collected in a single dictionary `model_params`, which is turned into a :class:`tenpy.tools.params.Config` object.

Parameters
----------

*model_params : :class:`tenpy.tools.params.Config`

Parameters for the model. See :cfg:config:`TFIModel` below.

Options
-------

.. cfg:config :: TFIModel

:include: CouplingMPOModel

conserve : None | 'parity'

J, g : float | array
    Coupling as defined for the Hamiltonian above.

```python
def init_sites(self, model_params):
    conserve = model_params.get('conserve', 'parity')
    assert conserve != 'Sz'
    if conserve == 'best':
        conserve = 'parity'
        if self.verbose >= 1.:
            print(self.name + ': set conserve to', conserve)
    site = SpinHalfSite(conserve=conserve)
    return site

def init_terms(self, model_params):
    J = np.asarray(model_params.get('J', 1.))
    g = np.asarray(model_params.get('g', 1.))
    for u in range(len(self.lat.unit_cell)):
        self.add_onsite(-g, u, 'Sigmaz')
    for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
        self.add_coupling(-J, u1, 'Sigmax', u2, 'Sigmax', dx)
    # done
```

class TFIChain(TFIModel, NearestNeighborModel):
    """The :class:`TFIModel` on a Chain, suitable for TEBD.

See the :class:`TFIModel` for the documentation of parameters."

```python
def __init__(self, model_params):
    model_params = asConfig(model_params, self.__class__.__name__)
    model_params.setdefault('lattice', "Chain")
    CouplingMPOModel.__init__(self, model_params)
```
Automation of Hermitian conjugation

As most physical Hamiltonians are Hermitian, these Hamiltonians are fully determined when only half of the mutually conjugate terms is defined. For example, a simple Hamiltonian:

$$H = \sum_{(i,j),i<j} -J(c_i^\dagger c_j + c_j^\dagger c_i)$$

is fully determined by the term $c_i^\dagger c_j$ if we demand that Hermitian conjugates are included automatically. In TeNPy, whenever you add a coupling using `add_onsite()`, `add_coupling()`, or `add_multi_coupling()`, you can use the optional argument `plus_hc` to automatically create and add the Hermitian conjugate of that coupling term - as shown above.

Additionally, in an MPO, explicitly adding both a non-Hermitian term and its conjugate increases the bond dimension of the MPO, which increases the memory requirements of the `MPOEnvironment`. Instead of adding the conjugate terms explicitly, you can set a flag `explicit_plus_hc` in the `MPOCouplingModel` parameters, which will ensure two things:

1. The model and the MPO will only store half the terms of each Hermitian conjugate pair added, but the flag `explicit_plus_hc` indicates that they represent `self + h.c.`. In the example above, only the term $c_i^\dagger c_j$ would be saved.

2. At runtime during DMRG, the Hermitian conjugate of the (now non-Hermitian) MPO will be computed and applied along with the MPO, so that the effective Hamiltonian is still Hermitian.

**Note:** The model flag `explicit_plus_hc` should be used in conjunction with the flag `plus_hc` in `add_coupling()` or `add_multi_coupling()`. If `plus_hc` is `False` while `explicit_plus_hc` is `True` the MPO bond dimension will not be reduced, but you will still pay the additional computational cost of computing the Hermitian conjugate at runtime.

Thus, we end up with several use cases, depending on your preferences. Consider the `FermionModel`. If you do not care about the MPO bond dimension, and want to add Hermitian conjugate terms manually, you would set `model_par['explicit_plus_hc'] = False` and write:

```python
self.add_coupling(-J, u1, 'Cd', u2, 'C', dx)
self.add_coupling(np.conj(-J), u2, 'Cd', u1, 'C', -dx)
```

If you wanted to save the trouble of the extra line of code (but still did not care about MPO bond dimension), you would keep the `model_par`, but instead write:

```python
self.add_coupling(-J, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```

Finally, if you wanted a reduction in MPO bond dimension, you would need to set `model_par['explicit_plus_hc'] = True`, and write:

```python
self.add_coupling(-J, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```
Some random remarks on models

- Needless to say that we have also various predefined models under `tenpy.models`.

- Of course, an MPO is all you need to initialize a `MPOModel` to be used for DMRG; you don’t have to use the `CouplingModel` or `CouplingMPOModel`. For example an exponentially decaying long-range interactions are not supported by the coupling model but straight-forward to include to an MPO, as demonstrated in the example `examples/mpo_exponentially_decaying.py`.

- If the model of your interest contains Fermions, you should read the `Fermions and the Jordan-Wigner transformation`.

- We suggest writing the model to take a single parameter dictionary for the initialization, as the `CouplingMPOModel` does. The `CouplingMPOModel` converts the dictionary to a dict-like `Config` with some additional features before passing it on to the `init_lattice`, `init_site`, ... methods. It is recommended to read out providing default values with `model_params.get("key", default_value).see get()`.

- When you write a model and want to include a test that it can be at least constructed, take a look at `tests/test_model.py`.

7.3.4 Details on the lattice geometry

The `Lattice` class defines the geometry of the system. In the basic form, it represents a unit cell of a few sites repeated in one or multiple directions. Moreover, it maps this higher-dimensional geometry to a one-dimensional chain for MPS-based algorithms.

Visualization

A plot of the lattice can greatly help to understand which sites are connected by what couplings. The methods `plot_*` of the `Lattice` can do a good job for a quick illustration. Let’s look at the Honeycomb lattice as an example.

```python
import matplotlib.pyplot as plt
from tenpy.models import lattice

plt.figure(figsize=(5, 6))
ax = plt.gca()
latt = lattice.Honeycomb(Lx=4, Ly=4, sites=None, bc='periodic')
latt.plot_coupling(ax)
latt.plot_order(ax, linestyle=':')
latt.plot_sites(ax)
latt.plot_basis(ax, origin=-0.5*(latt.basis[0] + latt.basis[1]))
ax.set_aspect('equal')
ax.set_xlim(-1)
ax.set_ylim(-1)
plt.show()
```

In this case, the unit cell (shaded green) consists of two sites, which for the purpose of plotting we just set to `sites=None`; in general you should specify instances of `Site` for that. The unit cell gets repeated in the directions given by the lattice basis (green arrows at the unit cell boundary). Hence, we can label each site by a `lattice index` \((x, y, u)\) in this case, where \(x\) in `range(Lx)` , \(y\) in `range(Ly)` specify the translation of the unit cell and \(u\) in `range(len(unit_cell))` , here \(u\) in `[0, 1]`, specifies the index within the unit cell.
How an MPS winds through the lattice: the order

For MPS-based algorithms, we need to map a 2D lattice like the one above to a 1D chain. The red, dashed line in the plot indicates how an MPS winds through the 2D lattice. The MPS index $i$ is a simple enumeration of the sites along this line, shown as numbers next to the sites in the plot. The methods $\text{mps2lat_idx()}$ and $\text{lat2mps_idx()}$ map indices of the MPS to and from indices of the lattice.

The MPS class itself is (mostly) agnostic of the underlying geometry. For example, $\text{expectation_value()}$ will return a 1D array of the expectation value on each site indexed by the MPS index $i$. If you have a two-dimensional lattice, you can use $\text{mps2lat_values()}$ to map this result to a 2D array index by the lattice indices.

A suitable order is critical for the efficiency of MPS-based algorithms. On one hand, different orderings can lead to different MPO bond-dimensions, with direct impact on the complexity scaling. On the other hand, it influences how much entanglement needs to go through each bonds of the underlying MPS, e.g., the ground state to be found in DMRG, and therefore influences the required MPS bond dimensions. For the latter reason, the “optimal” ordering can not be known a priori and might even depend on your coupling parameters (and the phase you are in). In the end, you can just try different orderings and see which one works best.

The simplest way to change the order is to use a non-default value for the initialization parameter $\text{order}$ of the $\text{Lattice}$ class. This gets passed on to $\text{ordering()}$, which you an override in a custom lattice class to define new possible orderings. Alternatively, you can go the most general way and simply set the attribute $\text{order}$ to be a 2D numpy array with lattice indices as rows, in the order you want.

```python
import matplotlib.pyplot as plt
from tenpy.models import lattice

Lx, Ly = 3, 3
fig, axes = plt.subplots(2, 2, figsize=(7, 8))

lat1 = lattice.Honeycomb(Lx, Ly, sites=None, bc='periodic')  # default order
lat2 = lattice.Honeycomb(Lx, Ly, sites=None, bc='periodic',
                        order='Cstyle')  # first method to change order
# alternative: directly set "Cstyle" order
lat3 = lattice.Honeycomb(Lx, Ly, sites=None, bc='periodic')
lat3.order = lat2.ordering("Cstyle")  # now equivalent to lat2

# general: can apply arbitrary permutation to the order
lat4 = lattice.Honeycomb(Lx, Ly, sites=None, bc='periodic',
                        order='Cstyle')

old_order = lat4.order
permutation = []
for i in range(0, len(old_order), 2):
    permutation.append(i+1)
    permutation.append(i)
lat4.order = old_order[permutation, :]

for lat, label, ax in zip([lat1, lat2, lat3, lat4],
                          ['order='default',
                           "order='Cstyle'",
                           "order='Cstyle',
                           "custom permutation"],
                          axes.flatten()):
    lat.plot_coupling(ax)
    lat.plot_sites(ax)
    lat.plot_order(ax, linestyle=':', linewidth=2.)
    ax.set_aspect('equal')
    ax.set_title('order = ' + repr(label))
```

(continues on next page)
Boundary conditions

The Lattice defines the boundary conditions $bc$ in each direction. It can be one of the usual 'open' or 'periodic' in each direction.

On top of that, there is the $bc_MPS$ boundary condition of the MPS, one of 'finite', 'segment', 'infinite'. For an 'infinite' MPS, the whole lattice is repeated in the direction of the first basis vector of the lattice. For $bc_MPS$='infinite', the first direction should always be 'periodic', but you can also define a lattice with $bc_MPS$='finite', $bc$=['periodic', 'periodic'] for a finite system on the torus. This is discouraged, though, because the ground state MPS will require the squared bond dimension for the same precision in this case!

For two (or higher) dimensional lattices, e.g for DMRG on an infinite cylinder, you can also specify an integer shift instead of just saying 'periodic': Rolling the 2D lattice up into a cylinder, you have a degree of freedom which sites to connect. This is illustrated in the figure below for a Square lattice with $bc$=['periodic', shift] for shift in [-1, 0, 1] (different columns). In the first row, the orange markers indicate a pair of identified sites (see plot_bc_shift()). The dashed orange line indicates the direction of the cylinder axis. The line where the cylinder is "cut open" therefore winds around the the cylinder for a non-zero shift. (A similar thing happens even for shift=0 for more complicated lattices with non-orthogonal basis.) In the second row, we directly draw lines between all sites connected by nearest-neighbor couplings, as they appear in the MPO.

Irregular Lattices

The IrregularLattice allows to add or remove sites from/to an existing regular lattice. The doc-string of IrregularLattice contains several examples, let us consider another one here, where we use the IrregularLattice to "fix" the boundary of the Honeycomb lattice: when we use "open" boundary conditions for a finite system, there are two sites (on the lower left, and upper right), wich are not included into any hexagonal. The following example shows how to remove them from the system:

```python
import matplotlib.pyplot as plt
from tenpy.models import lattice

Lx, Ly = 3, 3
fig, axes = plt.subplots(1, 2, sharex=True, sharey=True, figsize=(6, 4))

reg_lat = lattice.Honeycomb(Lx=Lx, Ly=Ly, sites=None, bc='open')
irr_lat = lattice.IrregularLattice(reg_lat, remove=[[0, 0, 0], [-1, -1, 1]])
for lat, label, ax in zip([reg_lat, irr_lat],
                         ['regular', 'irregular'],
                         axes.flatten()):
    lat.plot_coupling(ax)
    lat.plot_order(ax, linestyle=':')
    lat.plot_sites(ax)
    ax.set_aspect('equal')
    ax.set_title(label)

plt.show()
```
order = "order='default'"

order = "order='Cstyle'"

order = "order='Cstyle'"

order = 'custom permutation'
7.3. Introductions
7.3.5 Fermions and the Jordan-Wigner transformation

The Jordan-Wigner transformation maps fermionic creation- and annihilation operators to (bosonic) spin-operators.

Spinless fermions in 1D

Let’s start by explicitly writing down the transformation. With the Pauli matrices \( \sigma^x, \sigma^y, \sigma^z \) and \( \sigma^\pm = (\sigma^x \pm i\sigma^y)/2 \) on each site, we can map

\[
  n_j \leftrightarrow (\sigma^z_j + 1)/2 \\
  c_j \leftrightarrow (-1)^{\sum_{l<j} n_l} \sigma^-_j \\
  c_j^\dagger \leftrightarrow (-1)^{\sum_{l<j} n_l} \sigma^+_j
\]

The \( n_l \) in the second and third row are defined in terms of Pauli matrices according to the first row. We do not interpret the Pauli matrices as spin-1/2; they have nothing to do with the spin in the spin-full case. If you really want to interpret them physically, you might better think of them as hard-core bosons \( b_j = \sigma^-_j, b_j^\dagger = \sigma^+_j \), with a spin of the fermions mapping to a spin of the hard-core bosons.

Note that this transformation maps the fermionic operators \( c_j \) and \( c_j^\dagger \) to global operators; although they carry an index \( j \) indicating a site, they actually act on all sites \( 1 \leq l < j \)! Thus, clearly the operators \( C \) and \( C_d \) defined in the FermionSite do not directly correspond to \( c_j \) and \( c_j^\dagger \). The part \( (-1)^{\sum_{l<j} n_l} \) is called Jordan-Wigner string and in the FermionSite is given by the local operator \( JW := (-1)^{n_j} \) acting all sites \( 1 < j \). Since this important, let me stress it again:

**Warning:** The fermionic operator \( c_j \) (and similar \( c_j^\dagger \)) maps to a global operator consisting of the Jordan-Wigner string built by the local operator \( JW \) on sites \( 1 \leq l < j \) and the local operator \( C \) (or \( C_d \), respectively) on site \( j \).

On the sites itself, the onsite operators \( C \) and \( C_d \) in the FermionSite fulfill the correct anti-commutation relation, without the need to include \( JW \) strings. The \( JW \) string is necessary to ensure the anti-commutation for operators acting on different sites.

Written in terms of onsite operators defined in the FermionSite, with the \( i \)-th entry in the list acting on site \( i \), the relations are thus:

\[
  \begin{array}{c}
  \text{["JW", 
  ..., "JW", "C", 
  ..., "Id"]} \quad \text{# for the annihilation operator} \\
  \text{["JW", 
  ..., "JW", "Cd", 
  ..., "Id"]} \quad \text{# for the creation operator}
  \end{array}
\]

Note that "JW" squares to the identity, "JW JW" = "Id", which is the reason that the Jordan-Wigner string completely cancels in \( n_j = c_j^\dagger c_j \). In the above notation, this can be written as:

\[
  \begin{array}{c}
  \text{["JW", 
  ..., "JW", "Cd", 
  ..., "Id"]} \times \text{["JW", 
  ..., "JW", "C", 
  ..., "Id"]} \\
  \Rightarrow \text{["JW JW", 
  ..., "JW JW", "Cd C", 
  "Id Id", 
  ..., "Id Id"]} \quad \text{# by definition of tensor product} \\
  \Rightarrow \text{["Id", 
  ..., "Id", 
  "N", 
  ..., "Id"]} \quad \text{# by definition of the local operators} \\
  \Rightarrow \text{("X Y" stands for the local operators X and Y applied on the same site. We assume that the "Cd" and "C" on the first line act on the same site.)}
  \end{array}
\]

For a pair of operators acting on different sites, \( JW \) strings have to be included for every site between the operators. For example, taking \( i < j \), \( c_i^\dagger c_j \leftrightarrow \sigma^+_i (-1)^{\sum_{l<i} n_l} \sigma^-_j \). More explicitly, for \( j = i+2 \) we get:
In other words, the Jordan-Wigner string appears only in the range \( i \leq l < j \), i.e. between the two sites and on the smaller/left one of them. (You can easily generalize this rule to cases with more than two \( c \) or \( c^\dagger \).)

This last line (as well as the last line of the previous example) can be rewritten by changing the order of the operators \( Cd \ JW \) to "JW Cd" \( = - "Cd" \). (This is valid because either site \( i \) is occupied, yielding a minus sign from the JW, or it is empty, yielding a 0 from the Cd.)

This is also the case for \( j < i \), say \( j = i-2 \):

\[
\begin{align*}
\mathcal{N}_{s,i}^1 \mathcal{N}_{s,i+1}^1 & \leftrightarrow (-1)^{\sum_{l<i} n^1_{i,l} \sigma^+_l \sigma^-_j}.
\end{align*}
\]

As shown in the following, the JW again appears on the left site, but this time acting after \( C \):

Higher dimensions

For an MPO or MPS, you always have to define an ordering of all your sites. This ordering effectively maps the higher-dimensional lattice to a 1D chain, usually at the expense of long-range hopping/interactions. With this mapping, the Jordan-Wigner transformation generalizes to higher dimensions in a straightforward way.

Spinful fermions

As illustrated in the above picture, you can think of spin-1/2 fermions on a chain as spinless fermions living on a ladder (and analogous mappings for higher dimensional lattices). Each rung (a blue box in the picture) forms a \texttt{SpinHalfFermionSite} which is composed of two \texttt{FermionSite} (the circles in the picture) for spin-up and spin-down. The mapping of the spin-1/2 fermions onto the ladder induces an ordering of the spins, as the final result must again be a one-dimensional chain, now containing both spin species. The solid line indicates the convention for the ordering, the dashed lines indicate spin-preserving hopping \( c^\dagger_{s,i}c_{s,i+1} + h.c. \) and visualize the ladder structure. More generally, each species of fermions appearing in your model gets a separate label, and its Jordan-Wigner string includes the signs \((-1)^n\) of all species of fermions to the ‘left’ of it (in the sense of the ordering indicated by the solid line in the picture).

In the case of spin-1/2 fermions labeled by \( \uparrow \) and \( \downarrow \) on each site, the complete mapping is given (where \( j \) and \( l \) are indices of the \texttt{FermionSite}):

\[
\begin{align*}
\mathcal{N}^\uparrow_{s,j} & \leftrightarrow (\sigma^z_{s,j} + 1)/2, \\
\mathcal{N}^\downarrow_{s,j} & \leftrightarrow (\sigma^z_{s,j} + 1)/2, \\
c_{s,j} \leftrightarrow (-1)^{\sum_{l<j} n^\uparrow_{1,l} + n^\downarrow_{1,l} \sigma^+_l \sigma^-_j}, \\
c_{s,j}^\dagger \leftrightarrow (-1)^{\sum_{l<j} n^\uparrow_{1,l} + n^\downarrow_{1,l} \sigma^+_l \sigma^-_j}, \\
c_{s,j}^\uparrow \leftrightarrow (-1)^{\sum_{l<j} n^\downarrow_{1,l} (1 - n^\downarrow_{1,l}) \sigma^+_l \sigma^-_j}, \\
c_{s,j}^\downarrow \leftrightarrow (-1)^{\sum_{l<j} n^\downarrow_{1,l} (1 - n^\uparrow_{1,l}) \sigma^+_l \sigma^-_j}.
\end{align*}
\]
In each of the above mappings the operators on the right hand sides commute; we can rewrite \((-1)\sum_{l<j} n_{\uparrow,j} n_{\downarrow,l} = \prod_{l<j} (-1)^{n_{\uparrow,j} - n_{\downarrow,l}}\), which resembles the actual structure in the code more closely. The parts of the operator acting in the same box of the picture, i.e. which have the same index \(j\) or \(l\), are the ‘onsite’ operators in the SpinHalfFermionSite: for example JW on site \(j\) is given by \((-1)^{n_{\uparrow,j}}(1)^{n_{\downarrow,j}}\), Cu is just the \(\sigma^+_{\uparrow,j}\), Cd is \((-1)^{n_{\uparrow,j}}\sigma^+_{\downarrow,j}\), and Cdd is \((-1)^{n_{\uparrow,j}}\sigma^+_{\downarrow,j}\). Note the asymmetry regarding the spin in the definition of the onsite operators: the spin-down operators include Jordan-Wigner signs for the spin-up fermions on the same site. This asymmetry stems from the ordering convention introduced by the solid line in the picture, according to which the spin-up site is “left” of the spin-down site. With the above definition, the operators within the same SpinHalfFermionSite fulfill the expected commutation relations, for example "Cu Cdd" == "Cdd Cu", but again the JW on sites left of the operator pair is crucial to get the correct commutation relations globally.

**Warning:** Again, the fermionic operators \(c_{l,j},c^\dagger_{l,j},c_{l+1,j},c^\dagger_{l+1,j}\) correspond to global operators consisting of the Jordan-Wigner string built by the local operator JW on sites \(l < j\) and the local operators 'Cu', 'Cdu', 'Cd', 'Cdd' on site \(j\).

Written explicitly in terms of onsite operators defined in the FermionSite, with the \(j\)-th entry in the list acting on site \(j\), the relations are:

```
["JW", ..., "JW", "Cu", "Id", ..., "Id"]  # for the annihilation operator spin-up
["JW", ..., "JW", "Cd", "Id", ..., "Id"]  # for the annihilation operator spin-down
["JW", ..., "JW", "Cdu", "Id", ..., "Id"]  # for the creation operator spin-up
["JW", ..., "JW", "Cd", "Id", ..., "Id"]  # for the creation operator spin-down
```

As you can see, the asymmetry regarring the spins in the definition of the local onsite operators "Cu", "Cd", "Cdu" and "Cdd" lead to a symmetric definition in the global sense. If you look at the definitions very closely, you can see that in terms like ["Id", "Cd JW", "JW", "Cd"] the Jordan-Wigner sign \((-1)^{n_{\uparrow,j}}\) appears twice (namely once in the definition of "Cd" and once in the "JW" on site 2) and could in principle be canceled, however in favor of a simplified handling in the code we do not recommend you to cancel it. Similar, within a spinless FermionSite, one can simplify "Cd JW" == "Cd" and "JW C" == "C", but these relations do not hold in the SpinHalfSite, and for consistency we recommend to explicitly keep the "JW" operator string even in nearest-neighbor models where it is not strictly necessary.

**How to handle Jordan-Wigner strings in practice**

There are only a few pitfalls where you have to keep the mapping in mind: When building a model, you map the physical fermionic operators to the usual spin/bosonic operations. The algorithms don’t care about the mapping, they just use the given Hamiltonian, be it given as MPO for DMRG or as nearest neighbor couplings for TEBD. Only when you do a measurement (e.g. by calculating an expectation value or a correlation function), you have to reverse this mapping. Be aware that in certain cases, e.g. when calculating the entanglement entropy on a certain bond, you cannot reverse this mapping in a straightforward way, and thus your results might depend on how you defined the Jordan-Wigner string.

Whatever you do, you should first think about if (and how much of) the Jordan-Wigner string cancels. For example for many of the onsite operators (like the particle number operator \(N\) or the spin operators in the SpinHalfFermionSite) the Jordan-Wigner string cancels completely and you can just ignore it both in onsite-terms and couplings. In case of two operators acting on different sites, you typically have a Jordan-Wigner string inbetween (e.g. for the \(c_{l,j}^\dagger c_{l+1,j}\) examples described above and below) or no Jordan-Wigner strings at all (e.g. for density-density interactions \(n_i n_j\)). In fact, the case that the Jordan Wigner string on the left of the first non-trivial operator does not cancel is currently not supported for models and expectation values, as it usually doesn’t appear in practice. For terms involving more operators, things tend to get more complicated, e.g. \(c_{l,j}^\dagger c_{l,k}^\dagger c_{l,j}\) with \(i < j < k < l\) requires a Jordan-Wigner string on sites \(m\) with \(i \leq m < j\) or \(k \leq m < l\), but not for \(j < m < k\).
TeNPy keeps track of which onsite operators need a Jordan-Wigner string in the Site class, specifically in need_JW_string and op_needs_JW(). Hence, when you define custom sites or add extra operators to the sites, make sure that op_needs_JW() returns the expected results.

When building a model the Jordan-Wigner strings need to be taken into account. If you just specify the $H_MPO$ or $H_bond$, it is your responsibility to use the correct mapping. However, if you use the add_coupling() method of the CouplingModel, (or the generalization add_multi_coupling() for more than 2 operators), TeNPy can use the information from the Site class to automatically add Jordan-Wigner strings as needed. Indeed, with the default argument op_string=None, add_coupling will automatically check whether the operators need Jordan-Wigner strings and correspondingly set op_string='JW', str_on_first=True, if necessary. For add_multi_coupling, you can’t even explicitly specify the correct Jordan-Wigner strings, but you must use op_string=None, from which it will automatically determine where Jordan-Wigner strings are needed.

Obviously, you should be careful about the convention which of the operators is applied first (in a physical sense as an operator acting on a state), as this corresponds to a sign of the prefactor. Read the doc-strings of add_coupling() add_multi_coupling() for details.

As a concrete example, let us specify a hopping $\sum_i (c_i^\dagger c_{i+1} + \text{h.c.}) = \sum_i (c_i^\dagger c_{i+1} + c_i^\dagger c_{i-1})$ in a 1D chain of FermionSite with add_coupling(). The recommended way is just:

```python
self.add_coupling(strength, 0, 'Cd', 0, 'C', 1, plus_hc=True)
```

If you want to specify both the Jordan-Wigner string and the h.c. term explicitly, you can use:

```python
self.add_coupling(strength, 0, 'Cd', 0, 'C', 1, op_string='JW', str_on_first=True)
self.add_coupling(strength, 0, 'Cd', 0, 'C', -1, op_string='JW', str_on_first=True)
```

Slightly more complicated, to specify the hopping $\sum_{\langle i,j \rangle} (c_{s,i}^\dagger c_{s,j} + \text{h.c.})$ in the Fermi-Hubbard model on a 2D square lattice, we could use:

```python
for (dx, dy) in [(1, 0), (0, 1)]:
    self.add_coupling(strength, 0, 'Cd', 0, 'C', (dx, dy), op_string='JW', str_on_first=True) # spin up
    self.add_coupling(strength, 0, 'Cd', 0, 'C', (dx, dy), op_string='JW', str_on_first=True) # spin down

# or without 'plus_hc'
for (dx, dy) in [(1, 0), (-1, 0), (0, 1), (0, -1)]: # include -dx!
    self.add_coupling(strength, 0, 'Cd', 0, 'Cu', (dx, dy)) # spin up
    self.add_coupling(strength, 0, 'Cd', 0, 'Cu', (dx, dy)) # spin down

# or specifying the 'JW' string explicitly
for (dx, dy) in [(1, 0), (-1, 0), (0, 1), (0, -1)]:
    self.add_coupling(strength, 0, 'Cd', 0, 'Cu', (dx, dy), 'JW', True) # spin up
    self.add_coupling(strength, 0, 'Cd', 0, 'Cu', (dx, dy), 'JW', True) # spin down
```

The most important functions for doing measurements are probably expectation_value() and correlation_function(). Again, if all the Jordan-Wigner strings cancel, you don’t have to worry about them at all, e.g. for many onsite operators or correlation functions involving only number operators. If you build multi-site operators to be measured by expectation_value, take care to include the Jordan-Wigner string correctly.

Some MPS methods like correlation_function(), expectation_value_term() and expectation_value_terms_sum() automatically add Jordan-Wigner strings (at least with default arguments). Other more low-level functions like expectation_value_multi_sites() don’t do it. Hence, you should always watch out during measurements, if the function used needs special treatment for Jordan-Wigner strings.

7.3. Introductions 87
7.3.6 Saving to disk: input/output

**Using pickle**

A simple and pythonic way to store data of TeNPy arrays is to use pickle from the Python standard library. Pickle allows to store (almost) arbitrary python objects, and the `Array` is no exception (and neither are other TeNPy classes).

Say that you have run DMRG to get a ground state $\psi$ as an MPS. With pickle, you can save it to disk as follows:

```python
import pickle
with open('my_psi_file.pkl', 'wb') as f:
    pickle.dump(psi, f)
```

Here, the `with ... :` structure ensures that the file gets closed after the pickle dump, and the `'wb'` indicates the file opening mode “write binary”. Reading the data from disk is as easy as (`'rb'` for reading binary):

```python
with open('my_psi_file.pkl', 'rb') as f:
    psi = pickle.load(f)
```

**Note:** It is a good (scientific) practice to include meta-data to the file, like the parameters you used to generate that state. Instead of just the $\psi$, you can simply store a dictionary containing $\psi$ and other data, e.g., `data = {'psi': psi, 'dmrg_params': dmrg_params, 'model_params': model_params}`. This can save you a lot of pain, when you come back looking at the files a few month later and forgot what you’ve done to generate them!

In some cases, compression can significantly reduce the space needed to save the data. This can for example be done with `gzip` (as well in the Python standard library). However, be warned that it might cause longer loading and saving times, i.e. it comes at the penalty of more CPU usage for the input/output. In Python, this requires only small adjustments:

```python
import pickle
import gzip

# to save:
with gzip.open('my_data_file.pkl', 'wb') as f:
    pickle.dump(data, f)
# and to load:
with gzip.open('my_data_file.pkl', 'rb') as f:
    data = pickle.load(f)
```

**Using HDF5 with h5py**

While pickle is great for simple input/output of python objects, it also has disadvantages. The probably most dramatic one is the limited portability: saving data on one PC and loading it on another one might fail! Even exporting data from Python 2 to load them in Python 3 on the same machine can give quite some troubles. Moreover, pickle requires to load the whole file at once, which might be unnecessary if you only need part of the data, or even lead to memory problems if you have more data on disk than fits into RAM.

Hence, we support saving to HDF5 files as an alternative. The h5py package provides a dictionary-like interface for the file/group objects with numpy-like data sets, and is quite easy to use. If you don’t know about HDF5, read the quickstart of the h5py documentation (and this guide).

The implementation can be found in the `tenpy.tools.hdf5_io` module with the `Hdf5Saver` and `Hdf5Loader` classes and the wrapper functions `save_to_hdf5()`, `load_from_hdf5()`.

The usage is very similar to pickle:
import h5py
from tenpy.tools import hdf5_io

data = {"psi": psi,  # e.g. an MPS
        "model": my_model,
        "parameters": {"L": 6, "g": 1.3}}

with h5py.File("file.h5", 'w') as f:
    hdf5_io.save_to_hdf5(f, data)
# ...

with h5py.File("file.h5", 'r') as f:
    data = hdf5_io.load_from_hdf5(f)
# or for partial reading:
    pars = hdf5_io.load_from_hdf5(f, "/parameters")

**Warning:** Like loading a pickle file, loading data from a manipulated HDF5 file with the functions described has the potential to cause arbitrary code execution. Only load data from trusted sources!

**Note:** The hickle package imitates the pickle functionality while saving the data to HDF5 files. However, since it aims to be close to pickle, it results in a more complicated data structure than we want here.

**Note:** To use the export/import features to HDF5, you need to install the h5py python package (and hence some version of the HDF5 library).

### Data format specification for saving to HDF5

This section motivates and defines the format how we save data of TeNPy-defined classes. The goal is to have the `save_to_hdf5()` function for saving sufficiently simple enough python objects (supported by the format) to disk in an HDF5 file, such that they can be reconstructed with the `load_from_hdf5()` function, as outlined in the example code above.

**Guidelines of the format:**

1. **Store enough data such that `load_from_hdf5()` can reconstruct a copy of the object (provided that the save did not fail with an error).**

2. **Objects of a type supported by the HDF5 datasets (with the h5py interface) should be directly stored as h5py Dataset.** Such objects are for example numpy arrays (of non-object dtype), scalars and strings.

3. **Allow to save (nested) python lists, tuples and dictionaries with values (and keys) which can be saved.**

4. **Allow user-defined classes to implement a well-defined interface which allows to save instances of that class, hence extending what data can be saved.** An instance of a class supporting the interface gets saved as an HDF5 Group. Class attributes are stored as entries of the group, metadata like the type should be stored in HDF5 attributes, see attributes.

5. **Simple and intuitive, human-readable structure for the HDF5 paths.** For example, saving a simple dictionary `{"a": np.arange(10), "b": 123.45}` should result in an HDF5 file with just the two data sets /a and /b.

6. **Allow loading only a subset of the data by specifying the path of the HDF5 group to be loaded.** For the above example, specifying the path /b should result in loading the float 123.45, not the array.
6. Avoid unnecessary copies if the same python object is referenced by different names, e.g., for the data {'c': large_obj, 'd': large_obj} with to references to the same large_obj, save it only once and use HDF5 hard-links such that /c and /d are the same HDF5 dataset/group. Also avoid the copies during the loading, i.e., the loaded dictionary should again have two references to a single object large_obj. This is also necessary to allow saving and loading of objects with cyclic references.

The full format specification is given by what the code in hdf5_io does… Since this is not trivial to understand, let me summarize it here:

- Following 1), simple scalars, strings, and numpy arrays are saved as Dataset. Other objects are saved as a HDF5 Group, with the actual data being saved as group members (as sub-groups and sub-datasets) or as attributes (for metadata or simple data).

- The type of the object is stored in the HDF5 attribute 'type', which is one of the global REPR_* variables in tenpy.tools.hdf5_io. The type determines the format for saving/loading of builtin types (list, …)

- Userdefined classes which should be possible to export/import need to implement the methods save_hdf5 and from_hdf5 as specified in Hdf5Exportable. When saving such a class, the attribute 'type' is automatically set to 'instance', and the class name and module are saved under the attributes 'module' and 'class'. During loading, this information is used to automatically import the module, get the class and call the classmethod from_hdf5 for reconstruction. This can only work if the class definition already exists, i.e., you can only save class instances, not classes itself.

- For most (python) classes, simply subclassing Hdf5Exportable should work to make the class exportable. The latter saves the contents of __dict__, with the extra attribute 'format' specifying whether the dictionary is “simple” (see below.).

- The None object is saved as a group with the attribute 'type' being 'None' and no subgroups.

- For iterables (list, tuple and set), we simple enumerate the entries and save entries as group members under the names '0', '1', '2', …, and a maximum 'len' attribute.

- The format for dictionaries depends on whether all keys are “simple”, which we define as being strings which are valid path names in HDF5, see valid_hdf5_path_component(). Following 4), the keys of a simple dictionary are directly used as names for group members, and the values being whatever object the group member represents.

- Partial loading along 5) is possible by directly specifying the subgroup or the path to load_from_hdf5().

- Guideline 6) is ensured as much as possible. However, there is a bug/exception: tuples with cyclic references are not re-constructed correctly; the inner objects will be lists instead of tuples (but with the same object entries).

Finally, we have to mention that many TeNPy classes are Hdf5Exportable. In particular, the Array supports this. To see what the exact format for those classes is, look at the save_hdf5 and from_hdf5 methods of those classes.

**Note:** There can be multiple possible output formats for the same object. The dictionary – with the format for simple keys or general keys – is such an example, but userdefined classes can use the same technique in their from_hdf5 method. The user might also explicitly choose a “lossy” output format (e.g., “flat” for np_conserved Arrays and LegCharges).

**Tip:** The above format specification is quite general and not bound to TeNPy. Feel free to use it in your own projects :-) To separate the development, versions and issues of the format clearly from TeNPy, we maintain the code for it in a separate git repository, [https://github.com/tenpy/hdf5_io](https://github.com/tenpy/hdf5_io)
7.3.7 Protocol for using (i)DMRG

While this documentation contains extensive guidance on how to interact with the tenpy, it is often unclear how to approach a physics question using these methods. This page is an attempt to provide such guidance, describing a protocol on how to go from a model implementation to an answered question.

The basic workflow for an (i)DMRG project is as follows, with individual steps expanded on later where necessary.

1. Confirm the correctness of the model implementation.
2. Run some low-effort tests to see whether the question seems answerable.
3. If the tests are successful, run production-quality simulations. This will be entirely particular to the project you’re working on.
4. Confirm that your results are converged.

Confirming the model is correct

Although TeNPy makes model implementation much easier than constructing the MPO by hand, one should still ensure that the MPO represents the intended model faithfully. There are several possible ways to do this. Firstly, for sufficiently small system sizes, one can contract the entire MPO into a matrix, and inspect the matrix elements. In TeNPy, this can be done using `get_full_hamiltonian()`. These should reproduce the analytical Hamiltonian up to machine precision, or any other necessary cut-off (e.g., long-range interactions may be truncated at some finite distance).

Secondly, if the model basis allows it, one can construct (product state) MPSs for known eigenstates of the model and evaluate whether these reproduce the correct eigenvalues upon contraction with the MPO.

Finally, one can sometimes construct a basis of single- or even two-particle MPSs in some basis, and evaluate the MPO on this basis to get a representation of the single- and two-particle Hamiltonian. If the model contains only single- and two-body terms, this latter approach should reproduce all terms in the Hamiltonian.

Low-effort tests

As not every state can be accurately represented by an MPS, some results are outside the reach of (i)DMRG. To prevent wasting considerable numerical resources on a fruitless project, it is recommended to run some low-effort trials first, and see whether any indication of the desired result can be found. If so, one can then go on to more computationally expensive simulations. If not, one should evaluate:

1. Whether there is a mistake in the model or simulation set-up,
2. Whether a slightly more computationally expensive test would potentially yield a result, or
3. Whether your approach is unfortunately out of reach of (i)DMRG.

To set up low-effort trials, one should limit system size, bond dimension and the range of interactions, as well as (if possible) target a non-critical region of phase space. All these measures reduce the size of and/or entanglement entropy needing to be captured by the MPS, which yields both memory and run time advantages. Of course, one introduces a trade-off between computational cost and accuracy, which is why one should be careful to not put too much faith into results obtained at this stage.
Detecting convergence issues

Ensuring that the results of an (i)DMRG simulation are well-converged and thus reliable is a hugely important part of any (i)DMRG study. Possible indications that there might be a convergence issue include:

1. The simulation shows a non-monotonous decrease of energy, and/or a non-monotonous increase of entanglement entropy. An increase of energy or decrease of entanglement entropy on subsequent steps within a sweep, or between subsequent sweeps, are particularly suspicious.
2. The simulation does not halt because it reached a convergence criterion, but because it reached its maximum number of sweeps.
3. Results vary wildly under small changes of parameters. In particular, if a small change in bond dimension yields a big change in results, one should be suspicious of the data.

Combating convergence issues

To combat convergence issues of the (i)DMRG algorithm, several strategies (short of switching to a different method) can be attempted:

1. Ensure that there are no errors in the model (see above) or the simulation set-up.
2. Increase the maximum bond dimension.
3. Ramp up the maximum bond dimension during simulation, rather than starting at the highest value. I.e., define a schedule wherein the first $N_{\text{sweeps}}$ sweeps run at some $\chi_1 < \chi_{\text{max}}$, the next $N_{\text{sweeps}}$ at $\chi_1 < \chi_2 < \chi_{\text{max}}$, etc. This can be done through the chi_list option of the DMRGEngine. You should also make sure that the max_hours option is set to sufficiently long runtimes.
4. Increase the maximum number of sweeps the algorithm is allowed to make, through the max_sweeps option of the DMRGEngine.
5. Change the Mixer settings to in- or decrease the effects of the mixer.
6. Change convergence criteria. This will not overcome convergence issues in itself, but can help fine tune the (i)DMRG simulation if it takes a long time to converge (relax the convergence constraints), or if the simulation finishes too soon (tighten the constraints). Criteria to consider are max_E_err and max_S_err, in DMRGEngine.
7. Increase the minimum number of sweeps taken by the algorithm. Again, this will not resolve issues due to bad convergence, but might prevent bad results due to premature convergence. This can be done through the min_sweeps option of the DMRGEngine.
8. Change the size and shape of the MPS unit cell (where possible), in case an artificially enforced translational invariance prevents the algorithm from finding a true ground state which is incommensurate with this periodicity. For example, a chain system which has a true ground state that is periodic in three sites, will not be accurately represented by a two-site MPS unit cell, as the latter enforces two-site periodicity.

In some instances, it is essentially unavoidable to encounter convergence issues. In particular, a simulation of a critical state can cause problems with (i)DMRG convergence, as these states violate the area law underlying an accurate MPS approximation. In these cases, one should acknowledge the difficulties imposed by the method and take care to be very careful in interpreting the data.
7.4 Examples

7.4.1 Toycodes

These toycodes are meant to give you a flavor of the different algorithms, while keeping the codes as readable and simple as possible. The scripts are included in the [TeNPySource] repository in the folder `toycodes/`, but not part of the basic TeNpy library; the only requirements to run them are Python 3, Numpy, and Scipy.

**a_mps.py**

on github.

```python
"""Toy code implementing a matrix product state."""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import numpy as np
from scipy.linalg import svd
# if you get an error message "LinAlgError: SVD did not converge",
# uncomment the following line. (This requires TeNPy to be installed.)
# from tenpy.linalg.svd_robust import svd  # (works like scipy.linalg.svd)

class SimpleMPS:
    """Simple class for a matrix product state.
    We index sites with `i` from 0 to L-1; bond `i` is left of site `i`.
    We *assume* that the state is in right-canonical form.
    Parameters
    ----------
    Bs, Ss, bc:
    Same as attributes.
    Attributes
    ----------
    Bs : list of np.Array[ndim=3]
        The 'matrices' in right-canonical form, one for each physical site
        (within the unit-cell for an infinite MPS).
        Each `B[i]` has legs (virtual left, physical, virtual right), in short `vL i → vR`
    Ss : list of np.Array[ndim=1]
        The Schmidt values at each of the bonds, `Ss[i]` is left of `Bs[i]`.
    bc : 'infinite', 'finite'
        Boundary conditions.
    L : int
        Number of sites (in the unit-cell for an infinite MPS).
    nbonds : int
        Number of (non-trivial) bonds: L-1 for 'finite' boundary conditions
    """
    def __init__(self, Bs, Ss, bc='finite'):
        assert bc in ['finite', 'infinite']
        self.Bs = Bs
        self.Ss = Ss
        self.bc = bc
        self.L = len(Bs)
```

(continues on next page)
self.nbonds = self.L - 1 if self.bc == 'finite' else self.L

def copy(self):
    return SimpleMPS([B.copy() for B in self.Bs], [S.copy() for S in self.Ss],
                     self.bc)

def get_thetal(self, i):
    """Calculate effective single-site wave function on sites i in mixed canonical form."
    The returned array has legs 'vL, i, vR' (as one of the Bs).
    """
    return np.tensordot(np.diag(self.Ss[i]), self.Bs[i], [1, 0])  # vL [vL'], vL i vR

def get_theta2(self, i):
    """Calculate effective two-site wave function on sites i,j=(i+1) in mixed canonical form.
    The returned array has legs 'vL, i, j, vR'..
    """
    j = (i + 1) % self.L
    return np.tensordot(self.get_thetal(i), self.Bs[j], [2, 0])  # vL i [vR], vL j vR

def get_chi(self):
    """Return bond dimensions.""

def site_expectation_value(self, op):
    """Calculate expectation values of a local operator at each site.""
    result = []
    for i in range(self.L):
        theta = self.get_thetal(i)  # vL i vR
        op_theta = np.tensordot(op, theta, axes=[1, 1])  # i [i*], vL [i] vR
        result.append(np.tensordot(theta.conj(), op_theta, [[0, 1, 2], [1, 0, 2]]))  # [vL*] [i*] [vR*], [i] [vL] [vR]
    return np.real_if_close(result)

def bond_expectation_value(self, op):
    """Calculate expectation values of a local operator at each bond.""
    result = []
    for i in range(self.nbonds):
        theta = self.get_theta2(i)  # vL i j vR
        op_theta = np.tensordot(op[i], theta, axes=[2, 3])  # i [i*] [j*], vL [i] [j] vR
        result.append(np.tensordot(theta.conj(), op_theta, [[0, 1, 2, 3], [2, 0, 1, 3]]))  # [vL*] [i*] [j*] [vR*], [i] [j] [vL] [vR]
    return np.real_if_close(result)

def entanglement_entropy(self):
    """Return the (von-Neumann) entanglement entropy for a bipartition at any of the bonds.""
    bonds = range(1, self.L) if self.bc == 'finite' else range(0, self.L)
    result = []
(continues on next page)
for i in bonds:
    S = self.Ss[i].copy()
    S[S < 1.e-20] = 0.  # 0*log(0) should give 0; avoid warning or NaN.
    S2 = S * S
    assert abs(np.linalg.norm(S) - 1.) < 1.e-14
    result.append(-np.sum(S2 * np.log(S2)))
return np.array(result)

def correlation_length(self):
    """Diagonalize transfer matrix to obtain the correlation length."""
    import scipy.sparse.linalg.eigen.arpack as arp
    assert self.bc == 'infinite'  # works only in the infinite case
    B = self.Bs[0]  # vL i vR
    chi = B.shape[0]
    T = np.tensordot(B, np.conj(B), axes=[1, 1])  # vL [i] vR, vL* [i*] vR*
    for i in range(1, self.L):
        B = self.Bs[i]
        T = np.tensordot(T, B, axes=[2, 0])  # vL vL* [i] vR, [vL*] [i*] vR*
    T = np.reshape(T, (chi**2, chi**2))
    eta = arp.eigs(T, k=2, which='LM', return_eigenvectors=False, ncv=20)
    return -self.L / np.log(np.min(np.abs(eta))

def init_FM_MPS(L, d, bc='finite'):
    """Return a ferromagnetic MPS (= product state with all spins up)"""
    B = np.zeros([1, d, 1], np.float)
    B[0, 0, 0] = 1.
    S = np.ones([1], np.float)
    Bs = [B.copy() for i in range(L)]
    Ss = [S.copy() for i in range(L)]
    return SimpleMPS(Bs, Ss, bc)

def split_truncate_theta(theta, chi_max, eps):
    """Split and truncate a two-site wave function in mixed canonical form.
    Split a two-site wave function as follows:--
    \[(\theta)--vL \quad \rightarrow \quad \text{(A)}--\text{diag}(S)--\text{(B)}--vR\]
    \[| \quad | \quad |\]
    \[i \quad j \quad i \quad j\]
    Afterwards, truncate in the new leg (labeled `vC`)."
    Parameters
    -----------
    theta : np.Array[ndim=4]
        Two-site wave function in mixed canonical form, with legs `vL, i, j, vR`.
    chi_max : int
        Maximum number of singular values to keep
    eps : float
        Discard any singular values smaller than that.

    Returns

(continues on next page)
A : np.Array[ndim=3]
  Left-canonical matrix on site i, with legs `vL, i, vC`.
S : np.Array[ndim=1]
  Singular/Schmidt values.
B : np.Array[ndim=3]
  Right-canonical matrix on site j, with legs `vC, j, vR`.

chivL, dL, dR, chivR = theta.shape
theta = np.reshape(theta, [chivL * dL, dR * chivR])
X, Y, Z = svd(theta, full_matrices=False)

# truncate
chivC = min(chi_max, np.sum(Y > eps))
piv = np.argsort(Y)[::-1][:chivC]  # keep the largest `chivC` singular values
X, Y, Z = X[:, piv], Y[piv], Z[piv, :]

# renormalize
S = Y / np.linalg.norm(Y)  # == Y/sqrt(sum(Y**2))

# split legs of X and Z
A = np.reshape(X, [chivL, dL, chivC])
B = np.reshape(Z, [chivC, dR, chivR])

return A, S, B

b_model.py

on github.

"""Toy code implementing the transverse-field Ising model."""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import numpy as np

class TFIModel:
    """Simple class generating the Hamiltonian of the transverse-field Ising model.
    The Hamiltonian reads
    .. math::
        H = - J \ \sum_{i} \ \sigma^x_i \ \sigma^x_{i+1} - g \ \sum_{i} \ \sigma^z_i
    Parameters
    -----------
    L : int
        Number of sites.
    J, g : float
        Coupling parameters of the above defined Hamiltonian.
    bc : 'infinite', 'finite'
        Boundary conditions.
    Attributes
    -----------
    L : int
        Number of sites.
    bc : 'infinite', 'finite'
        Boundary conditions.
    sigmax, sigmay, sigmaz, id :

(continues on next page)
Local operators, namely the Pauli matrices and identity.

\( H_{\text{bonds}} \) : list of np.Array[ndim=4]

The Hamiltonian written in terms of local 2-site operators, \( `H = \sum_i H_{\text{bonds}[i]}` \).

Each \( `H_{\text{bonds}[i]}` \) has (physical) legs (i out, (i+1) out, i in, (i+1) in),
in short \( `i j i^* j^*` \).

\( H_{\text{mpo}} \) : list of np.Array[ndim=4]

The Hamiltonian written as an MPO.

Each \( `H_{\text{mpo}[i]}` \) has legs (virtual left, virtual right, physical out, \( \rightarrow \) physical in),
in short \( `wL wR i i^*` \).

```python
# (note: not required for TEBD)
def init_H_mpo(self):
    ```
```
```
```
```
```
```
```
```
```
w[1, 2] = -self.J * self.sigmax
w_list.append(w)
self.H_mpo = w_list

c_tebd.py

on github.

"""Toy code implementing the time evolving block decimation (TEBD)."""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import numpy as np
from scipy.linalg import expm
from a_mps import split_truncate_theta

def calc_U_bonds(H_bonds, dt):
    """Given the H_bonds, calculate \( U_bonds[i] = \expm(-dt \cdot H_bonds[i]) \)."
    
    Each local operator has legs (i out, (i+1) out, i in, (i+1) in), in short \( i \rightarrow i/j \rightarrow i*j \).
    
    Note that no imaginary 'i' is included, thus real 'dt' means 'imaginary time' evolution!
    """
    d = H_bonds[0].shape[0]
    U_bonds = []
    for H in H_bonds:
        H = np.reshape(H, [d * d, d * d])
        U = expm(-dt * H)
        U_bonds.append(np.reshape(U, [d, d, d, d]))
    return U_bonds

def run_TEBD(psi, U_bonds, N_steps, chi_max, eps):
    """Evolve for \( N\) steps with TEBD."""
    Nbonds = psi.L - 1 if psi.bc == 'finite' else psi.L
    assert len(U_bonds) == Nbonds
    for n in range(N_steps):
        for k in [0, 1]:  # even, odd
            for i_bond in range(k, Nbonds, 2):
                update_bond(psi, i_bond, U_bonds[i_bond], chi_max, eps)
            # done

def update_bond(psi, i, U_bond, chi_max, eps):
    """Apply \( U_bond \) acting on \( i, j=(i+1) \) to \( \psi \)."""
    j = (i + 1) % psi.L
    # construct theta matrix
    theta = psi.get_theta2(i)  # vL i j vR
    # apply U
    Utheta = np.tensordot(U_bond, theta, axes=[[2, 3], [1, 2]])  # vL [i*] [j*], vL_\rightarrow[i] [j] vR
    Utheta = np.transpose(Utheta, [2, 0, 1, 3])  # vL i j vR
    # split and truncate
    Ai, Sj, Bj = split_truncate_theta(Utheta, chi_max, eps)
# put back into MPS

\[
Gi = \text{np.tensordot}(\text{np.diag}(\text{psi.Ss[i]**(-1)}), \text{Ai}, \text{axes}=[1, 0]) \quad # \text{vL} \quad [\text{vL}^*], \quad [\text{vL}] \quad i \quad \rightarrow \text{VC}
\]

\[
\text{psi.Bs[i]} = \text{np.tensordot}(Gi, \text{np.diag}(Sj), \text{axes}=[2, 0]) \quad # \text{vL} \quad [\text{vC}], \quad [\text{vC}] \quad j \quad \text{vR}
\]

\[
\text{psi.Ss[j]} = Sj \quad # \text{VC}
\]

\[
\text{psi.Bs[j]} = Bj \quad # \text{vC} \quad j \quad \text{vR}
\]

def example_TEBD_gs_tf_ising_finite(L, g):
    print("finite TEBD, imaginary time evolution, transverse field Ising")
    print("L=" + str(L) + ", g=" + str(g) + ")
    import a_mps
    import b_model
    M = b_model.TFIModel(L=L, J=1., g=g, bc='finite')
    psi = a_mps.init_FM_MPS(M.L, M.d, M.bc)
    for dt in [0.1, 0.01, 1.e-4, 1.e-5]:
        U_bonds = calc_U_bonds(M.H_bonds, dt)
        run_TEBD(psi, U_bonds, N_steps=500, chi_max=30, eps=1.e-10)
        E = np.sum(psi.bond_expectation_value(M.H_bonds))
        print("dt = \{dt:.5f\}: E = \{E:.13f\}".format(dt=dt, E=E))
        print("final bond dimensions: ", psi.get_chi())
        mag_x = np.sum(psi.site_expectation_value(M.sigmax))
        mag_z = np.sum(psi.site_expectation_value(M.sigmaz))
        print("magnetization in X = \{mag_x:.5f\}".format(mag_x=mag_x))
        print("magnetization in Z = \{mag_z:.5f\}".format(mag_z=mag_z))
        if L < 20:
            # compare to exact result
            from tfi_exact import finite_gs_energy
            E_exact = finite_gs_energy(L=L, g=g)
            print("Exact diagonalization: E = \{E:.13f\}".format(E=E_exact))
            print("relative error: ", abs((E - E_exact) / E_exact))
            return E, psi, M

def example_TEBD_gs_tf_ising_infinite(g):
    print("infinite TEBD, imaginary time evolution, transverse field Ising")
    print("g=" + str(g) + ")
    import a_mps
    import b_model
    M = b_model.TFIModel(L=2, J=1., g=g, bc='infinite')
    psi = a_mps.init_FM_MPS(M.L, M.d, M.bc)
    for dt in [0.1, 0.01, 1.e-4, 1.e-5]:
        U_bonds = calc_U_bonds(M.H_bonds, dt)
        run_TEBD(psi, U_bonds, N_steps=500, chi_max=30, eps=1.e-10)
        E = np.mean(psi.bond_expectation_value(M.H_bonds))
        print("dt = \{dt:.5f\}: E (per site) = \{E:.13f\}".format(dt=dt, E=E))
        print("final bond dimensions: ", psi.get_chi())
        mag_x = np.mean(psi.site_expectation_value(M.sigmax))
        mag_z = np.mean(psi.site_expectation_value(M.sigmaz))
        print("<\sigma_x> = \{mag_x:.5f\}".format(mag_x=mag_x))
        print("<\sigma_z> = \{mag_z:.5f\}".format(mag_z=mag_z))
        print("correlation length: ", psi.correlation_length())
        # compare to exact result
        from tfi_exact import infinite_gs_energy
        E_exact = infinite_gs_energy(g)
        print("Analytic result: E (per site) = \{E:.13f\}".format(E=E_exact))
        print("relative error: ", abs((E - E_exact) / E_exact))
        return E, psi, M
def example_TEBD_tf_ising_lightcone(L, g, tmax, dt):
    print("finite TEBD, real time evolution, transverse field Ising")
    print("L={L:d}, g={g:.2f}, tmax={tmax:.2f}, dt={dt:.3f}".format(L=L, g=g,
    →tmax=tmax, dt=dt))
    # find ground state with TEBD or DMRG
    # E, psi, M = example_TEBD_gs_tf_ising_finite(L, g)
    from d_dmrg import example_DMRG_tf_ising_finite
    E, psi, M = example_DMRG_tf_ising_finite(L, g)
    i0 = L // 2
    # apply sigmaz on site i0
    SzB = np.tensordot(M.sigmaz, psi.Bs[i0], axes=[1, 1]) # i [i*], vL [i] vR
    psi.Bs[i0] = np.transpose(SzB, [1, 0, 2]) # vL i vR
    U_bonds = calc_U_bonds(M.H_bonds, 1.j * dt) # (imaginary dt -> realtime,
    →evolution)
    S = [psi.entanglement_entropy()]
    Nsteps = int(tmax / dt + 0.5)
    for n in range(Nsteps):
        if abs((n * dt + 0.1) % 0.2 - 0.1) < 1.e-10:
            print("t = {t:.2f}, chi =".format(t=n * dt), psi.get_chi())
        run_TEBD(psi, U_bonds, 1, chi_max=50, eps=1.e-10)
        S.append(psi.entanglement_entropy())
    import matplotlib.pyplot as plt
    plt.figure()
    plt.imshow(S[::-1], vmin=0.,
    →aspect='auto',
    →interpolation='nearest',
    →extent=(0, L - 1., -0.5 * dt, (Nsteps + 0.5) * dt))
    plt.xlabel('site $i$')
    plt.ylabel('time $t/J$')
    plt.xlim(0., tmax)
    plt.colorbar().set_label('entropy $S$')
    filename = 'c_tebd_lightcone_[g:.2f].pdf'.format(g=g)
    plt.savefig(filename)
    print("saved " + filename)

if __name__ == "__main__":
    example_TEBD_gs_tf_ising_finite(L=10, g=1.)
    print("-
    →\n    →100)
    example_TEBD_gs_tf_ising_infinite(g=1.5)
    print("-
    →\n    →100)
    example_TEBD_tf_ising_lightcone(L=20, g=1.5, tmax=3., dt=0.01)
"""Toy code implementing the density-matrix renormalization group (DMRG)."""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import numpy as np
from a_mps import split_truncate_theta
import scipy.sparse
import scipy.sparse.linalg.eigen.arpack as arp

class SimpleHeff(scipy.sparse.linalg.LinearOperator):
    '''Class for the effective Hamiltonian.
    To be diagonalized in `SimpleDMRGE-engine.update_bond`. Looks like this:
    .--vL* vR*--.
    |   i* j* |
    | | | |
    (LP)--(W1)--(W2)----(RP)
    | | | |
    | i j |
    .--vL vR--.
    '''
    def __init__(self, LP, RP, W1, W2):
        self.LP = LP
        self.RP = RP
        self.W1 = W1
        self.W2 = W2
        chi1, chi2 = LP.shape[0], RP.shape[2]
d1, d2 = W1.shape[2], W2.shape[2]
        self.theta_shape = (chi1, d1, d2, chi2)
        self.shape = (chi1 * d1 * d2 * chi2, chi1 * d1 * d2 * chi2)
        self.dtype = W1.dtype

    def _matvec(self, theta):
        x = np.reshape(theta, self.theta_shape)
        x = np.tensordot(self.LP, x, axes=(2, 0))
        x = np.tensordot(x, self.W1, axes=(1, 2))
        x = np.tensordot(x, self.W2, axes=(3, 1))
        x = np.tensordot(x, self.RP, axes=(1, 3))
        x = np.reshape(x, self.shape[0])
        return x

class SimpleDMRGE-engine:
    '''DMRG algorithm, implemented as class holding the necessary data.'
Parameters
---------
psi, model, chi_max, eps:
See attributes

Attributes
---------
psi : SimpleMPS
The current ground-state (approximation).
model :
The model of which the groundstate is to be calculated.
chi_max, eps:
Truncation parameters, see :func:`a_mps.split_truncate_theta`.

LPs, RPs : list of np.Array[ndim=3]
Left and right parts ("environments") of the effective Hamiltonian.
``LPs[i]`` is the contraction of all parts left of site `i` in the network 
``<psi|H|psi>``,
and similar ``RPs[i]`` for all parts right of site `i`.
Each ``LPs[i]`` has legs `vL wL* vL*`, ``RPs[i]`` has legs `vR* wR* vR`.

```python
def __init__(self, psi, model, chi_max, eps):
    assert psi.L == model.L and psi.bc == model.bc  # ensure compatibility
    self.H_mpo = model.H_mpo
    self.psi = psi
    self.LPs = [None] * psi.L
    self.RPs = [None] * psi.L
    self.chi_max = chi_max
    self.eps = eps
    # initialize left and right environment
    D = self.H_mpo[0].shape[0]
    chi = psi.Bs[0].shape[0]
    LP = np.zeros([chi, D, chi], dtype=np.float)  # vL wL* vL*
    RP = np.zeros([chi, D, chi], dtype=np.float)  # vR* wR* vR
    LP[:, 0, :] = np.eye(chi)
    RP[:, D - 1, :] = np.eye(chi)
    self.LPs[0] = LP
    self.RPs[-1] = RP
    # initialize necessary RPs
    for i in range(psi.L - 1, 1, -1):
        self.update_RP(i)

def sweep(self):
    # sweep from left to right
    for i in range(self.psi.nbonds - 1):
        self.update_bond(i)
    # sweep from right to left
    for i in range(self.psi.nbonds - 1, 0, -1):
        self.update_bond(i)

def update_bond(self, i):
    j = (i + 1) % self.psi.L
    # get effective Hamiltonian
    Heff = SimpleHeff(self.LPs[i], self.RPs[j], self.H_mpo[i], self.H_mpo[j])
    # Diagonalize Heff, find ground state `theta`
    theta0 = np.reshape(self.psi.get_theta2(i), [Heff.shape[0]])  # initial guess
    e, v = arp.eigsh(Heff, k=1, which='SA', return_eigenvectors=True, v0=theta0)
```
\( \theta = \text{np.reshape}(v[:, 0], \text{Heff.theta_shape}) \)

# split and truncate
\( A_i, S_j, B_j = \text{split_truncate_theta}(\theta, \text{self.chi_max}, \text{self.eps}) \)

# put back into MPS
\( G_i = \text{np.tensordot}(\text{np.diag}(\text{self.psi.Ss}[i]**(-1)), A_i, \text{axes}=[1, 0]) \)  # \( vL [vL^*] \)
\( \to \{vL\} \ i \ vC \)
\( \text{self.psi.Bs}[i] = \text{np.tensordot}(G_i, \text{np.diag}(S_j), \text{axes}=[2, 0]) \)  # \( vL \ i \ [vC]^* \)
\( \to \{vC^*\} \) \( vC \)
\( \text{self.psi.Ss}[j] = S_j \)  # \( vC \)
\( \text{self.psi.Bs}[j] = B_j \)  # \( vC \ j \ vR \)
\( \text{self.update_LP}(i) \)
\( \text{self.update_RP}(j) \)

```python
def update_RP(self, i):
    """Calculate RP right of site \('i-1\)' from RP right of site \('i\')."""
    j = (i - 1) % self.psi.L
    RP = self.RPs[i]  # \( vR^* \ wR^* \ vR \)
    B = self.psi.Bs[i]  # \( vL \ i \ vR \)
    Bc = B.conj()  # \( vL^* \ i^* \ vR^* \)
    W = self.H_mpo[i]  # \( wL \ wR \ i \ i^* \)
    RP = np.tensordot(B, RP, axes=[2, 0])  # \( vL \ i \ [vR]^* \ vR^* \)
    RP = np.tensordot(RP, W, axes=[1, [2], [3, 1]])  # \( vL \ [vL^*] \ wR, wL \ [wR] \ i \)
    \( \to \{i\} \)
    RP = np.tensordot(RP, Bc, axes=[i, 1, 2, 1])  # \( vL \ [vR] \ wL \ [i], vL^* \ [i^*] \)
    \( \to \{vR^*\} \)
    self.RPs[j] = RP  # \( vL \ wL \ vL^* \ (== vR^* \ wR^* \ vR \ on \ site \ i-1) \)

def update_LP(self, i):
    """Calculate LP left of site \('i+1\)' from LP left of site \('i\')."""
    j = (i + 1) % self.psi.L
    LP = self.LPs[i]  # \( vL \ wL \ vL^* \)
    B = self.psi.Bs[i]  # \( vL \ i \ vR \)
    G = np.tensordot(np.diag(self.psi.Ss[i]), B, axes=[1, 0])  # \( vL \ [vL^*], \ [vL] \)
    \( \to \{vR^*\} \ vR \)
    A = np.tensordot(G, np.diag(self.psi.Ss[j]**-1), axes=[2, 0])  # \( vL \ i \ [vR]^* \)
    Ac = A.conj()  # \( vL^* \ i^* \ vR^* \)
    W = self.H_mpo[i]  # \( wL \ wR \ i \ i^* \)
    LP = np.tensordot(LP, A, axes=[2, 0])  # \( vL \ wL^* \ [vL^*], \ [vL] \ i \ vR \)
    LP = np.tensordot(LP, W, axes=[[0, 3], [1, 2]])  # \( [wL] \ wR \ i \ [i^*], \ vL \ [wL^*] \)
    \( \to \{i\} \ vR \)
    LP = np.tensordot(Ac, LP, axes=[0, 1, 2, 1])  # \( [vL^*] \ [i^*] \ vR^* \ wR \ [i] \)
    \( \to \{vL\} \ vR \)
    self.LPs[j] = LP  # \( vL \ wL^* \ vL^* \ on \ site \ i+1 \)
```

```python
def example_DMRG_tf_ising_finite(L, g):
    print("finite DMRG, transverse field Ising")
    print("L={L:d}, g={g:.2f}".format(L=L, g=g))
    import a_mps
    import b_model
    M = b_model.TFIModel(L=L, J=1., g=g, bc='finite')
    psi = a_mps.init_FM_MPS(M.L, M.d, M.bc)
    eng = SimpleDMRGEngine(psi, M, chi_max=30, eps=1.e-10)
    for i in range(10):
        eng.sweep()
        E = np.sum(psi.bond_expectation_value(M.H_bonds))
```

(continues on next page)
print("sweep \{i\:2d\}: E = \{E:.13f\}\).format(i=i + 1, E=E))
print("final bond dimensions: ", psi.get_chi())
mag_x = np.sum(psi.site_expectation_value(M.sigmax))
mag_z = np.sum(psi.site_expectation_value(M.sigmaz))
print("magnetization in X = \{mag_x:.5f\}\).format(mag_x=mag_x))
print("magnetization in Z = \{mag_z:.5f\}\).format(mag_z=mag_z))
if L < 20:  # compare to exact result
    from tfi_exact import finite_gs_energy
    E_exact = finite_gs_energy(L, 1., g)
    print("Exact diagonalization: E = \{E:.13f\}\).format(E=E_exact))
    print("relative error: ", abs((E - E_exact) / E_exact))
return E, psi, M

def example_DMRG_tf_ising_infinite(g):
    print("infinite DMRG, transverse field Ising")
    print("g=\{g:.2f\}\).format(g=g))
    import a_mps
    import b_model
    M = b_model.TFIModel(L=2, J=1., g=g, bc='infinite')
    psi = a_mps.init_FM_MPS(M.L, M.d, M.bc)
    eng = SimpleDMRGEngine(psi, M, chi_max=20, eps=1.e-14)
    for i in range(20):
        eng.sweep()
        E = np.mean(psi.bond_expectation_value(M.H_bonds))
        print("sweep \{i\:2d\}: E (per site) = \{E:.13f\}\).format(i=i + 1, E=E))
    print("final bond dimensions: ", psi.get_chi())
mag_x = np.mean(psi.site_expectation_value(M.sigmax))
mag_z = np.mean(psi.site_expectation_value(M.sigmaz))
print("<\sigma_x> = \{mag_x:.5f\}\).format(mag_x=mag_x))
print("<\sigma_z> = \{mag_z:.5f\}\).format(mag_z=mag_z))
print("correlation length: ", psi.correlation_length())
    # compare to exact result
    from tfi_exact import infinite_gs_energy
    E_exact = infinite_gs_energy(1., g)
    print("Analytic result: E (per site) = \{E:.13f\}\).format(E=E_exact))
    print("relative error: ", abs((E - E_exact) / E_exact))
return E, psi, M

if __name__ == "__main__":
    example_DMRG_tf_ising_finite(L=10, g=1.)
    print("---")
    example_DMRG_tf_ising_infinite(g=1.5)

tfi_exact.py

on github.

"""Provides exact ground state energies for the transverse field ising model for comparison.

The Hamiltonian reads

.. math ::
\[ H = -J \sum_{i} \sigma_i^x \sigma_{i+1}^x - g \sum_{i} \sigma_i^z \]

(continues on next page)
def finite_gs_energy(L, J, g):
    """For comparison: obtain ground state energy from exact diagonalization.
    Exponentially expensive in L, only works for small enough \'L\' \(<\sim 20."
    
    if L > 20:
        warnings.warn("Large L: Exact diagonalization might take a long time!")
    # get single site operaors
    sx = sparse.csr_matrix(np.array([[0., 1.], [1., 0.]])
    sz = sparse.csr_matrix(np.array([[1., 0.], [0., -1.]])
    id = sparse.csr_matrix(np.eye(2))
    sx_list = []  # sx_list[i] = kron([id, id, ..., id, sx, id, .... id])
    sz_list = []
    for i_site in range(L):
        x_ops = [id] * L
        z_ops = [id] * L
        x_ops[i_site] = sx
        z_ops[i_site] = sz
        X = x_ops[0]
        Z = z_ops[0]
        for j in range(1, L):
            X = sparse.kron(X, x_ops[j], 'csr')
            Z = sparse.kron(Z, z_ops[j], 'csr')
        sx_list.append(X)
        sz_list.append(Z)
    H_xx = sparse.csr_matrix((2**L, 2**L))
    H_z = sparse.csr_matrix((2**L, 2**L))
    for i in range(L - 1):
        H_xx = H_xx + sx_list[i] * sx_list[(i + 1) % L]
    for i in range(L):
        H_z = H_z + sz_list[i]
    H = -J * H_xx - g * H_z
    E, V = arp.eigsh(H, k=1, which='SA', return_eigenvectors=True, ncv=20)
    return E[0]

def infinite_gs_energy(J, g):
    """For comparison: Calculate groundstate energy density from analytic formula.
    The analytic formula stems from mapping the model to free fermions, see P. Pfeuty,
    The one-dimensional Ising model with a transverse field, Annals of Physics 57, p. 79
    (1970). Note that we use Pauli matrices compared this reference using spin-1/2 matrices and replace
    the sum_k -> integral dk/2pi to obtain the result in the N \(\rightarrow\) infinity limit.
    """

7.4. Examples

105
def f(k, lambda_):
    return np.sqrt(1 + lambda_**2 + 2 * lambda_ * np.cos(k))

E0_exact = -g / (J * 2. * np.pi) * scipy.integrate.quad(f, -np.pi, np.pi, args=(J/ g, ))[0]
    return E0_exact

7.4.2 Basic scripts

These example scripts illustrate the very basic interface for calling TeNPy. They are included in the [TeNPySource] repository in the folder examples/, we include them here in the documentation for reference. You need to install TeNPy to call them (see Installation instructions), but you can copy them anywhere before execution. (Some scripts include other files from the same folder, though; copy those as well.)

**a_np_conserved.py**

on github.

```python
"""An example code to demonstrate the usage of :class:`~tenpy.linalg.np_conserved.Array`.

This example includes the following steps:
1) create Arrays for an Neel MPS
2) create an MPO representing the nearest-neighbour AFM Heisenberg Hamiltonian
3) define 'environments' left and right
4) contract MPS and MPO to calculate the energy
5) extract two-site hamiltonian ``H2`` from the MPO
6) calculate ``exp(-1.j*dt*H2)`` by diagonalization of H2
7) apply ``exp(H2)`` to two sites of the MPS and truncate with svd

Note that this example uses only np_conserved, but no other modules.
Compare it to the example `b_mps.py`, which does the same steps using a few predefined classes like MPS and MPO.
"""

# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import tenpy.linalg.np_conserved as npc
import numpy as np

# model parameters
Jxx, Jz = 1., 1.
L = 20
dt = 0.1
cutoff = 1.e-10
print("Jxx=\{Jxx\}, Jz=\{Jz\}, L=\{L:d\}\".format(Jxx=Jxx, Jz=Jz, L=L))

print("1) create Arrays for an Neel MPS")

# vL ->--B-->- vR
# /
# ^
# /
# p
```
# create a ChargeInfo to specify the nature of the charge
chinfo = npc.ChargeInfo([1], ['2*Sz'])  # the second argument is just a descriptive name

# create LegCharges on physical leg and even/odd bonds
p_leg = npc.LegCharge.from_qflat(chinfo, [[1], [-1]])  # charges for up, down
v_leg_even = npc.LegCharge.from_qflat(chinfo, [[0]])

v_leg_odd = npc.LegCharge.from_qflat(chinfo, [[1]])

B_even = npc.zeros([v_leg_even, v_leg_odd.conj(), p_leg], labels=['vL', 'vR', 'p'])  # virtual left/right, physical
B_odd = npc.zeros([v_leg_odd, v_leg_even.conj(), p_leg], labels=['vL', 'vR', 'p'])

B_even[0, 0, 0] = 1.  # up
B_odd[0, 0, 1] = 1.  # down

Bs = [B_even, B_odd] * (L // 2) + [B_even] * (L % 2)  # (right-canonical)
Ss = [np.ones(1)] * L  # Ss[i] are singular values between Bs[i-1] and Bs[i]

# Side remark:
# An MPS is expected to have non-zero entries everywhere compatible with the charges.
# In general, we recommend to use `sort_legcharge` (or `as_completely_blocked`) to ensure complete blocking. (But the code will also work, if you don't do it.)
# The drawback is that this might introduce permutations in the indices of single legs,
# which you have to keep in mind when converting dense numpy arrays to and from npc.Arrays.

print("2) create an MPO representing the AFM Heisenberg Hamiltonian")

# p *
# /|
# | ^
# | |
# wL -->W--> wR
# |
# |
# |
# p

# create physical spin-1/2 operators Sz, S+, S-
Sz = npc.Array.from_ndarray([[0.5, 0.], [0., -0.5]], [p_leg, p_leg.conj()], labels=['p', 'p*'])
Sp = npc.Array.from_ndarray([[0., 1.], [0., 0.]], [p_leg, p_leg.conj()], labels=['p', 'p*'])
Sm = npc.Array.from_ndarray([[0., 0.], [1., 0.]], [p_leg, p_leg.conj()], labels=['p', 'p*'])
Id = npc.eye_like(Sz, labels=Sz.get_leg_labels())  # identity

mpo_leg = npc.LegCharge.from_qflat(chinfo, [[0], [2], [-2], [0], [0]])

W_grid = [[Id, Sp, Sm, Sz, None],
          [None, None, None, None, 0.5 * Jxx * Sm],
          [None, None, None, None, 0.5 * Jxx * Sp],
          [None, None, None, None, Jz * Sz ],
          [None, None, None, None, Id]]  # yapf: disable

W = npc.grid_outer(W_grid, [mpo_leg, mpo_leg.conj()], grid_labels=['wL', 'wR'])
# wL/wR = virtual left/right of the MPO
# Ws = [W] * L

print("3) define 'environments' left and right")

envL = npc.zeros([W.get_leg('wL').conj(), Bs[0].get_leg('vL').conj(), Bs[0].get_leg('vL').conj()], labels=['wR', 'vR', 'vR*'])
envL[0, :, :] = npc.diag(1., envL.legs[1])
envR = npc.zeros([W.get_leg('wR').conj(), Bs[-1].get_leg('vR').conj(), Bs[-1].get_leg('vR').conj()], labels=['wL', 'vL', 'vL*'])
envR[-1, :, :] = npc.diag(1., envR.legs[1])

print("4) contract MPS and MPO to calculate the energy <psi|H|psi>")
for i in range(L):
    contr = npc.tensordot(contr, Bs[i], axes=('vR', 'vL'))
    contr = npc.tensordot(contr, Ws[i], axes=('p', 'wR'))
    contr = npc.tensordot(contr, Bs[i].conj(), axes=('p', 'vR*'))
E = npc.inner(contr, envR, axes=('vR', 'wR', 'vR*'), ('vL', 'wL', 'vL*'))

print("5) calculate two-site hamiltonian \"H2\" from the MPO")
# label left, right physical legs with p, q
W0 = W.replace_labels(['p', 'p*'], ['p0', 'p0*'])
W1 = W.replace_labels(['p', 'p*'], ['p1', 'p1*'])
H2 = npc.tensordot(W0, W1, axes=('wR', 'wL')).itranspose(['wL', 'wR', 'p0', 'p1', 'p0*', 'p1*'])
H2 = H2[0, -1]

print("H2 labels:", H2.get_leg_labels())

print("6) calculate exp(H2) by diagonalization of H2")
# diagonalization requires to view H2 as a matrix
E2, U2 = npc.eigh(H2)
print("Eigenvalues of H2:", E2)
U_expE2 = U2.scale_axis(np.exp(-1.j * dt * E2), axis=1)  # scale_axis ~= apply an
exp_H2 = npc.tensordot(U_expE2, U2.conj(), axes=(1, 1))
exp_H2.iset_leg_labels(H2.get_leg_labels())
exp_H2 = exp_H2.split_legs()  # by default split all legs which are "LegPipe"
# (this restores the original labels ['p0', 'p1', 'p0*', 'p1*'] of H2 in 'exp_H2')
print("7) apply \( \exp(H2) \) to even/odd bonds of the MPS and truncate with svd")
# (this implements one time step of first order TEBD)
for even_odd in [0, 1]:
    for i in range(even_odd, L - 1, 2):
        B_L = Bs[i].scale_axis(Ss[i], 'vL').ireplace_label('p', 'p0')
        B_R = Bs[i + 1].replace_label('p', 'p1')
        theta = npc.tensordot(B_L, B_R, axes=('vR', 'vL'))
        theta = npc.tensordot(exp_H2, theta, axes=[['p0*', 'p1*'], ['p0', 'p1']])
    # view as matrix for SVD
    theta = theta.combine_legs([('vL', 'p0'), ('p1', 'vR')], new_axes=[0, 1], qconj=[+1, -1])
    # now theta has labels '(vL.p0)', '(p1.vR)'
    U, S, V = npc.svd(theta, inner_labels=['vR', 'vL'])
    # truncate
    keep = S > cutoff
    S = S[keep]
    invsq = np.linalg.norm(S)
    Ss[i + 1] = S / invsq
    U = U.iscale_axis(S / invsq, 'vR')
    Bs[i + 1] = V.split_legs('(p1.vR)').ireplace_label('p1', 'p')
    Bs[i] = U.split_legs('(vL.p0)').iscale_axis(Ss[i]**(-1), 'vL').ireplace_label('p0', 'p')
print("finished")

import tenpy.linalg.np_conserved as npc
import numpy as np
# some more imports
from tenpy.networks.site import SpinHalfSite
from tenpy.models.lattice import Chain
from tenpy.networks.mps import MPS
from tenpy.networks.mpo import MPO, MPOEnvironment
from tenpy.algorithms.truncation import svd_theta

b_mps.py

on github.

"""Simplified version of `a_np_conserved.py` making use of other classes (like MPS, MPO).

This example includes the following steps:
1) create Arrays for an Neel MPS
2) create an MPO representing the nearest-neighbour AFM Heisenberg Hamiltonian
3) define 'environments' left and right
4) contract MPS and MPO to calculate the energy
5) extract two-site hamiltonian \( \`H2` \) from the MPO
6) calculate \( \`\exp(-1.j*dt*H2)` \) by diagonalization of \( H2 \)
7) apply \( \`\exp(H2)` \) to two sites of the MPS and truncate with svd

Note that this example performs the same steps as `a_np_conserved.py`, but makes use of other predefined classes except npc.
"""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import tenpy.linalg.np_conserved as npc
import numpy as np
# some more imports
from tenpy.networks.site import SpinHalfSite
from tenpy.models.lattice import Chain
from tenpy.networks.mps import MPS
from tenpy.networks.mpo import MPO, MPOEnvironment
from tenpy.algorithms.truncation import svd_theta

(continues on next page)
# model parameters
Jxx, Jz = 1., 1.
L = 20
dt = 0.1
cutoff = 1.e-10
print("Jxx=\{Jxx\}, Jz=\{Jz\}, L=\{L:d\}".format(Jxx=Jxx, Jz=Jz, L=L))

print("1) create Arrays for an Neel MPS")
site = SpinHalfSite(conserve='Sz')  # predefined charges and Sp,Sm,Sz operators
p_leg = site.leg
chinfo = p_leg.chinfo
# make lattice from unit cell and create product state MPS
lat = Chain(L, site, bc_MPS='finite')
state = ["up", "down"] * (L // 2) + ["up"] * (L % 2)  # Neel state
print("state = ", state)
psi = MPS.from_product_state(lat.mps_sites(), state, lat.bc_MPS)

print("2) create an MPO representing the AFM Heisenberg Hamiltonian")
# predefined physical spin-1/2 operators Sz, S+, S-
Sz, Sp, Sm, Id = site.Sz, site.SP, site.Sm, site.Id
mpo_leg = npc.LegCharge.from_qflat(chinfo, [[0], [2], [-2], [0], [0]])

W_grid = [[Id, Sp, Sm, Sz, None],
          [None, None, None, None, 0.5 * Jxx * Sm],
          [None, None, None, None, 0.5 * Jxx * Sp],
          [None, None, None, None, Jz * Sz],
          [None, None, None, None, Id]]  # yapf:disable
W = npc.grid_outer(W_grid, [mpo_leg, mpo_leg.conj()], grid_labels=['wL', 'wR'])
# wL/wR = virtual left/right of the MPO
Ws = [W] * L
Ws[0] = W[:, :, :]
Ws[-1] = W[:, :, :-1]
H = MPO(psi.sites, Ws, psi.bc, IdL=0, IdR=-1)

print("3) define 'environments' left and right")
# this is automatically done during initialization of MPOEnvironment
env = MPOEnvironment(psi, H, psi)
envL = env.get_LP(0)
envR = env.get_RP(L - 1)

print("4) contract MPS and MPO to calculate the energy <\psi|H|\psi>")
E = env.full_contraction(L - 1)
print("E =", E)

print("5) calculate two-site hamiltonian `\`H2\`\` from the MPO")
# label left, right physical legs with p, q
W0 = H.get_W(0).replace_labels([p', p*'], [p0', p0*'])
W1 = H.get_W(1).replace_labels([p', p*'], [p1', p1*'])
H2 = npc.tensordot(W0, W1, axes=([wR', wL']), itranspose([wL', wR', p0', p1', p0* →', p1*'])
H2 = H2[H.IdL[0], H.IdR[2]]  # (If H has single-site terms, it's not that simple anymore)
print("H2 labels: ", H2.get_leg_labels())

print("6) calculate exp(H2) by diagonalization of H2")
# diagonalization requires to view H2 as a matrix
H2 = H2.combine_legs([['p0', 'p1'], ['p0*', 'p1*']], conj=[+1, -1])
print("labels after combine_legs: ", H2.get_leg_labels())
E2, U2 = npc.eigh(H2)
print("Eigenvalues of H2: ", E2)
U_expE2 = U2.scale_axis(np.exp(-1.j*dt*E2), axis=1)  # scale_axis ~= apply a diagonal matrix
exp_H2 = npc.tensordot(U_expE2, U2.conj(), axes=(1, 1))
exp_H2.iset_leg_labels(H2.get_leg_labels())
exp_H2 = exp_H2.split_legs()  # by default split all legs which are 'LegPipe'
# (this restores the original labels ['p0', 'p1', 'p0*', 'p1*'] of 'H2' in 'exp_H2')

assert(npc.norm(exp_H2_alternative - exp_H2) < 1.e-14)

print("7) apply exp(H2) to even/odd bonds of the MPS and truncate with svd")
# (this implements one time step of first order TEBD)
trunc_par = {'svd_min': cutoff, 'trunc_cut': None, 'verbose': 0}
for even_odd in [0, 1]:
    for i in range(even_odd, L - 1, 2):
        theta = psi.get_theta(i, 2)  # handles canonical form (i.e. scaling with 'S')
        theta = npc.tensordot(exp_H2, theta, axes=[['p0*', 'p1*'], ['p0', 'p1']])
        # view as matrix for SVD
        theta = theta.combine_legs([['vL', 'p0'], ['p1', 'vR']], new_axes=[0, 1],
        conj=[+1, -1])  # now theta has labels '(vL,p0)', '(p1,vR)'
        U, S, V, err, invsq = svd_theta(theta, trunc_par, inner_labels=['vR', 'vL'])
        psi.set_SR(i, S)
        A_L = U.split_legs('(vL,p0)').ireplace_label('p0', 'p')
        B_R = V.split_legs('(p1,vR)').ireplace_label('p1', 'p')
        psi.set_B(i, A_L, form='A')  # left-canonical form
        psi.set_B(i + 1, B_R, form='B')  # right-canonical form
print("finished")

c_tebd.py

on github.

"""Example illustrating the use of TEBD in tenpy.
The example functions in this class do the same as the ones in 'toycodes/c_tebd.py',
but make use of the classes defined in tenpy.
"""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import numpy as np

from tenpy.networks.mps import MPS
from tenpy.models.tf_ising import TFIChain
from tenpy.algorithms import tebd

(continues on next page)
def example_TEBD_gs_tf_ising_finite(L, g, verbose=True):
    print("finite TEBD, imaginary time evolution, transverse field Ising")
    print("L={L:d}, g={g:.2f}".format(L=L, g=g))
    model_params = dict(L=L, J=1., g=g, bc_MPS='finite', conserve=None, verbose=verbose)
    M = TFIChain(model_params)
    product_state = ["up"] * M.lat.N_sites
    psi = MPS.from_product_state(M.lat.mps_sites(), product_state, bc=M.lat.bc_MPS)
    tebd_params = {
        'order': 2,
        'delta_tau_list': [0.1, 0.01, 0.001, 1.e-4, 1.e-5],
        'N_steps': 10,
        'max_error_E': 1.e-6,
        'trunc_params': {
            'chi_max': 30,
            'svd_min': 1.e-10
        },
        'verbose': verbose
    }
    eng = tebd.Engine(psi, M, tebd_params)
    eng.run_GS()  # the main work...

    # expectation values
    E = np.sum(M.bond_energies(psi))  # M.bond_energies() works only a for NearestNeighborModel
    if L < 20:  # compare to exact result
        from tfi_exact import finite_gs_energy
        E_exact = finite_gs_energy(L, 1., g)
        print("Exact diagonalization: E = {E:.13f}".format(E=E_exact))
        print("relative error: ", abs((E - E_exact) / E_exact))
    return E, psi, M

def example_TEBD_gs_tf_ising_infinite(g, verbose=True):
    print("infinite TEBD, imaginary time evolution, transverse field Ising")
    print("g={g:.2f}".format(g=g))
    model_params = dict(L=2, J=1., g=g, bc_MPS='infinite', conserve=None, verbose=verbose)
    M = TFIChain(model_params)
    product_state = ["up"] * M.lat.N_sites
    psi = MPS.from_product_state(M.lat.mps_sites(), product_state, bc=M.lat.bc_MPS)
    tebd_params = {
        'order': 2,
        'delta_tau_list': [0.1, 0.01, 0.001, 1.e-4, 1.e-5],
        'N_steps': 10,
        'max_error_E': 1.e-8,
        'trunc_params': {
            'chi_max': 30,
        },
        'verbose': verbose
    }
    eng = tebd.Engine(psi, M, tebd_params)
TeNPy, Release 0.7.2.dev55+68eae2c

(continued from previous page)

```python
'svd_min': 1.e-10
},
'verbose': verbose,
}
eng = tebd.Engine(psi, M, tebd_params)
eng.run_GS()  # the main work...
E = np.mean(M.bond_energies(psi))  # M.bond_energies() works only a for
# alternative: directly measure E2 = np.mean(psi.expectation_value(M.H_bond))
print("E (per site) = \{E:.13f\}".format(E=E))
print("final bond dimensions: ", psi.chi)
mag_x = np.mean(psi.expectation_value("Sigmax"))
mag_z = np.mean(psi.expectation_value("Sigmaz"))
print("<sigma_x> = \{mag_x:.5f\}".format(mag_x=mag_x))
print("<sigma_z> = \{mag_z:.5f\}".format(mag_z=mag_z))
print("correlation length:", psi.correlation_length())
# compare to exact result
from tfi_exact import infinite_gs_energy
E_exact = infinite_gs_energy(1., g)
print("Analytic result: E (per site) = \{E:.13f\}".format(E=E_exact))
print("relative error: \{abs((E - E_exact) / E_exact):.8f\}")
return E, psi, M
```

```python
def example_TEBD_tf_ising_lightcone(L, g, tmax, dt, verbose=True):
    print("finite TEBD, real time evolution")
    print("L=\{L:d\}, g=\{g:.2f\}, tmax=\{tmax:.2f\}, dt=\{dt:.3f\}".format(L=L, g=g,
    tmax=tmax, dt=dt))
    # find ground state with TEBD or DMRG
    # E, psi, M = example_TEBD_gs_tf_ising_finite(L, g)
    from d_dmrg import example_DMRG_tf_ising_finite
    print("(run DMRG to get the groundstate)")
    E, psi, M = example_DMRG_tf_ising_finite(L, g, verbose=False)
    print("(DMRG finished)")
    i0 = L // 2
    # apply sigmaz on site i0
    psi.apply_local_op(i0, 'Sigmaz', unitary=True)
    dt_measure = 0.05
    # tebd.Engine makes 'N_steps' steps of `dt` at once; for second order this is
    # more efficient.
    tebd_params = {
        'order': 2,
        'dt': dt,
        'N_steps': int(dt_measure / dt + 0.5),
        'trunc_params': {
            'chi_max': 50,
            'svd_min': 1.e-10,
            'trunc_cut': None
        },
        'verbose': verbose,
    }
    eng = tebd.Engine(psi, M, tebd_params)
    S = [psi.entanglement_entropy()]
    for n in range(int(tmax / dt_measure + 0.5)):
        eng.run()
        S.append(psi.entanglement_entropy())
import matplotlib.pyplot as plt
```

(continues on next page)

7.4. Examples 113
```python
plt.figure()
plt.imshow(S[::-1],
vmin=0.,
aspect='auto',
interpolation='nearest',
extent=(0, L - 1., -0.5 * dt_measure, eng.evolved_time + 0.5 * dt_measure))
plt.xlabel('site $i$')
plt.ylabel('time $t/J$')
plt.ylim(0., tmax)
plt.colorbar().set_label('entropy $S$')
filename = 'c_tebd_lightcone_{g:.2f}.pdf'.format(g=g)
plt.savefig(filename)
print("saved " + filename)

def example_TEBD_gs_tf_ising_next_nearest_neighbor(L, g, Jp, verbose=True):
    from tenpy.models.spins_nnn import SpinChainNNN2
    from tenpy.models.model import NearestNeighborModel
    print("finite TEBD, imaginary time evolution, transverse field Ising next-nearest-neighbor")
    print("L=\{L:d\}, g=\{g:.2f\}, Jp=\{Jp:.2f\}".format(L=L, g=g, Jp=Jp))
    model_params = dict(L=L,
            Jx=1.,
            Jy=0.,
            Jz=0.,
            Jxp=Jp,
            Jyp=0.,
            Jzp=0.,
            hz=g,
            bc_MPS='finite',
            conserve=None,
            verbose=verbose)
    # we start with the non-grouped sites, but next-nearest neighbor interactions,
    # building the MPO
    M = SpinChainNNN2(model_params)
    product_state = ['up'] * M.lat.N_sites
    psi = MPS.from_product_state(M.lat.mps_sites(), product_state, bc=M.lat.bc_MPS)
    # now we group each to sites ...
    psi.group_sites(n=2)  # ... in the state
    M.group_sites(n=2)  # ... and model
    # now, M has only 'nearest-neighbor' interactions with respect to the grouped sites
    # thus, we can convert the MPO into H_bond terms:
    M_nn = NearestNeighborModel.from_MPOModel(M)  # hence, we can initialize H_bond from the MPO
    # now, we continue to run TEBD as before
    tebd_params = {
        'order': 2,
        'delta_tau_list': [0.1, 0.01, 0.001, 1.e-4, 1.e-5],
        'N_steps': 10,
        'max_error_E': 1.e-6,
        'trunc_params': {
            'chi_max': 30,
            'svd_min': 1.e-10
        }}
```
TeNPy, Release 0.7.2.dev55+68eae2c

import numpy as np
from tenpy.networks.mps import MPS
from tenpy.models.tf_ising import TFIChain
from tenpy.models.spins import SpinModel
from tenpy.algorithms import dmrg

def example_DMRG_tf_ising_finite(L, g, verbose=True):
    print("finite DMRG, transverse field Ising model")
    print("L={L:d}, g={g:.2f}".format(L=L, g=g))
    model_params = dict(L=L, J=1., g=g, bc_MPS='finite', conserve=None)
    # verbose=verbose)
    M = TFIChain(model_params)

if __name__ == '__main__':
    example_DMRG_tf_ising_finite(L=10, g=1.)
    print("-" * 100)
    example_DMRG_tf_ising_finite(L=10, g=1.5)
    print("-" * 100)
    example_DMRG_tf_ising_finite(L=20, g=1.5, tmax=3., dt=0.01)
    print("-" * 100)
    example_DMRG_tf_ising_finite(L=10, g=1.0, Jp=0.1)

(d_continues on previous page)

7.4. Examples 115
product_state = ['up'] * M.lat.N_sites
psi = MPS.from_product_state(M.lat.mps_sites(), product_state, bc=M.lat.bc_MPS)
dmrg_params = {
    'mixer': None,  # setting this to True helps to escape local minima
    'max_E_err': 1.e-10,
    'trunc_params': {
        'chi_max': 30,
        'svd_min': 1.e-10
    },
    'verbose': verbose,
    'combine': True
}
info = dmrg.run(psi, M, dmrg_params)  # the main work...
E = info['E']
print("E = \{E:.13f\}".format(E=E))
print("final bond dimensions: ", psi.chi)
mag_x = np.sum(psi.expectation_value("Sigmax"))
mag_z = np.sum(psi.expectation_value("Sigmaz"))
print("magnetization in X = \{mag_x:.5f\}".format(mag_x=mag_x))
print("magnetization in Z = \{mag_z:.5f\}".format(mag_z=mag_z))
if L < 20:  # compare to exact result
    from tfi_exact import finite_gs_energy
    E_exact = finite_gs_energy(L, 1., g)
    print("Exact diagonalization: E = \{E:.13f\}".format(E=E_exact))
    print("relative error: ", abs((E - E_exact) / E_exact))
return E, psi, M

def example_1site_DMRG_tf_ising_finite(L, g, verbose=True):
    print("single-site finite DMRG, transverse field Ising model")
    print("L=\{L:d\}, g=\{g:.2f\}".format(L=L, g=g))
    model_params = dict(L=L, J=1., g=g, bc_MPS='finite', conserve=None, ...
    verbose=verbose)
    M = TFIChain(model_params)
    product_state = ['up'] * M.lat.N_sites
    psi = MPS.from_product_state(M.lat.mps_sites(), product_state, bc=M.lat.bc_MPS)
dmrg_params = {
    'mixer': True,  # setting this to True is essential for the 1-site algorithm
    'max_E_err': 1.e-10,
    'trunc_params': {
        'chi_max': 30,
        'svd_min': 1.e-10
    },
    'verbose': verbose,
    'combine': False,
    'active_sites': 1 # specifies single-site
}
info = dmrg.run(psi, M, dmrg_params)
E = info['E']
print("E = \{E:.13f\}".format(E=E))
print("final bond dimensions: ", psi.chi)
mag_x = np.sum(psi.expectation_value("Sigmax"))
mag_z = np.sum(psi.expectation_value("Sigmaz"))
print("magnetization in X = \{mag_x:.5f\}".format(mag_x=mag_x))
print("magnetization in Z = \{mag_z:.5f\}".format(mag_z=mag_z))
if L < 20:  # compare to exact result
from tfi_exact import finite_gs_energy
E_exact = finite_gs_energy(L, 1., g)
print("Exact diagonalization: E = \{E:\.13f\}".format(E=E_exact))
print("relative error: ", abs((E - E_exact) / E_exact))
return E, psi, M

def example_DMRG_tf_ising_infinite(g, verbose=True):
    print("infinite DMRG, transverse field Ising model")
    print("g=\{g\:.2f\}".format(g=g))
    model_params = dict(L=2, J=1., g=g, bc_MPS='infinite', conserve=None, ...
    verbose=verbose)
    M = TFIChain(model_params)
    product_state = ["up"] * M.lat.N_sites
    psi = MPS.from_product_state(M.lat.mps_sites(), product_state, bc=M.lat.bc_MPS)
    dmrg_params = {
        "mixer": True,  # setting this to True helps to escape local minima
        "trunc_params": {
            "chi_max": 30,
            "svd_min": 1.e-10
        },
        "max_E_err": 1.e-10,
        "verbose": verbose,
    }
    # Sometimes, we want to call a 'DMRG engine' explicitly
    eng = dmrg.TwoSiteDMRGEngine(psi, M, dmrg_params)
    E, psi = eng.run()  # equivalent to dmrg.run() up to the return parameters.
    print("E = \{E:\.13f\}".format(E=E))
    print("final bond dimensions: ", psi.chi)
    mag_x = np.mean(psi.expectation_value("Sigmax"))
    mag_z = np.mean(psi.expectation_value("Sigmaz"))
    print("<\sigma_x> = \{mag_x:\.5f\}".format(mag_x=mag_x))
    print("<\sigma_z> = \{mag_z:\.5f\}".format(mag_z=mag_z))
    print("correlation length: ", psi.correlation_length())
    # compare to exact result
    from tfi_exact import infinite_gs_energy
    E_exact = infinite_gs_energy(1., g)
    print("Analytic result: E (per site) = \{E\:.13f\}".format(E=E_exact))
    print("relative error: ", abs((E - E_exact) / E_exact))
    return E, psi, M

def example_1site_DMRG_tf_ising_infinite(g, verbose=True):
    print("single-site infinite DMRG, transverse field Ising model")
    print("g=\{g\:.2f\}".format(g=g))
    model_params = dict(L=2, J=1., g=g, bc_MPS='infinite', conserve=None, ...
    verbose=verbose)
    M = TFIChain(model_params)
    product_state = ["up"] * M.lat.N_sites
    psi = MPS.from_product_state(M.lat.mps_sites(), product_state, bc=M.lat.bc_MPS)
    dmrg_params = {
        "mixer": True,  # setting this to True is essential for the 1-site algorithm
        "trunc_params": {
            "chi_max": 30,
            "svd_min": 1.e-10
        },
    }
    # Sometimes, we want to call a 'DMRG engine' explicitly
    eng = dmrg.TwoSiteDMRGEngine(psi, M, dmrg_params)
    E, psi = eng.run()  # equivalent to dmrg.run() up to the return parameters.
    print("E = \{E\:.13f\}".format(E=E))
    print("final bond dimensions: ", psi.chi)
    mag_x = np.mean(psi.expectation_value("Sigmax"))
    mag_z = np.mean(psi.expectation_value("Sigmaz"))
    print("<\sigma_x> = \{mag_x\:.5f\}".format(mag_x=mag_x))
    print("<\sigma_z> = \{mag_z\:.5f\}".format(mag_z=mag_z))
    print("correlation length: ", psi.correlation_length())
    # compare to exact result
    from tfi_exact import infinite_gs_energy
    E_exact = infinite_gs_energy(1., g)
    print("Analytic result: E (per site) = \{E\:.13f\}".format(E=E_exact))
    print("relative error: ", abs((E - E_exact) / E_exact))
    return E, psi, M

7.4. Examples 117
'max_E_err': 1.e-10,
'verbose': verbose,
'combine': True
}

eng = dmrg.SingleSiteDMRGEngine(psi, M, dmrg_params)
E, psi = eng.run()  # equivalent to dmrg.run() up to the return parameters.
print("E = \{E:.13f\}".format(E=E))
print("final bond dimensions: ", psi.chi)
mag_x = np.mean(psi.expectation_value("Sigmax"))
mag_z = np.mean(psi.expectation_value("Sigmaz"))
print("<\sigma_x> = \{mag_x:.5f\}".format(mag_x=mag_x))
print("<\sigma_z> = \{mag_z:.5f\}".format(mag_z=mag_z))
print("correlation length:", psi.correlation_length())

# compare to exact result
from tfi_exact import infinite_gs_energy
E_exact = infinite_gs_energy(1., g)
print("Analytic result: E (per site) = \{E:.13f\}".format(E=E_exact))
print("relative error: ", abs((E - E_exact) / E_exact))

def example_DMRG_heisenberg_xxz_infinite(Jz, conserve='best', verbose=True):
    print("infinite DMRG, Heisenberg XXZ chain")
    print("Jz=\{Jz:.2f\}, conserve=\{conserve!r\}".format(Jz=Jz, conserve=conserve))
    model_params = dict(
        L=2,
        S=0.5,  # spin 1/2
        Jx=1.,
        Jy=1.,
        Jz=Jz,  # couplings
        bc_MPS='infinite',
        conserve=conserve,
        verbose=verbose)
    M = SpinModel(model_params)
    product_state = ["up", "down"]  # initial Neel state
    psi = MPS.from_product_state(M.lat.mps_sites(), product_state, bc=M.lat.bc_MPS)
    dmrg_params = {
        'mixer': True,  # setting this to True helps to escape local minima
        'trunc_params': {
            'chi_max': 100,
            'svd_min': 1.e-10,
        },
        'max_E_err': 1.e-10,
        'verbose': verbose,
    }
    info = dmrg.run(psi, M, dmrg_params)
    E = info['E']
    print("E = \{E:.13f\}".format(E=E))
    print("final bond dimensions: ", psi.chi)
    Sz = psi.expectation_value("Sz")  # Sz instead of Sigma z: spin-1/2 operators!
    mag_z = np.mean(Sz)
    print("<S_z> = \{Sz0:.5f\}, \{Sz1:.5f\}; mean =\{mag_z:.5f\}".format(Sz0=Sz[0], Sz1=Sz[1], mag_z=mag_z))

    # note: it's clear that mean(<Sz>) is 0: the model has Sz conservation!
    print("correlation length:", psi.correlation_length())
    corrs = psi.correlation_function("Sz", "Sz", sites1=range(10))
    print("correlations <Sz_i Sz_j> =")
print(corrs)
return E, psi, M

if __name__ == '__main__':
    example_DMRG_tf_ising_finite(L=10, g=1., verbose=True)
    print("-" * 100)
    example_1site_DMRG_tf_ising_finite(L=10, g=1., verbose=True)
    print("-" * 100)
    example_DMRG_tf_ising_infinite(g=1.5, verbose=True)
    print("-" * 100)
    example_1site_DMRG_tf_ising_infinite(g=1.5, verbose=True)
    print("-" * 100)
eexample_DMRG_heisenberg_xxz_infinite(Jz=1.5)

e_tdv.py

on github.

"""Example illustrating the use of TDVP in tenpy.
As of now, we have TDVP only for finite systems. The call structure is quite similar to TEBD. A difference is that we can run one-site TDVP or two-site TDVP. In the former, the bond dimension cannot grow; the latter allows to grow the bond dimension and hence requires a truncation."""

# Copyright 2019-2020 TeNPy Developers, GNU GPLv3
import numpy as np
import tenpy.linalg.np_conserved as npc
import tenpy.models.spins
import tenpy.networks.mps as mps
import tenpy.networks.site as site
from tenpy.algorithms import tdvp
from tenpy.networks.mps import MPS
import copy

def run_out_of_equilibrium():
    L = 10
    chi = 5
    delta_t = 0.1
    model_params = {
        'L': L,
        'S': 0.5,
        'conserve': 'Sz',
        'Jz': 1.0,
        'Jy': 1.0,
        'Jx': 1.0,
        'hx': 0.0,
        'hy': 0.0,
        'hz': 0.0,
        'muJ': 0.0,
        'bc_MPS': 'finite',
    }
heisenberg = tenpy.models.spins.SpinChain(model_params)
product_state = ["up"] * (L // 2) + ["down"] * (L - L // 2)
# starting from a domain-wall product state which is not an eigenstate of the
→Heisenberg model
psi = MPS.from_product_state(heisenberg.lat.mps_sites(),
    product_state,
    bc=heisenberg.lat.bc_MPS,
    form='B')

tdvp_params = {
    'start_time': 0,
    'dt': delta_t,
    'trunc_params': {
        'chi_max': chi,
        'svd_min': 1.e-10,
        'trunc_cut': None
    }
}

tdvp_engine = tdvp.Engine(psi, heisenberg, tdvp_params)
times = []
S_mid = []
for i in range(30):
    tdvp_engine.run_two_sites(N_steps=1)
    times.append(tdvp_engine.evolved_time)
    S_mid.append(psi.entanglement_entropy(bonds=[L // 2])[0])
for i in range(30):
    tdvp_engine.run_one_site(N_steps=1)
#psi_2=copy.deepcopy(psi)
#psi_2.canonical_form()
times.append(tdvp_engine.evolved_time)
S_mid.append(psi.entanglement_entropy(bonds=[L // 2])[0])

import matplotlib.pyplot as plt
plt.figure()
plt.plot(times, S_mid)
plt.xlabel('t')
plt.ylabel('S')
plt.axvline(x=3.1, color='red')
plt.text(0.0, 0.0000015, "Two sites update")
plt.text(3.1, 0.0000015, "One site update")
plt.show()

if __name__ == "__main__":
    run_out_of_equilibrium()
purification.py

from tenpy.models.tf_ising import TFIChain
from tenpy.networks.purification_mps import PurificationMPS
from tenpy.algorithms.purification import PurificationTEBD, PurificationApplyMPO

def imag_tebd(L=30, beta_max=3., dt=0.05, order=2, bc="finite"):
    model_params = dict(L=L, J=1., g=1.2)
    M = TFIChain(model_params)
    psi = PurificationMPS.from_infiniteT(M.lat.mps_sites(), bc=bc)
    options = {
        'trunc_params': {
            'chi_max': 100,
            'svd_min': 1.e-8
        },
        'order': order,
        'dt': dt,
        'N_steps': 1
    }
    beta = 0.
    eng = PurificationTEBD(psi, M, options)
    Szs = [psi.expectation_value("Sz")]
    betas = [0.]
    while beta < beta_max:
        beta += 2. * dt  # factor of 2: |psi> = exp^{- dt H}, but rho = |psi><psi|
        betas.append(beta)
        print("beta = {0:.2f}".format(beta))
        eng.run_imaginary(dt)  # cool down by dt
        Szs.append(psi.expectation_value("Sz"))  # and further measurements...
    return {'beta': betas, 'Sz': Szs}

def imag_apply_mpo(L=30, beta_max=3., dt=0.05, order=2, bc="finite", approx="II"):
    model_params = dict(L=L, J=1., g=1.2)
    M = TFIChain(model_params)
    psi = PurificationMPS.from_infiniteT(M.lat.mps_sites(), bc=bc)
    options = {'trunc_params': {'chi_max': 100, 'svd_min': 1.e-8}}
    beta = 0.
    if order == 1:
        Us = [M.H_MPO.make_U(-dt, approx)]
    elif order == 2:
        Us = [M.H_MPO.make_U(-d * dt, approx) for d in [0.5 + 0.5j, 0.5 - 0.5j]]
    eng = PurificationApplyMPO(psi, Us[0], options)
    Szs = [psi.expectation_value("Sz")]
    betas = [0.]
    while beta < beta_max:
        beta += 2. * dt  # factor of 2: |psi> = exp^{- dt H}, but rho = |psi><psi|
        betas.append(beta)
        print("beta = {0:.2f}".format(beta))
        for U in Us:
            eng.init_env(U)  # reset environment, initialize new copy of psi
            eng.run()  # apply U to psi
        Szs.append(psi.expectation_value("Sz"))  # and further measurements...
    return {'beta': betas, 'Sz': Szs}
if __name__ == "__main__":
    data_tebd = imag_tebd()
    data_mpo = imag_apply_mpo()

    import numpy as np
    from matplotlib.pyplot import plt

    plt.plot(data_mpo['beta'], np.sum(data_mpo['Sz'], axis=1), label='MPO')
    plt.plot(data_tebd['beta'], np.sum(data_tebd['Sz'], axis=1), label='TEBD')
    plt.xlabel(r'$\beta$')
    plt.ylabel(r'total $S^z$')
    plt.show()

tfi_exact.py

on github.

"""Provides exact ground state energies for the transverse field ising model for comparison."

The Hamiltonian reads
.. math ::
   \[ H = - J \sum_{i} \sigma^x_i \sigma^x_{i+1} - g \sum_{i} \sigma^z_i \]
"""

# Copyright 2019-2020 TeNPy Developers, GNU GPLv3

import numpy as np
import scipy.sparse as sparse
import scipy.sparse.linalg.eigen.arpack as arp
import warnings
import scipy.integrate

def finite_gs_energy(L, J, g):
    """For comparison: obtain ground state energy from exact diagonalization.
    Exponentially expensive in L, only works for small enough \'L\' \leq 20.
    """

    if L >= 20:
        warnings.warn("Large L: Exact diagonalization might take a long time!")
    # get single site operators
    sx = sparse.csr_matrix(np.array([[0., 1.], [1., 0.]]))
    sz = sparse.csr_matrix(np.array([[1., 0.], [0., -1.]]))
    id = sparse.csr_matrix(np.eye(2))
    sx_list = []  # sx_list[i] = kron([id, id, ..., id, sx, id, .... id])
    sz_list = []

    for i_site in range(L):
        x_ops = [id] * L
        z_ops = [id] * L
        x_ops[i_site] = sx
        z_ops[i_site] = sz
        X = x_ops[0]
        Z = z_ops[0]
        for j in range(i, L):
X = sparse.kron(X, x_ops[j], 'csr')  
Z = sparse.kron(Z, z_ops[j], 'csr')  
sx_list.append(X)  
sz_list.append(Z)  
H_xx = sparse.csr_matrix((2**L, 2**L))  
H_z = sparse.csr_matrix((2**L, 2**L))  
for i in range(L - 1):  
    H_xx = H_xx + sx_list[i] * sx_list[(i + 1) % L]  
for i in range(L):  
    H_z = H_z + sz_list[i]  
H = -J * H_xx - g * H_z  
E, V = arp.eigsh(H, k=1, which='SA', return_eigenvectors=True, ncv=20)  
return E[0]

def infinite_gs_energy(J, g):
    """For comparison: Calculate groundstate energy density from analytic formula."
    The analytic formula stems from mapping the model to free fermions, see P. Pfeuty,  
    The one-dimensional Ising model with a transverse field, Annals of Physics 57, p. 79  
    (1970). Note that  
    we use Pauli matrices compared this reference using spin-1/2 matrices and replace  
    the sum_k ->  
    integral dk/2pi to obtain the result in the N -> infinity limit.  
    """
    def f(k, lambda_):
        return np.sqrt(1 + lambda_**2 + 2 * lambda_ * np.cos(k))  
    E0_exact = -g / (J * 2. * np.pi) * scipy.integrate.quad(f, -np.pi, np.pi, args=(J / g, ))[0]  
    return E0_exact

z_exact_diag.py

on github.

"""A simple example comparing DMRG output with full diagonalization (ED).  
Sorry that this is not well documented! ED is meant to be used for debugging only ;)  
"""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import tenpy.linalg.np_conserved as npc
from tenpy.models.xxz_chain import XXZChain
from tenpy.networks.mps import MPS
from tenpy.algorithms.exact_diag import ExactDiag
from tenpy.algorithms import dmerg

def example_exact_diagonalization(L, Jz):
    xxz_pars = dict(L=L, Jxx=1., Jz=Jz, hz=0.0, bc_MPS='finite')
    M = XXZChain(xxz_pars)
product_state = ["up", "down"] * (xxz_pars['L'] // 2)  # this selects a charge

psi_DMRG = MPS.from_product_state(M.lat.mps_sites(), product_state)
charge_sector = psi_DMRG.get_total_charge(True)  # ED charge sector should match

ED = ExactDiag(M, charge_sector=charge_sector, max_size=2.e6)
# ED.build_full_H_from_mpo()  # whatever you prefer
print("start diagonalization")
ED.full_diagonalization()  # the expensive part for large L
E0_ED, psi_ED = ED.groundstate()  # return the ground state
print("psi_ED =", psi_ED)

print("run DMRG")
dmrg.run(psi_DMRG, M, {'verbose': 0})  # modifies psi_DMRG in place!
# first way to compare ED with DMRG: convert MPS to ED vector
psi_DMRG_full = ED.mps_to_full(psi_DMRG)
print("psi_DMRG_full =", psi_DMRG_full)
ov = npc.inner(psi_ED, psi_DMRG_full, axes='range', do_conj=True)
print("<psi_ED|psi_DMRG_full> =", ov)
assert (abs(abs(ov) - 1.) < 1.e-13)

# second way: convert ED vector to MPS
psi_ED_mps = ED.full_to_mps(psi_ED)
print("<psi_ED_mps|psi_ED> =", psi_ED_mps.expectation_value('Sz'))

if __name__ == "__main__":
    example_exact_diagonalization(10, 1.)

7.4.3 Notebooks

This is a collection of [jupyter] notebooks from the [TeNPyNotebooks] repository. You need to install TeNPy to execute them (see [Installation instructions]), but you can copy them anywhere before execution. Note that some of them might take a while to run, as they contain more extensive examples.

A first TEBD Example

Like examples/c_tebd.py, this notebook shows the basic interface for TEBD. It initialized the transverse field Ising model $H = JXX + gZ$ at the critical point $J = g = 1$, and an MPS in the all-up state $|↑\cdots↑\rangle$. It then performs a real-time evolution with TEBD and measures a few observables. This setup correspond to a global quench from $g = \infty$ to $g = 1$.

[1]: import numpy as np
import scipy
import matplotlib.pyplot as plt
import matplotlib
```python
[2]: import tenpy
import tenpy.linalg.np_conserved as npc
from tenpy.algorithms import tebd
from tenpy.networks.mps import MPS
from tenpy.models.tf_ising import TFIChain

[3]: L = 30

[4]: model_params = {
    'J': 1.,  # critical
    'g': 1.,
    'L': L,
    'bc_MPS': 'finite',
}
M = TFIChain(model_params)

MPS from_lat_product_state(M.lat, [['up']])

[5]: psi = MPS.from_lat_product_state(M.lat, [['up']])

[6]: tebd_params = {
    'N_steps': 1,
    'dt': 0.1,
    'order': 4,
    'trunc_params': {'chi_max': 100, 'svd_min': 1.e-12}
}
eng = tebd.Engine(psi, M, tebd_params)

Subconfig 'trunc_params'=Config(<3 options>, 'trunc_params') for config TEBD

[7]: def measurement(eng, data):
    keys = ['t', 'entropy', 'Sx', 'Sz', 'corr_XX', 'corr_ZZ', 'trunc_err']
    if data is None:
        data = dict([(k, []) for k in keys])
    data['t'].append(eng.evolved_time)
    data['entropy'].append(eng.psi.entanglement_entropy())
    data['Sx'].append(eng.psi.expectation_value('Sigmax'))
    data['Sz'].append(eng.psi.expectation_value('Sigmaz'))
    data['corr_XX'].append(eng.psi.correlation_function('Sigmax', 'Sigmax'))
    data['corr_ZZ'].append(eng.psi.correlation_function('Sigmaz', 'Sigmaz'))
    data['trunc_err'].append(eng.trunc_err.eps)
    return data

[8]: data = measurement(eng, None)

[9]: while eng.evolved_time < 5.:
    eng.run()
    measurement(eng, data)
```

(continues on next page)
--> time=0.100, max_chi=6, Delta_S=5.5243e-02, S=0.0552432967, since last update: 0.5s
--> time=0.200, max_chi=6, Delta_S=1.0453e-01, S=0.1597705686, since last update: 0.5s
--> time=0.300, max_chi=8, Delta_S=1.1368e-01, S=0.2734471407, since last update: 0.5s
--> time=0.400, max_chi=10, Delta_S=1.0226e-01, S=0.3757082127, since last update: 0.5s
--> time=0.500, max_chi=12, Delta_S=1.0453e-01, S=0.4581821173, since last update: 0.5s
--> time=0.600, max_chi=12, Delta_S=6.3393e-02, S=0.5215746922, since last update: 0.5s
--> time=0.700, max_chi=15, Delta_S=5.0837e-02, S=0.5724119006, since last update: 0.5s
--> time=0.800, max_chi=18, Delta_S=4.7046e-02, S=0.6194580889, since last update: 0.5s
--> time=0.900, max_chi=20, Delta_S=5.0606e-02, S=0.6700636890, since last update: 0.5s
--> time=1.000, max_chi=20, Delta_S=5.7462e-02, S=0.7275254979, since last update: 0.5s
--> time=1.100, max_chi=24, Delta_S=6.3115e-02, S=0.7906402648, since last update: 0.5s
--> time=1.200, max_chi=26, Delta_S=6.4779e-02, S=0.8554189184, since last update: 0.5s
--> time=1.300, max_chi=30, Delta_S=6.2269e-02, S=0.9176882429, since last update: 0.5s
--> time=1.400, max_chi=34, Delta_S=5.7451e-02, S=0.9751394599, since last update: 0.5s
--> time=1.500, max_chi=40, Delta_S=5.2899e-02, S=1.0280386118, since last update: 0.5s
--> time=1.600, max_chi=40, Delta_S=5.0543e-02, S=1.0785817862, since last update: 0.5s
--> time=1.700, max_chi=46, Delta_S=5.0852e-02, S=1.1294340516, since last update: 0.5s
--> time=1.800, max_chi=52, Delta_S=5.2841e-02, S=1.1822748827, since last update: 0.7s
--> time=1.900, max_chi=57, Delta_S=5.4804e-02, S=1.2370787276, since last update: 0.9s
--> time=2.000, max_chi=62, Delta_S=5.5311e-02, S=1.2923895877, since last update: 0.9s
--> time=2.100, max_chi=71, Delta_S=5.3906e-02, S=1.3462960135, since last update: 1.0s
--> time=2.200, max_chi=80, Delta_S=5.1209e-02, S=1.3975050668, since last update: 1.2s
--> time=2.300, max_chi=85, Delta_S=4.8446e-02, S=1.4459514729, since last update: 1.4s
--> time=2.400, max_chi=95, Delta_S=4.6732e-02, S=1.4926837515, since last update: 1.4s
--> time=2.500, max_chi=100, Delta_S=4.6486e-02, S=1.5391700161, since last update: 1.8s
--> time=2.600, max_chi=100, Delta_S=4.7282e-02, S=1.5864521162, since last update: 1.9s
--> time=2.700, max_chi=100, Delta_S=4.8160e-02, S=1.6346120966, since last update: 1.9s
--> time=2.800, max_chi=100, Delta_S=4.8202e-02, S=1.6828138289, since last update: 1.6s
--> time=2.900, max_chi=100, Delta_S=4.7044e-02, S=1.7298576742, since last update: 1.7s

(continues on next page)
(continued from previous page)

```python
[10]: plt.plot(data['t'], np.array(data['entropy'])[:, L//2])
plt.xlabel('time $t$')
plt.ylabel('entropy $S$')

[10]: Text(0, 0.5, 'entropy $SS$')
```

7.4. Examples
The growth of $S$ linear in time is typical for a global quench and to be expected from the quasi-particle picture

\begin{Verbatim}
[11]: plt.plot(data['t'], np.sum(data['Sx'], axis=1), label="X")
plt.plot(data['t'], np.sum(data['Sz'], axis=1), label="Z")
plt.xlabel('time $t$')
plt.ylabel('magnetization')
plt.legend(loc='best')
\end{Verbatim}

\begin{Verbatim}
[11]: <matplotlib.legend.Legend at 0x7f1018760e80>
\end{Verbatim}

The strict conservation of $X$ being zero is ensured by charge conservation, because $X$ changes the parity sector.

Nevertheless, the $XX$ correlation function can be nontrivial:

\begin{Verbatim}
[12]: corrs = np.array(data['corr_XX'])
tmax = data['t'][-1]
x = np.arange(L)
cmap = matplotlib.cm.viridis
for i, t in list(enumerate(data['t'])):
    (continues on next page)
If \( i = 0 \) or \( i = \text{len(data['t'])} - 1 \):

```python
deflect = '{t:.2f}'.format(t=t)
else:
    label = None
plt.plot(x, corrs[i, L//2, :], color=cmap(t/tmax), label=label)
```

```python
plt.xlabel(r'time $t$')
plt.ylabel(r'correlations $\langle X_i X_{j:d} \rangle$'.format(j=L//2))
plt.yscale('log')
plt.ylim(1.e-6, 1.)
plt.legend()
plt.show()
```

The output of the run showed that we gradually increased the bond dimension and only reached the maximum chi around \( t = 2.5 \). At this point we start to truncate significantly, because we cut off the tail whatever the singular values are. This is clearly visible if we plot the truncation error vs. time. Note the log-scale, though: if you are fine with an error of say 1 permille for expectation values, you can still go on for a bit more!

```python
[13]: plt.plot(data['t'], data['trunc_err'])
```

```python
plt.yscale('log')
# plt.ylim(1.e-15, 1.)
plt.xlabel('time $t$')
plt.ylabel('truncation error')
```

```
[13]: Text(0, 0.5, 'truncation error')
```
A first finite DMRG Example

Like examples/d_dmrg.py, this notebook shows the basic interface for DMRG. It initialized the transverse field Ising model $H = J XX + g Z$ at the critical point $J = g = 1$, and a finite MPS in the all-up state $|↑\cdots↑\rangle$. It then runs DMRG to find the ground state. Finally, we look at the profile of the entanglement-cuts.

```python
[1]: import numpy as np
    import scipy
    import matplotlib.pyplot as plt

[2]: import tenpy
    import tenpy.linalg.np_conserved as npc
    from tenpy.algorithms import dmrg
    from tenpy.networks.mps import MPS
    from tenpy.models.tf_ising import TFIChain

[3]: L = 100

[4]: model_params = {
    'J': 1., 'g': 1., # critical
    'L': L,
    'bc_MPS': 'finite',
}
M = TFIChain(model_params)
Reading 'bc_MPS'='finite' for config TFIChain
Reading 'L'=100 for config TFIChain
Reading 'J'=1.0 for config TFIChain
Reading 'g'=1.0 for config TFIChain

[5]: psi = MPS.from_lat_product_state(M.lat, [['up']])
```
```python
[6]:

dmrg_params = {
    'mixer': None,  # setting this to True helps to escape local minima
    'max_E_err': 1.e-10,
    'trunc_params': {
        'chi_max': 100,
        'svd_min': 1.e-10,
    },
    'verbose': True,
    'combine': True
}

eng = dmrg.TwoSiteDMRGEngine(psi, M, dmrg_params)
E, psi = eng.run()  # the main work; modifies psi in place
```
sweep 5, age = 100
Energy = -126.9618767396792691, S = 0.5277994025033066, norm_err = 2.1e-13
Current memory usage 115.4 MB, time elapsed: 20.4 s
Delta E = 6.3949e-13, Delta S = 7.3059e-11 (per sweep)
max_trunc_err = 6.5986e-20, max_E_trunc = 3.1264e-13
MPS bond dimensions: [2, 4, 8, 16, 22, 30, 34, 36, 41, 45, 47, 48, 52, 54, 57, 61, 61, 63, 64, 66, 67, 71, 71, 74, 77, 77, 78, 79, 81, 81, 83, 83, 84, 85, 85, 85, 85, 86, 88, 89, 90, 90, 90, 90, 90, 90, 90, 90, 90, 90, 90, 88, 86, 85, 85, 84, 83, 83, 81, 81, 81, 79, 78, 78, 77, 73, 71, 71, 67, 66, 64, 63, 61, 61, 57, 54, 52, 48, 47, 45, 41, 36, 34, 30, 22, 16, 8, 4, 2]
DMRG finished after 5 sweeps.
total size = 100, maximum chi = 91

Expectation Values

[7]: # the ground state energy was directly returned by dmrg.run()
    print("ground state energy = ", E)
    # there are other ways to extract the energy from psi:
    E1 = M.H_MPO.expectation_value(psi)  # based on the MPO
    E2 = np.sum(M.bond_energies(psi))    # based on bond terms of H, works only for a
    assert abs(E-E1) < 1.e-10 and abs(E-E2) < 1.e-10
    ground state energy = -126.96187673967927

[8]: # onsite expectation values
    X = psi.expectation_value("Sigmax")
    Z = psi.expectation_value("Sigmaz")
    x = np.arange(psi.L)
    plt.figure()
    plt.plot(x, Z, label="Z")
    plt.plot(x, X, label="X")  # note: it's clear that this is zero due to charge conservation!
    plt.xlabel("site")
    plt.ylabel("onsite expectation value")
    plt.legend()
    plt.show()
7.4. Examples

[9]: # correlation functions

i0 = psi.L // 4  # for fixed `i`
j = np.arange(i0 + 1, psi.L)
XX = psi.term_correlation_function_right([("Sigmax", 0)], ["Sigmax", 0]), i_L=i0, j_R=j
XX_disc = XX - X[i0] * X[j]
ZZ = psi.term_correlation_function_right(["Sigmaz", 0], ["Sigmaz", 0]), i_L=i0, j_R=j
ZZ_disc = ZZ - Z[i0] * Z[j]

dx = j - i0
plt.figure()
plt.plot(dx, XX_disc, label="X X")
plt.plot(dx, ZZ_disc, label="Z Z")
plt.xlabel(r"distance $|i-j|$")
plt.ylabel(r"disconnected correlations $\langle A_i A_j \rangle - \langle A_i \rangle \langle A_j \rangle$")
plt.legend()
plt.loglog()
plt.show()
We find power-law decaying correlations, as expected for a critical model. For a gapped model, we would expect exponentially decaying correlations.

We now look at the entanglement entropy. The transverse-field Ising model is critical at $g = J$. Conformal field theory, Calabrese-Cardy 2004, predicts an entanglement entropy profile of

$$S(l, L) = c_6 \log \left( \frac{2L \pi \sin \left( \frac{\pi l}{L} \right)}{a} \right) + \text{const}$$

where:
- $c_6$ is the central charge,
- $a$ is the lattice spacing (we set $a = 1$),
- $L$ is the total size of the system and we considers subsystems of size $l$ and $L - l$ as left/right.

Note that this yields the familiar

$$S(L/2, L) = c_6 \log (L) + \text{const}$$

for the half-chain entropy as a function of system size.

```python
[12]: S = psi.entanglement_entropy()

bonds = np.arange(0.5, psi.L-1)
plt.plot(bonds, S, 'o', label="S")

# perform fit to extract the central charge
central_charge, const, res = tenpy.tools.fit.central_charge_from_S_profile(psi)
fit = tenpy.tools.fit.entropy_profile_from_CFT(bonds + 0.5, psi.L, central_charge, ~const)
print(f"extracted central charge {central_charge:.5f} with residuum {res:.2e}\)
print("(Expect central charge = 0.5 for the transverse field Ising model.)")
plt.plot(bonds, fit, label=f"fit with $c={central_charge:.3f}$")
plt.xlabel("bond")
plt.ylabel("entanglement entropy $S$")
plt.legend()
plt.show()

extracted central charge 0.50788 with residuum 1.95e-09
(Expect central charge = 0.5 for the transverse field Ising model.)
Lattices: visualization and further examples

This notebook demonstrates a few ways to visualize lattices and couplings inside the lattice.

```python
import tenpy

import numpy as np
import matplotlib.pyplot as plt
from tenpy.models import lattice

In the following, we will focus on the Honeycomb lattice as an example with a non-trivial unit cell. If you want to try it out yourself for a different lattice, simply adjust the following alias:

```python
MyLattice = lattice.Honeycomb
Lu = MyLattice.Lu  # = 2 = the number of sites in the unit cell
fig_args = dict(figsize=(7, 5))
fig_args = dict(figsize=(7, 5), dpi=150)  # uncomment this if the figures appear too small to see something
```

plotting the lattice itself

To get started, let’s recall that a lattice consists of a unit cell that is repeated in the directions of the basis. The following plot visualizes the first unit cell and basis and plots the sites in the whole lattice. For the Honeycomb lattice, we have two different sites in the unit cell, which get visualized by different markers.

```python
lat = MyLattice(5, 4, sites=None, bc='periodic')
```

```python
plt.figure(**fig_args)
ax = plt.gca()
lat.plot_sites(ax)
ax.set_aspect('equal')
```
We can also plot the nearest- and next-nearest-neighbor bonds:

```python
plt.figure(**fig_args)
ax = plt.gca()
lat.plot_sites(ax)
lat.plot_coupling(ax)
lat.plot_coupling(ax, lat.pairs['next_nearest_neighbors'], linestyle=':', color='r')
ax.set_aspect('equal')
```
If you have a 1D MPS, it’s winding through the lattice is defined by the order. You can plot it as follows:

```python
[7]: plt.figure(**fig_args)
    ax = plt.gca()
    lat.plot_sites(ax)
    lat.plot_order(ax)
    ax.set_aspect('equal')
```

Visually verifying pairs of couplings by plotting them

In this section, we visually verify that the lattice pairs like the nearest_neighbors are indeed what they claim to be. To achieve this, we first get all the possible distances of them, plot circles with these distances and lines connecting the points for each distance.

Then, you have to stare at the plots and verify that these couplings include all pairs you want to have.

```python
[8]: lat = MyLattice(12, 12, sites=None, bc='periodic') # the lattice to plot
    lat_pairs = lat.pairs # the coupling pairs to plot

[9]: # get distances of the couplings
    dist_pair = {}
    for pair in lat_pairs:
        #print(pair)
        dist = None
        for u1, u2, dx in lat_pairs[pair]:
            d = lat.distance(u1, u2, dx)
            #print(u1, u2, dx, d)
            if dist is None:
                dist = d
                dist_pair[d] = pair
            else:
                # (continues on next page)
```
assert abs(dist-d) < 1.e-14

dists = sorted(dist_pair.keys())
if len(dists) != len(dist_pair):
    raise ValueError("no unique mapping dist -> pair")

[10]: print("(dist) (pairs)")
for d in dists:
    print("{0:.6f} {1}\n".format(d, dist_pair[d]))

(dist) (pairs)
0.577350 nearest_neighbors
1.000000 next_nearest_neighbors
1.154701 next_next_nearest_neighbors
1.527525 fourth_nearest_neighbors
1.732051 fifth_nearest_neighbors

[11]: colors = [plt.cm.viridis(r/dists[-1]) for r in dists]
centers = np.array([[3, 3, 0], [8, 3, 1], [3, 8, 2], [8, 8, 3]]) # one center for each site in the unit cell
us = list(range(Lu))

[12]: fig = plt.figure(**fig_args)
ax = plt.gca()
lat.plot_sites(ax, markersize=1.3)
for u, center in zip(us, centers):
    center = lat.position(center)
    for r, c in zip(dists, colors):
        circ = plt.Circle(center, r, fill=False, color=c)
        ax.add_artist(circ)
ax.set_aspect(1.)
t = ax.set_title("distances: " + ' '.join(['{0:.2f}'.format(d) for d in dists]))
for dist in dists:
    pair_name = dist_pair[dist]
print(dist, pair_name)
pairs = lat.pairs[pair_name]
fig = plt.figure(**fig_args)
ax = fig.gca()
lat.plot_sites(ax, markersize=1.3)
for u, center in zip(us, centers):
    center = lat.position(center)
    for r, c in zip(dists, colors):
        circ = plt.Circle(center, r, fill=False, color=c)
        ax.add_artist(circ)
pairs_with_reverse = pairs + [(u2, u1, -np.array(dx)) for u1, u2, dx in pairs]
for u1, u2, dx in pairs_with_reverse:
    print(u1, u2, dx, lat.distance(u1, u2, dx))
start = centers[u1]
end = start.copy()
end[-1] = u2
end[:-1] = start[:-1] + dx
x1, y1 = lat.position(start)
x2, y2 = lat.position(end)
ax.arrow(x1, y1, x2-x1, y2 - y1)
for u in us:
    x, y = lat.position(centers[u])
    number = lat.count_neighbors(u, pair_name)
    ax.text(x, y, str(number), color='r')
ax.set_aspect(1.)
ax.set_title(pair_name + ' distance = {0:.3f}'.format(dist))
0 1 [ 1 0]  1.5275252316519465
0 1 [ 1 -2]  1.5275252316519465
0 1 [ 0 -2]  1.5275252316519468
0 1 [-2 0]  1.5275252316519465
0 1 [-2 1]  1.5275252316519465
1 0 [ 0 -1]  1.5275252316519468
1 0 [-1 0]  1.5275252316519465
1 0 [-1 2]  1.5275252316519465
1 0 [ 0 2]  1.5275252316519468
1 0 [ 2 0]  1.5275252316519465
1 0 [ 2 -1]  1.5275252316519465
1.7320508075688772  fifth_nearest_neighbors
0 0 [ 1 1]  1.7320508075688772
0 0 [ 2 -1]  1.7320508075688772
0 0 [-1 2]  1.7320508075688772
1 1 [ 1 1]  1.7320508075688772
1 1 [ 2 -1]  1.7320508075688772
1 1 [-1 2]  1.7320508075688772
0 0 [-1 -1]  1.7320508075688772
0 0 [-2 1]  1.7320508075688772
0 0 [ 1 -2]  1.7320508075688772
1 1 [-1 -1]  1.7320508075688772
1 1 [-2 1]  1.7320508075688772
1 1 [ 1 -2]  1.7320508075688772
earest_neighbors distance = 0.577
7.4. Examples
fourth_nearest_neighbors distance = 1.528

fifth_nearest_neighbors distance = 1.732
7.5 Literature and References

This is a (by far non-exhaustive) list of some references for the various ideas behind the code. They can be cited like this:

- [TeNPyNotes] for TeNPy/software related sources
- [white1992] (lowercase first-author + year) for entries from literature.bib.

7.5.1 TeNPy related sources

[TeNPyNotes] are lecture notes, meant as an introduction to tensor networks (focusing on MPS), and introduced TeNPy to the scientific community by giving examples how to call the algorithms in TeNPy. [TeNPySource] is the location of the source code, and the place where you can report bugs. We have split example notebooks into [TeNPyNotebooks] to keep the git history of the original repository clean. [TeNPyDoc] is where the documentation is hosted online. [TeNPyForum] is the place where you can ask questions and look for help when you are stuck with implementing something.

7.5.2 Software-related

The following links are not physics-related, but are good to know if you want to work with TeNPy (or more generally Python).

7.5.3 General reading

[schollwoeck2011] is an extensive introduction to MPS, DMRG and TEBD with lots of details on the implementations, and a classic read, although a bit lengthy. Our [TeNPyNotes] are a shorter summary of the important concepts, similar as [orus2014]. [paeckel2019] is a very good, recent review focusing on time evolution with MPS. The lecture notes of [eisert2013] explain the area law as motivation for tensor networks very well. PEPS are for example reviewed in [verstraete2008], [eisert2013] and [orus2014]. [stoudenmire2012] reviews the use of DMRG for 2D systems. [cirac2009] discusses the different groups of tensor network states.

7.5.4 Algorithm developments

7.5.5 References

7.6 Papers using TeNPy

This page collects papers using (and citing) the TeNPy library, both as an inspiration what can be done, as well as to keep track of the usage, such that we can see how useful our work is to the community. It keeps us motivated!

To include your own work, you can either fill out this template on github, or you can directly add your citation in this Zotero online library (and notify us about it or just wait).

Entries in the following list are sorted by year-author.


### 7.7 Contributing

There are lots of things where you can help, even if you don’t want to dig deep into the source code. You are welcome to do any of the following things, all of them are very helpful!

- Report bugs and problems, such that they can be fixed.
- Implement new models.
- Update and extend the documentation.
- Give feedback on how you like TeNPy and what you would like to see improved.
- Help fixing bugs.
- Help fixing minor issues.
- Extend the functionality by implementing new functions, methods, and algorithms.

The code is maintained in a git repository, the official repository is on [github](https://github.com). Even if you’re not yet on the developer team, you can still submit pull requests on github. If you’re unsure how or what to do, you can ask for help in the [TeNPyForum](https://tenpy-forum.org). If you want to become a member of the developer team, just ask :-)  

**Thank You!**
7.7.1 Coding Guidelines

To keep consistency, we ask you to comply with the following guidelines for contributions. However, these are just guidelines - it still helps if you contribute something, even if it doesn’t follow these rules ;-) 

- Use a code style based on PEP 8. The git repo includes a config file `.style.yapf` for the python package `yapf`. `yapf` is a tool to auto-format code, e.g., by the command `yapf -i some/file (-i for “in place”). We run yapf on a regular basis on the github main branch. If your branch diverged, it might help to run yapf before merging.

  **Note:** Since no tool is perfect, you can format some regions of code manually and enclose them with the special comments `# yapf: disable` and `# yapf: enable`.

- Every function/class/module should be documented by its doc-string, see PEP 257. We auto-format the doc-strings with docformatter on a regular basis.

Additional documentation for the user guide is in the folder `doc/`.

The documentation uses reStructuredText. If you are new to reStructuredText, read this introduction. We use the `numpy` style for doc-strings (with the `napoleon` extension to sphinx). You can read about them in these Instructions for the doc strings. In addition, you can take a look at the following example file. Helpful hints on top of that:

```r
**"""< this r makes me a raw string, thus '\'' has no special meaning. Otherwise you would need to escape backslashes, e.g. in math formulas.

You can include cross references to classes, methods, functions, modules like :
:func:`tenpy.tools.math.toiterable`, :mod:`tenpy.linalg.np_conserved`. The ~ in the beginning makes only the last part of the name appear in the generated documentation.

Documents of the userguide can be referenced with :doc:`/intro_npc` even from inside the doc-strings.

You can also cross-link to other documentations, e.g. :class:`numpy.ndarray`, :
:func:`scipy.linalg.svd`, :mod: will work.

Moreover, you can link to github issues, arXiv papers, dois, and topics in the community forum with e.g. :issue:`5`, :arxiv:`1805.00055`, :doi:`10.1000/1` and :forum:`3`.

Citations from the literature list can be cited as :cite:`white1992` using the bibtex key.

Write inline formulas as :math:`H |\Psi\rangle = E |\Psi\rangle` or displayed equations as .. math::

\[ e^{i\pi} + 1 = 0 \]

In doc-strings, math can only be used in the Notes section. To refer to variables within math, use `\mathtt{varname}`.

.. todo ::

This block can describe things which need to be done and is automatically included in a section of :doc:`todo`.
```
(continues on next page)
• Use relative imports within TeNPy. Example:

```python
from ..linalg import np_conserved as npc
```

• Use the python package pytest for testing. Run it simply with `pytest` in `tests/`. You should make sure that all tests run through, before you `git push` back into the public repo. Long-running tests are marked with the attribute `slow`; for a quick check you can also run `pytest -m "not slow"`.

We have set up github actions to automatically run the tests.

• Reversely, if you write new functions, please also include suitable tests!

• During development, you might introduce `# TODO` comments. But also try to remove them again later! If you’re not 100% sure that you will remove it soon, please add a doc-string with a `.. todo ::` block, such that we can keep track of it.

Unfinished functions should raise `NotImplementedError()`.

• Summarize the changes you have made in the Changelog under `[latest]`.

• If you want to try out new things in temporary files: any folder named `playground` is ignored by `git`.

• If you add a new toycode or example: add a reference to include it in the documentation.

• We’ve created a sphinx extensions for documenting `config-option` dictionaries. If a class takes a dictionary of options, we usually call it `options`, convert it to a `Config` at the very beginning of the `__init__` with `asConfig()`, save it as `self.options`, and document it in the class doc-string with a `.. cfg:config :: directive. The name of the `config` should usually be the class-name (if that is sufficiently unique), or for algorithms directly the common name of the algorithm, e.g. “DMRG”; use the same name for the use the same name for the documentation of the `.. cfg:config :: directive as for the `Config` class instance. Attributes which are simply read-out options should be documented by just referencing the options with the `:cfg:option:` configname.optionname` role.

### 7.7.2 Building the documentation

You can use `Sphinx` to generate the full documentation in various formats (including HTML or PDF) yourself, as described in the following.

First, I will assume that you downloaded the [TeNPySource] repository with:

```bash
git clone --recursive https://github.com/tenpy/tenpy
```

This includes the [TeNPyNotebooks] as a git submodule; you might need to `git submodule update` if it is out of date.

Building the documentation requires a few more packages (including `Sphinx`). The recommended way is to create a separate conda environment for it with:

```bash
conda env create -f doc/environment.yml  # make sure to use the file from the doc/˓→subfolder!
conda activate tenpydoc
```

Alternatively, you can use `pip` and `pip install -r doc/requirements.txt`, but this will not be able to install all dependencies: some packages like `Graphviz` are not available from pip alone.

Afterwards, simply go to the folder `doc/` and run the following command:
This should generate the html documentation in the folder `doc/sphinx_build/html`. Open this folder (or to be precise: the file `index.html` in it) in your webbrowser and enjoy this and other documentation beautifully rendered, with cross links, math formulas and even a search function. Other output formats are available as other make targets, e.g., `make latexpdf`.

**Note:** Building the documentation with sphinx requires loading the TeNPy modules. The `conf.py` adjusts the python `sys.path` to include the `/tenpy` folder from root directory of the git repository. It will not use the cython-compiled parts.

### 7.7.3 To-Do list

You can check https://github.com/tenpy/tenpy/issues for things to be done.

The following list is auto-generated by sphinx, extracting `.. todo ::` blocks from doc-strings of the code.

**Todo:** TDVP is currently not implemented in with the sweep class.

(The original entry is located in `/home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/algorithms/mps_common.py:docstring` of `tenpy.algorithms.mps_common.Sweep`, line 6.)

**Todo:**

- implement or wrap `netcon.m`, a function to find optimal contraction sequences (arXiv:1304.6112)
- improve helpfulness of Warnings
- `.do_trace`: trace over all pairs of legs at once. need the corresponding `npc` function first.

(The original entry is located in `/home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/algorithms/network_contractor.py:docstring` of `tenpy.algorithms.network_contractor`, line 10.)

**Todo:** This is still a beta version, use with care. The interface might still change.

(The original entry is located in `/home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/algorithms/tdvp.py:docstring` of `tenpy.algorithms.tdvp`, line 12.)

**Todo:** long-term: Much of the code is similar as in DMRG. To avoid too much duplicated code, we should have a general way to sweep through an MPS and updated one or two sites, used in both cases.

(The original entry is located in `/home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/algorithms/tdvp.py:docstring` of `tenpy.algorithms.tdvp`, line 16.)

**Todo:** implement MPO for time evolution...

(The original entry is located in `/home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/models/model.py:docstring` of `tenpy.models.model.MPOModel`, line 7.)
Todo: This is a naive, expensive implementation contracting the full network. Try to follow arXiv:1711.01104 for a better estimate; would that even work in the infinite limit?

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/networks/mpo.py:docstring of tenpy.networks.mpo.MPO.variance, line 5.)

Todo: might be useful to add a “cleanup” function which removes operators cancelling each other and/or unused states. Or better use a ‘compress’ of the MPO?

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/networks/mpo.py:docstring of tenpy.networks.mpo.MPOGraph, line 17.)

Todo: Make more general: it should be possible to specify states as strings.

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/networks/mps.py:docstring of tenpy.networks.mps.build_initial_state, line 14.)

Todo: One can also look at the canonical ensembles by defining the conserved quantities differently, see [barthel2016] for details. Idea: usual charges on \( p \), trivial charges on \( q \); fix total charge to desired value. I think it should suffice to implement another from_infiniteT.

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/networks/purification_mps.py:docstring of tenpy.networks.purification_mps, line 106.)

Todo: For memory caching with big MPO environments, we need a Hdf5Cacher clearing the memo’s every now and then (triggered by what?).

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/tools/hdf5_io.py:docstring of tenpy.tools.hdf5_io, line 65.)

Todo: add further terms (e.g. \( c^\dagger c^\dagger + \text{h.c.} \)) to the Hamiltonian.

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/models/fermions_spinless.py:docstring of tenpy.models.fermions_spinless, line 3.)

Todo: WARNING: These models are still under development and not yet tested for correctness. Use at your own risk! Replicate known results to confirm models work correctly. Long term: implement different lattices. Long term: implement variable hopping strengths \( J_x, J_y \).

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/latest/tenpy/models/hofstadter.py:docstring of tenpy.models.hofstadter, line 3.)
7.8 Tenpy main module

- full name: tenpy
- parent module: tenpy
- type: module

Submodules

<table>
<thead>
<tr>
<th>Submodule</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>algorithms</td>
<td>A collection of algorithms such as TEBD and DMRG.</td>
</tr>
<tr>
<td>linalg</td>
<td>Linear-algebra tools for tensor networks.</td>
</tr>
<tr>
<td>models</td>
<td>Definition of the various models.</td>
</tr>
<tr>
<td>networks</td>
<td>Definitions of tensor networks like MPS and MPO.</td>
</tr>
<tr>
<td>tools</td>
<td>A collection of tools: mostly short yet quite useful functions.</td>
</tr>
<tr>
<td>version</td>
<td>Access to version of this library.</td>
</tr>
</tbody>
</table>

Module description

TeNPy - a Python library for Tensor Network Algorithms

TeNPy is a library for algorithms working with tensor networks, e.g., matrix product states and -operators, designed to study the physics of strongly correlated quantum systems. The code is intended to be accessible for newcommers and yet powerful enough for day-to-day research.

```python
tenpy.__version__ = '0.7.2'
    hard-coded version string

tenpy.__full_version__ = '0.7.2.dev55+68eae2c'
    full version from git description, and numpy/scipy/python versions

tenpy.show_config()
    Print information about the version of tenpy and used libraries.

    The information printed is tenpy.version.version_summary.
```

Submodules
7.9 algorithms

- full name: tenpy.algorithms
- parent module: tenpy
- type: module

Module description

A collection of algorithms such as TEBD and DMRG.

Submodules

<table>
<thead>
<tr>
<th>Submodule</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>truncation</td>
<td>Truncation of Schmidt values.</td>
</tr>
<tr>
<td>tebd</td>
<td>Time evolving block decimation (TEBD).</td>
</tr>
<tr>
<td>mps_common</td>
<td>'Sweep' algorithm and effective Hamiltonians.</td>
</tr>
<tr>
<td>dmrng</td>
<td>Density Matrix Renormalization Group (DMRG).</td>
</tr>
<tr>
<td>tdvp</td>
<td>Time Dependant Variational Principle (TDVP) with MPS (finite version only).</td>
</tr>
<tr>
<td>purification</td>
<td>Algorithms for using Purification.</td>
</tr>
<tr>
<td>mpo_evolution</td>
<td>Time evolution using the WI or WII approximation of the time evolution operator.</td>
</tr>
<tr>
<td>network_contractor</td>
<td>Network Contractor.</td>
</tr>
<tr>
<td>exact_diag</td>
<td>Full diagonalization (ED) of the Hamiltonian.</td>
</tr>
</tbody>
</table>

7.9.1 truncation

- full name: tenpy.algorithms.truncation
- parent module: tenpy.algorithms
- type: module

Classes

```
Hdf5Exportable
  └── TruncationError
```
TruncationError

- full name: tenpy.algorithms.truncation.TruncationError
- parent module: tenpy.algorithms.truncation
- type: class

Inheritance Diagram

```
Hdf5Exportable
    ▼
    TruncationError
```

Methods

- `TruncationError.__init__((eps, ov))` Initialize self.
- `TruncationError.copy()` Return a copy of self.
- `TruncationError.from_S(S_discarded[, norm_old])` Construct TruncationError from discarded singular values.
- `TruncationError.from_hdf5(hdf5_loader, h5gr, ...)` Load instance from a HDF5 file.
- `TruncationError.from_norm(norm_new[, norm_old])` Construct TruncationError from norm after and before the truncation.
- `TruncationError.save_hdf5(hdf5_saver, h5gr, ...)` Export self into a HDF5 file.

Class Attributes and Properties

- `TruncationError.ov_err` Error $1-\text{ov}$ of the overlap with the correct state.

```python
class tenpy.algorithms.truncation.TruncationError(eps=0.0, ov=1.0)
    Bases: tenpy.tools.hdf5_io.Hdf5Exportable

    Class representing a truncation error.
    The default initialization represents “no truncation”.
```
Warning: For imaginary time evolution, this is not the error you are interested in!

Parameters

- **eps** *(float)* – See below.
- **ov** *(float)* – See below.

**eps**

The total sum of all discarded Schmidt values squared. Note that if you keep singular values up to 1.e-14 (= a bit more than machine precision for 64bit floats), *eps* is on the order of 1.e-28 (due to the square!)

Type float

**ov**

A lower bound for the overlap \(|\langle \psi_{\text{trunc}} | \psi_{\text{correct}} \rangle|^2\) (assuming normalization of both states). This is probably the quantity you are actually interested in. Takes into account the factor 2 explained in the section on Errors in the TEBD Wikipedia article [https://en.wikipedia.org/wiki/Time-evolving_block_decimation].

Type float

**copy()**

Return a copy of self.

**classmethod from_norm** *(norm_new, norm_old=1.0)*

Construct TruncationError from norm after and before the truncation.

Parameters

- **norm_new** *(float)* – Norm of Schmidt values kept, \(\sqrt{\sum_{\text{kept}} \lambda_a^2}\) (before re-normalization).
- **norm_old** *(float)* – Norm of all Schmidt values before truncation, \(\sqrt{\sum \lambda_a^2}\).

**classmethod from_S** *(S_discarded, norm_old=None)*

Construct TruncationError from discarded singular values.

Parameters

- **S_discarded** *(1D numpy array)* – The singular values discarded.
- **norm_old** *(float)* – Norm of all Schmidt values before truncation, \(\sqrt{\sum \lambda_a^2}\). Default (None) is 1.

**property ov_err**

Error 1. -ov of the overlap with the correct state.

**classmethod from_hdf5** *(hdf5_loader, h5gr, subpath)*

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

Parameters

- **hdf5_loader** *(Hdf5Loader)* – Instance of the loading engine.
- **h5gr** *(Group)* – HDF5 group which is represent the object to be constructed.
- **subpath** *(str)* – The name of h5gr with a '/' in the end.

Returns **obj** – Newly generated class instance containing the required data.

Return type **cls**
**save_hdf5** *(hdf5_saver, h5gr, subpath)*

Export *self* into a HDF5 file.

This method saves all the data it needs to reconstruct *self* with *from_hdf5()*.

This implementation saves the content of *__dict__* with *save_dict_content()* , storing the format under the attribute 'format'.

**Parameters**

- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.
- **h5gr** (:class:`Group`) – HDF5 group which is supposed to represent *self*.
- **subpath** *(str)* – The name of *h5gr* with a '/' in the end.

**Functions**

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>svd_theta</em> <em>(theta, trunc_par[, qtotal_LR, ...])</em></td>
<td>Performs SVD of a matrix <em>theta</em> (= the wavefunction) and truncates it.</td>
</tr>
<tr>
<td><em>truncate</em> <em>(S, options)</em></td>
<td>Given a Schmidt spectrum <em>S</em>, determine which values to keep.</td>
</tr>
</tbody>
</table>

**svd_theta**

- full name: tenpy.algorithms.truncation.svd_theta
- parent module: tenpy.algorithms.truncation
- type: function

*tenpy.algorithms.truncation.svd_theta* *(theta, trunc_par, qtotal_LR=[None, None], inner_labels=['vR', 'vL'])*

Performs SVD of a matrix *theta* (= the wavefunction) and truncates it.

Perform a singular value decomposition (SVD) with *svd()* and truncates with *truncate()* . The result is an approximation *theta ~= tensordot(U.scale_axis(S*renormalization, 1), VH, axes=1)*

**Parameters**

- **theta** *(Array, shape (M, N))* – The matrix, on which the singular value decomposition (SVD) is performed. Usually, *theta* represents the wavefunction, such that the SVD is a Schmidt decomposition.
- **trunc_par** *(dict)* – truncation parameters as described in *truncate()*.
- **qtotalLR** *((charges, charges))* – The total charges for the returned *U* and *VH*.
- **inner_labels** *((string, string))* – Labels for the *U* and *VH* on the newly-created bond.

**Returns**

- **U** *(Array)* – Matrix with left singular vectors as columns. Shape (M, M) or (M, K) depending on *full_matrices*.
- **S** *(1D ndarray)* – The singular values of the array. If no *cutoff* is given, it has length *min(M, N)*. Normalized to *np.linalg.norm(S)==1*. 

156 Chapter 7. License
• **VH** (*Array*) – Matrix with right singular vectors as rows. Shape \((N, N)\) or \((K, N)\) depending on *full_matrices*.

• **err** (*TruncationError*) – The truncation error introduced.

• **renormalization** (*float*) – Factor, by which S was renormalized.

### Module description

Truncation of Schmidt values.

Often, it is necessary to truncate the number of states on a virtual bond of an MPS, keeping only the state with the largest Schmidt values. The function `truncatematrix()` picks exactly those from a given Schmidt spectrum \(\lambda_a\), depending on some parameters explained in the doc-string of the function.

Further, we provide `TruncationError` for a simple way to keep track of the total truncation error.

The SVD on a virtual bond of an MPS actually gives a Schmidt decomposition \(|\psi\rangle = \sum_a \lambda_a |L_a\rangle |R_a\rangle\) where \(|L_a\rangle\) and \(|R_a\rangle\) form orthonormal bases of the parts left and right of the virtual bond. Let us assume that the state is properly normalized, \(\langle \psi | \psi \rangle = \sum_a \lambda_a^2 = 1\). Assume that the singular values are ordered descending, and that we keep the first \(\chi_c\) of the initially \(\chi\) Schmidt values.

Then we decompose the untruncated state as \(|\psi\rangle = \sqrt{1 - \epsilon} |\psi_{tr}\rangle + \sqrt{\epsilon} |\psi_{\perp tr}\rangle\) where \(|\psi_{tr}\rangle = \frac{1}{\sqrt{1 - \epsilon}} \sum_{a<\chi_c} \lambda_a |L_a\rangle |R_a\rangle\) is the truncated state kept (normalized to 1), \(|\psi_{\perp tr}\rangle = \frac{1}{\sqrt{\epsilon}} \sum_{a=\chi_c} \lambda_a |L_a\rangle |R_a\rangle\) is the discarded part (orthogonal to the kept part) and the *truncation error of a single truncation* is defined as \(\epsilon = 1 - |\langle \psi | \psi_{tr}\rangle|^2 = \sum_{a=\chi_c} \lambda_a^2\).

**Warning:** For imaginary time evolution (e.g. with TEBD), you try to project out the ground state. Then, looking at the truncation error defined in this module does not give you any information how good the found state coincides with the actual ground state! (Instead, the returned truncation error depends on the overlap with the initial state, which is arbitrary \(>0\))

**Warning:** This module takes only track of the errors coming from the truncation of Schmidt values. There might be other sources of error as well, for example TEBD has also an discretisation error depending on the chosen time step.

### 7.9.2 tebd

• full name: tenpy.algorithms.tebd

• parent module: tenpy.algorithms

• type: module
Classes

**Engine**

`Engine(psi, model, options)` Time Evolving Block Decimation (TEBD) algorithm.

**RandomUnitaryEvolution**

`RandomUnitaryEvolution(psi, options)` Evolution of an MPS with random two-site unitaries in a TEBD-like fashion.

### Module description

Time evolving block decimation (TEBD).

The TEBD algorithm (proposed in [vidal2004]) uses a trotter decomposition of the Hamiltonian to perform a time evolution of an MPS. It works only for nearest-neighbor hamiltonians (in tenpy given by a `NearestNeighborModel`), which can be written as $H = H_{\text{even}} + H_{\text{odd}}$, such that $H_{\text{even}}$ contains the terms on even bonds (and similar $H_{\text{odd}}$ the terms on odd bonds). In the simplest case, we apply first $U = \exp(-i * dt * H_{\text{even}})$, then $U = \exp(-i * dt * H_{\text{odd}})$ for each time step $dt$. This is correct up to errors of $O(dt^2)$, but to evolve until a time $T$, we need $T/dt$ steps, so in total it is only correct up to error of $O(T * dt)$. Similarly, there are higher order schemata (in $dt$) (for more details see `Engine.update()`).

Remember, that bond $i$ is between sites $(i-1, i)$, so for a finite MPS it looks like:

```
|   - B0 - B1 - B2 - B3 - B4 - B5 - B6 -   |
|    |      |      |      |      |      |      |      |
| U1 | U3   | U5   |      |      |      |      |      |
|----|------|------|-----|------|------|-----|
|    |      |      |      |      |      |      |      |
| U2 | U4   | U6   |      |      |      |      |      |
|----|------|------|-----|------|------|-----|
.   .   .   .   .   .   .   .
```

After each application of a $U_i$, the MPS needs to be truncated - otherwise the bond dimension $\chi$ would grow indefinitely. A bound for the error introduced by the truncation is returned.

If one chooses imaginary $dt$, the exponential projects (for sufficiently long ‘time’ evolution) onto the ground state of the Hamiltonian.

**Note:** The application of DMRG is typically much more efficient than imaginary TEBD! Yet, imaginary TEBD might be usefull for cross-checks and testing.
### 7.9.3 mps_common

- full name: tenpy.algorithms.mps_common
- parent module: tenpy.algorithms
- type: module

#### Classes

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>EffectiveH</td>
<td>Prototype class for local effective Hamiltonians used in sweep algorithms.</td>
</tr>
<tr>
<td>OneSiteH</td>
<td>Class defining the one-site effective Hamiltonian for Lanczos.</td>
</tr>
<tr>
<td>Sweep</td>
<td>Prototype class for a ‘sweeping’ algorithm.</td>
</tr>
<tr>
<td>TwoSiteH</td>
<td>Class defining the two-site effective Hamiltonian for Lanczos.</td>
</tr>
<tr>
<td>VariationalApplyMPO</td>
<td>Variational compression for applying an MPO to an MPS (in place).</td>
</tr>
<tr>
<td>VariationalCompression</td>
<td>Variational compression of an MPS (in place).</td>
</tr>
</tbody>
</table>

### EffectiveH

- full name: tenpy.algorithms.mps_common.EffectiveH
- parent module: tenpy.algorithms.mps_common
- type: class
Inheritance Diagram

```
NpcLinearOperator
  |__ EffectiveH
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>EffectiveH.__init__(env, i0[, combine, ...])</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>EffectiveH.adjoint()</code></td>
<td>Return the hermitian conjugate of <code>self</code>.</td>
</tr>
<tr>
<td><code>EffectiveH.combine_theta(theta)</code></td>
<td>Combine the legs of <code>theta</code>, such that it fits to how we combined the legs of <code>self</code>.</td>
</tr>
<tr>
<td><code>EffectiveH.matvec(vec)</code></td>
<td>Calculate the action of the operator on a vector <code>vec</code>.</td>
</tr>
<tr>
<td><code>EffectiveH.to_matrix()</code></td>
<td>Contract <code>self</code> to a matrix.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

```
EffectiveH.acts_on
EffectiveH.length
```

class tenpy.algorithms.mps_common.EffectiveH(env, i0, combine=False, move_right=True)
Bases: tenpy.linalg.sparse.NpcLinearOperator

Prototype class for local effective Hamiltonians used in sweep algorithms.

As an example, the local effective Hamiltonian for a two-site (DMRG) algorithm looks like:

```
|   | .--- | .--- |
|   |     |     |
|   | LP----H0--H1---RP |
|   |     |     |
|   | .--- | .--- |
```

where $H_0$ and $H_1$ are MPO tensors.

Parameters

- `env (MPOEnvironment)` – Environment for contraction $\langle \psi \mid H \mid \psi \rangle$.
- `i0 (int)` – Index of the active site if length=1, or of the left-most active site if length>1.
- `combine (bool, optional)` – Whether to combine legs into pipes as far as possible. This reduces the overhead of calculating charge combinations in the contractions.
• `move_right (bool, optional) – Whether the sweeping algorithm that calls for an
  EffectiveH is moving to the right.

`length`
  Number of (MPS) sites the effective hamiltonian covers. NB: Class attribute.
  
  `Type` int

`dtype`
  The data type of the involved arrays.
  
  `Type` np.dtype

`N`
  Contracting `self` with `as_matrix()` will result in an \( N \times N \) matrix.
  
  `Type` int

`acts_on`
  Labels of the state on which `self` acts. NB: class attribute. Overwritten by normal attribute, if `combine`.
  
  `Type` list of str

`combine`
  Whether to combine legs into pipes as far as possible. This reduces the overhead of calculating charge
  combinations in the contractions.
  
  `Type` bool

`move_right`
  Whether the sweeping algorithm that calls for an EffectiveH is moving to the right.
  
  `Type` bool

`combine_theta (theta)`
  Combine the legs of `theta`, such that it fits to how we combined the legs of `self`.
  
  `Parameters` `theta (Array)` – Wave function to apply the effective Hamiltonian to, with un-
  combined legs.
  
  `Returns` `theta` – Wave function with labels as given by `self.acts_on`.
  
  `Return type` Array

`adjoint ()`
  Return the hermitian conjugate of `self`
  
  If `self` is hermitian, subclasses can choose to implement this to define the adjoint operator of `self`.

`matvec (vec)`
  Calculate the action of the operator on a vector `vec`.
  
  Note that we don’t require `vec` to be one-dimensional. However, for square operators we require that the
  result of `matvec` has the same legs (in the same order) as `vec` such that they can be added. Note that this
  excludes a non-trivial `qtotal` for square operators.

`to_matrix ()`
  Contract `self` to a matrix.
  
  If `self` represents an operator with very small shape, e.g. because the MPS bond dimension is very small,
  an algorithm might choose to contract `self` to a single tensor.
  
  `Returns` `matrix` – Contraction of the represented operator.
  
  `Return type` Array
OneSiteH

- full name: tenpy.algorithms.mps_common.OneSiteH
- parent module: tenpy.algorithms.mps_common
- type: class

Inheritance Diagram

![Inheritance Diagram](image)

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>OneSiteH.<strong>init</strong>(env, i0[, combine, move_right])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>OneSiteH.adjoint()</td>
<td>Return the hermitian conjugate of self.</td>
</tr>
<tr>
<td>OneSiteH.combine_Heff()</td>
<td>Combine LP and RP with W to form LHeff and RHeff, depending on the direction.</td>
</tr>
<tr>
<td>OneSiteH.combine_theta(theta)</td>
<td>Combine the legs of theta, such that it fits to how we combined the legs of self.</td>
</tr>
<tr>
<td>OneSiteH.matvec(theta)</td>
<td>Apply the effective Hamiltonian to theta.</td>
</tr>
<tr>
<td>OneSiteH.to_matrix()</td>
<td>Contract self to a matrix.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
</tr>
</thead>
<tbody>
<tr>
<td>OneSiteH.acts_on</td>
</tr>
<tr>
<td>OneSiteH.length</td>
</tr>
</tbody>
</table>

```python
class tenpy.algorithms.mps_common.OneSiteH (env, i0, combine=False, move_right=True)
    Bases: tenpy.algorithms.mps_common.EffectiveH

Class defining the one-site effective Hamiltonian for Lanczos.

The effective one-site Hamiltonian looks like this:
If `combine` is True, we define either \( L_{\text{Heff}} \) as contraction of \( LP \) with \( W \) (in the case `move_right` is True) or \( R_{\text{Heff}} \) as contraction of \( RP \) and \( W \).

**Parameters**

- `env (MPOEnvironment)` – Environment for contraction \( \langle \psi | H | \psi \rangle \).
- `i0 (int)` – Index of the active site if length=1, or of the left-most active site if length>1.
- `combine (bool)` – Whether to combine legs into pipes. This combines the virtual and physical leg for the left site (when moving right) or right side (when moving left) into pipes. This reduces the overhead of calculating charge combinations in the contractions, but one `matvec()` is formally more expensive, \( O(2d^3\chi^3D) \). Is originally from the wo-site method; unclear if it works well for 1 site.
- `move_right (bool)` – Whether the sweep is moving right or left for the next update.

**length**

Number of (MPS) sites the effective Hamiltonian covers.

**Type** `int`

**acts_on**

Labels of the state on which `self` acts. NB: class attribute. Overwritten by normal attribute, if `combine`.

**Type** `list of str`

**combine, move_right**

See above.

**Type** `bool`

**L_{\text{Heff}}, R_{\text{Heff}}**

Only set if `combine`, and only one of them depending on `move_right`. If `move_right` was True, \( L_{\text{Heff}} \) is set with labels \( '(vR*.p0)', 'wR', '(vR.p0*)' \) for bra, MPO, ket; otherwise \( R_{\text{Heff}} \) is set with labels \( '(p0*.vL)', 'wL', '(p0, vL*)' \).

**Type** `Array`

**LP, W0, RP**

Tensors making up the network of `self`.

**Type** `Array`

**matvec (theta)**

Apply the effective Hamiltonian to `theta`.

**Parameters**

- `theta (Array)` – Labels: \( vL, p0, vR \) if `combine=False`, \( (vL.p0), vR \) or \( vL, (p0.vR) \) if `True` (depending on the direction of movement)

**Returns** Product of `theta` and the effective Hamiltonian.

**Return type** `theta Array`

**combine_Heff ()**

Combine LP and RP with W to form \( L_{\text{Heff}} \) and \( R_{\text{Heff}} \), depending on the direction.

In a move to the right, we need \( L_{\text{Heff}} \). In a move to the left, we need \( R_{\text{Heff}} \). Both contain the same W.
**combine_theta** *(theta)*

Combine the legs of *theta*, such that it fits to how we combined the legs of *self*.

**Parameters**

- **theta** *(Array)* – Wave function with labels 'vL', 'p0', 'p1', 'vR'

**Returns**

- **theta** – Wave function with labels 'vL', 'p0', 'p1', 'vR'

**Return type** *Array*

**to_matrix()**

Contract *self* to a matrix.

**adjoint()**

Return the hermitian conjugate of *self*.

---

### TwoSiteH

- **full name**: `tenpy.algorithms.mps_common.TwoSiteH`
- **parent module**: `tenpy.algorithms.mps_common`
- **type**: class

#### Inheritance Diagram

```
NpcLinearOperator
    ↓
  EffectiveH
    ↓
TwoSiteH
```

#### Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>TwoSiteH.__init__(env, i0[, combine, move_right])</code></td>
<td>Initialize <em>self</em>.</td>
</tr>
<tr>
<td><code>TwoSiteH.adjoint()</code></td>
<td>Return the hermitian conjugate of <em>self</em>.</td>
</tr>
<tr>
<td><code>TwoSiteH.combine_Heff()</code></td>
<td>Combine LP and RP with W to form LHeff and RHeff.</td>
</tr>
<tr>
<td><code>TwoSiteH.combine_theta(theta)</code></td>
<td>Combine the legs of <em>theta</em>, such that it fits to how we combined the legs of <em>self</em>.</td>
</tr>
<tr>
<td><code>TwoSiteH.matvec(theta)</code></td>
<td>Apply the effective Hamiltonian to <em>theta</em>.</td>
</tr>
<tr>
<td><code>TwoSiteH.to_matrix()</code></td>
<td>Contract <em>self</em> to a matrix.</td>
</tr>
</tbody>
</table>
Class Attributes and Properties

```python
class TwoSiteH acts_on
TwoSiteH.length

class tenpy.algorithms.mps_common.TwoSiteH(env, i0, combine=False, move_right=True)
Bases: tenpy.algorithms.mps_common.EffectiveH

Class defining the two-site effective Hamiltonian for Lanczos.

The effective two-site Hamiltonian looks like this:

```
|   ---   --- |
|   |   |   |
| LP----W0--W1---RP |
|   |   |   |
|   ---   --- |
```

If `combine` is True, we define $L_{\text{Heff}}$ and $R_{\text{Heff}}$, which are the contractions of $LP$ with $W0$, and $RP$ with $W1$, respectively.

Parameters

- `env` (*MPOEnvironment*) – Environment for contraction $<\psi|H|\psi>$.
- `i0` (*int*) – Index of the active site if length=1, or of the left-most active site if length>1.
- `combine` (*bool*) – Whether to combine legs into pipes. This combines the virtual and physical leg for the left site (when moving right) or right side (when moving left) into pipes. This reduces the overhead of calculating charge combinations in the contractions, but one `matvec()` is formally more expensive, $O(2d^3\chi^3D)$.
- `move_right` (*bool*) – Whether the the sweep is moving right or left for the next update.

- `combine` (*bool*) – Whether to combine legs into pipes. This combines the virtual and physical leg for the left site and right site into pipes. This reduces the overhead of calculating charge combinations in the contractions, but one `matvec()` is formally more expensive, $O(2d^3\chi^3D)$.

- `length` (*int*) – Number of (MPS) sites the effective hamiltonian covers.

- `acts_on` (*list of str*) – Labels of the state on which `self` acts. NB: class attribute. Overwritten by normal attribute, if `combine`.

- `LHeff` (*Array*) – Left part of the effective Hamiltonian. Labels '($v_{R.}*p0$)', 'wR', '($v_{R.p0}$)' for bra, MPO, ket.

- `RHeff` (*Array*) – Right part of the effective Hamiltonian. Labels '($p1.*vL$)', 'wL', '($p1.vL$)' for ket, MPO, bra.
LP, W0, W1, RP
Tensors making up the network of self.

Type Array

matvec(theta)
Apply the effective Hamiltonian to theta.

Parameters theta (Array) — Labels: vL, p0, p1, vR if combine=False, (vL.p0), (p1.vR) if True

Returns Product of theta and the effective Hamiltonian.

Return type theta Array

combine_Heff()
Combine LP and RP with W to form LHeff and RHeff.

Combine LP with W0 and RP with W1 to get the effective parts of the Hamiltonian with piped legs.

combine_theta(theta)
Combine the legs of theta, such that it fits to how we combined the legs of self.

Parameters theta (Array) — Wave function with labels 'vL', 'p0', 'p1', 'vR'

Returns theta — Wave function with labels 'vL', 'p0', 'p1', 'vR'

Return type Array

to_matrix()
Contract self to a matrix.

adjoint()
Return the hermitian conjugate of self.

Module description

‘Sweep’ algorithm and effective Hamiltonians.

Many MPS-based algorithms use a ‘sweep’ structure, wherein local updates are performed on the MPS tensors sequentially, first from left to right, then from right to left. This procedure is common to DMRG, TDVP, sequential time evolution, etc.

Another common feature of these algorithms is the use of an effective local Hamiltonian to perform the local updates. The most prominent example of this is probably DMRG, where the local MPS object is optimized with respect to the rest of the MPS-MPO-MPS network, the latter forming the effective Hamiltonian.

The Sweep class attempts to generalize as many aspects of ‘sweeping’ algorithms as possible. EffectiveH and its subclasses implement the effective Hamiltonians mentioned above. Currently, effective Hamiltonians for 1-site and 2-site optimization are implemented.

The VariationalCompression and VariationalApplyMPO implemented here also directly use the Sweep class.
7.9.4 dmrg

- full name: tenpy.algorithms.dmrg
- parent module: tenpy.algorithms
- type: module

Classes

<table>
<thead>
<tr>
<th>Class Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DMRGEngine(psi, model, options)</td>
<td>DMRG base class; 'Engine' for the DMRG algorithm.</td>
</tr>
<tr>
<td>DensityMatrixMixer(options)</td>
<td>Mixer based on density matrices.</td>
</tr>
<tr>
<td>EngineCombine(psi, model, DMRG_params)</td>
<td>Engine which combines legs into pipes as far as possible.</td>
</tr>
<tr>
<td>EngineFracture(psi, model, DMRG_params)</td>
<td>Engine which keeps the legs separate.</td>
</tr>
<tr>
<td>Mixer(options)</td>
<td>Base class of a general Mixer.</td>
</tr>
<tr>
<td>SingleSiteDMRGEngine(psi, model, options)</td>
<td>'Engine' for the single-site DMRG algorithm.</td>
</tr>
<tr>
<td>TwoSiteDMRGEngine(psi, model, options)</td>
<td>'Engine' for the two-site DMRG algorithm.</td>
</tr>
<tr>
<td>TwoSiteMixer(options)</td>
<td>Mixer for two-site DMRG.</td>
</tr>
</tbody>
</table>
DensityMatrixMixer

- full name: tenpy.algorithms.dmrg.DensityMatrixMixer
- parent module: tenpy.algorithms.dmrg
- type: class

Inheritance Diagram

![Inheritance Diagram](image)

Methods

<table>
<thead>
<tr>
<th>Method Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DensityMatrixMixer.<strong>init</strong>(options)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>DensityMatrixMixer.get_xL(wL_leg, Id_L, Id_R)</td>
<td>Generate the coupling of the MPO legs for the reduced density matrix.</td>
</tr>
<tr>
<td>DensityMatrixMixer.get_xR(wR_leg, Id_L, Id_R)</td>
<td>Generate the coupling of the MPO legs for the reduced density matrix.</td>
</tr>
<tr>
<td>DensityMatrixMixer.mix_rho_L(engine, theta, ...)</td>
<td>Calculated mixed reduced density matrix for left site.</td>
</tr>
<tr>
<td>DensityMatrixMixer.mix_rho_R(engine, theta, ...)</td>
<td>Calculated mixed reduced density matrix for left site.</td>
</tr>
<tr>
<td>DensityMatrixMixer.perturb_svd(engine, theta, ...)</td>
<td>Mix extra terms to theta and perform an SVD.</td>
</tr>
<tr>
<td>DensityMatrixMixer.update_amplitude(sweeps)</td>
<td>Update the amplitude, possibly disable the mixer.</td>
</tr>
</tbody>
</table>

```python
class tenpy.algorithms.dmrg.DensityMatrixMixer(options)
Bases: tenpy.algorithms.dmrg.Mixer

Mixer based on density matrices.

This mixer constructs density matrices as described in the original paper [white2005].

perturb_svd(engine, theta, i0, update_LP, update_RP)
Mix extra terms to theta and perform an SVD.

We calculate the left and right reduced density using the mixer (which might include applications of \( H \)).
These density matrices are diagonalized and truncated such that we effectively perform a svd for the case mixer.amplitude=0.

Parameters```
• **engine** (`SingleSiteDMRGEngine | TwoSiteDMRGEngine`) – The DMRG engine calling the mixer.

• **theta** (`Array`) – The optimized wave function, prepared for svd.

• **i0** (`int`) – Site index; `theta` lives on `i0, i0+1`.

• **update_LP** (`bool`) – Whether to calculate the next `env.LP[i0+1]`.

• **update_RP** (`bool`) – Whether to calculate the next `env.RP[i0]`.

**Returns**

• **U** (`Array`) – Left-canonical part of `theta`. Labels `'vL.p0)' , 'vR'`

• **S** (`1D ndarray | 2D Array`) – Without mixer just the singular values of the array; with mixer it might be a general matrix; see comment above.

• **VH** (`Array`) – Right-canonical part of `theta`. Labels 'vL', '(p1.vR)'.

• **err** (`TruncationError`) – The truncation error introduced.

**mix_rho_L** (`engine, theta, i0, mix_enabled`)
Calculated mixed reduced density matrix for left site.

Pictorially:

```
+------------------mix_enabled=False  mix_enabled=True------------------+
|                   |
| .---theta---.     |
| | | | | | | | |
| | | | | | | | |
| LP---H0--H1--.    |
| | | | | | | | |
| .---theta *--.    |
| | | | | | | |
| LP *--H0*-H1*-    |
| | | | | |
| .---theta *------|
```

**Parameters**

• **engine** (`Engine`) – The DMRG engine calling the mixer.

• **theta** (`Array`) – Ground state of the effective Hamiltonian, prepared for svd.

• **i0** (`int`) – Site index; `theta` lives on `i0, i0+1`.

• **mix_enabled** (`bool`) – Whether we should perturb the density matrix.

**Returns**

• **rho_L** – A (hermitian) square array with labels `'vL.p0)' , '(vL*.p0*)' Mainly the reduced density matrix of the left part, but with some additional mixing.

**Return type** `Array`

**mix_rho_R** (`engine, theta, i0, mix_enabled`)
Calculated mixed reduced density matrix for left site.

Pictorially:

```
+------------------mix_enabled=False  mix_enabled=True------------------+
|                   |
| .---theta---.     |
| | | | | | | | |
| | | | | | | | |
| LP---H0--H1--.    |
| | | | | | | | |
| .---theta *--.    |
| | | | | | | |
| LP *--H0*-H1*-    |
| | | | | |
| .---theta *------|
```

(continues on next page)
Parameters

- **engine** (*Engine*) – The DMRG engine calling the mixer.
- **theta** (*Array*) – Ground state of the effective Hamiltonian, prepared for svd.
- **i0** (*int*) – Site index; theta lives on i0, i0+1.
- **mix_enabled** (*bool*) – Whether we should perturb the density matrix.

Returns **rho_R** – A (hermitian) square array with labels `(p1.vR)`, `(p1*.vR*)`. Mainly the reduced density matrix of the right part, but with some additional mixing.

Return type *Array*

### get_xR(*wR_leg*, *Id_L*, *Id_R*)
Generate the coupling of the MPO legs for the reduced density matrix.

Parameters

- **wR_leg** (*LegCharge*) – LegCharge to be connected to.
- **IdL** (*int | None*) – Index within the leg for which the MPO has only identities to the left.
- **IdR** (*int | None*) – Index within the leg for which the MPO has only identities to the right.

Returns

- **mixed_xR** (*Array*) – Connection of the MPOs on the right for the reduced density matrix rhoL. Labels (`wL`, `wL*`).
- **add_separate_Id** (*bool*) – If Id_L is None, we can’t include the identity into mixed_xR, so it has to be added directly in mix_rho_L().

### get_xL(*wL_leg*, *Id_L*, *Id_R*)
Generate the coupling of the MPO legs for the reduced density matrix.

Parameters

- **wL_leg** (*LegCharge*) – LegCharge to be connected to.
- **Id_L** (*int | None*) – Index within the leg for which the MPO has only identities to the left.
- **Id_R** (*int | None*) – Index within the leg for which the MPO has only identities to the right.

Returns

- **mixed_xL** (*Array*) – Connection of the MPOs on the left for the reduced density matrix rhoR. Labels (`wR`, `wR*`).
- **add_separate_Id** (*bool*) – If Id_R is None, we can’t include the identity into mixed_xL, so it has to be added directly in mix_rho_R().

### update_amplitude(*sweeps*)
Update the amplitude, possibly disable the mixer.
Parameters `sweeps` (int) – The number of performed sweeps, to check if we need to disable the mixer.

Returns `mixer` – Returns `self` if we should continue mixing, or `None`, if the mixer should be disabled.

Return type `Mixer | None`

EngineCombine

- full name: `tenpy.algorithms.dmrgr.EngineCombine`
- parent module: `tenpy.algorithms.dmrgr`
- type: `class`

Inheritance Diagram

```
DMRGEngine
  
TwoSiteDMRGEngine
  
EngineCombine
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>EngineCombine.__init__</code>(psi, model, DMRG_params)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>EngineCombine.diag</code>(theta_guess)</td>
<td>Diagonalize the effective Hamiltonian represented by self.</td>
</tr>
<tr>
<td><code>EngineCombine.environment_sweeps</code>(N_sweeps)</td>
<td>Perform (N_{sweeps}) sweeps without optimization to update the environment.</td>
</tr>
<tr>
<td><code>EngineCombine.get_sweep_schedule</code>()</td>
<td>Define the schedule of the sweep.</td>
</tr>
<tr>
<td><code>EngineCombine.init_env</code>([model])</td>
<td>(Re-)initialize the environment.</td>
</tr>
</tbody>
</table>

continues on next page
Table 18 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>EngineCombine.make_eff_H()</code></td>
<td>Create new instance of <code>self.EffectiveH</code> at <code>self.i0</code> and set it to <code>self.eff_H</code>.</td>
</tr>
<tr>
<td><code>EngineCombine.mixed_svd(theta)</code></td>
<td>Get (truncated) $\mathcal{B}$ from the new theta (as returned by <code>diag</code>).</td>
</tr>
<tr>
<td><code>EngineCombine.mixer_activate()</code></td>
<td>Set <code>self.mixer</code> to the class specified by <code>options['mixer']</code>.</td>
</tr>
<tr>
<td><code>EngineCombine.mixer_cleanup()</code></td>
<td>Cleanup the effects of a mixer.</td>
</tr>
<tr>
<td><code>EngineCombine.plot_sweep_stats([axes, ...])</code></td>
<td>Plot sweep_stats to display the convergence with the sweeps.</td>
</tr>
<tr>
<td><code>EngineCombine.plot_update_stats([axes[, ...]])</code></td>
<td>Plot update_stats to display the convergence during the sweeps.</td>
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<tr>
<td><code>EngineCombine.prepare_svd(theta)</code></td>
<td>Transform theta into matrix for svd.</td>
</tr>
<tr>
<td><code>EngineCombine.prepare_update()</code></td>
<td>Prepare <code>self</code> for calling <code>update_local()</code> on sites <code>i0 : i0+n_optimize</code>.</td>
</tr>
<tr>
<td><code>EngineCombine.reset_stats()</code></td>
<td>Reset the statistics, useful if you want to start a new sweep run.</td>
</tr>
<tr>
<td><code>EngineCombine.run()</code></td>
<td>Run the DMRG simulation to find the ground state.</td>
</tr>
<tr>
<td><code>EngineCombine.set_B(U, S, VH)</code></td>
<td>Update the MPS with the $U, S, VH$ returned by <code>self.mixed_svd</code>.</td>
</tr>
<tr>
<td><code>EngineCombine.sweep([optimize, meas_E_trunc])</code></td>
<td>One ‘sweep’ of the algorithm.</td>
</tr>
<tr>
<td><code>EngineCombine.update_LP(U)</code></td>
<td>Update left part of the environment.</td>
</tr>
<tr>
<td><code>EngineCombine.update_RP(VH)</code></td>
<td>Update right part of the environment.</td>
</tr>
<tr>
<td><code>EngineCombine.update_local(theta[, optimize])</code></td>
<td>Perform site-update on the site <code>i0</code>.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

- `EngineCombine.DMRG_params`
- `EngineCombine.engine_params`
- `EngineCombine.n_optimize` the number of sites to be optimized over at once.

```python
class tenpy.algorithms.dmrg.EngineCombine (psi, model, DMRG_params)
    Bases: tenpy.algorithms.dmrg.TwoSiteDMRGEengine

    Engine which combines legs into pipes as far as possible.
    This engine combines the virtual and physical leg for the left site and right site into pipes. This reduces the overhead of calculating charge combinations in the contractions, but one `matvec()` is formally more expensive, $O(2d^3\chi^3D)$.

    Deprecated since version 0.5.0: Directly use the `TwoSiteDMRGEengine` with the DMRG parameter `combine=True`.
```

```python
DefaultMixer
    alias of `DensityMatrixMixer`

EffectiveH
    alias of `tenpy.algorithms.mps_common.TwoSiteH`

diag(theta_guess)
    Diagonalize the effective Hamiltonian represented by self.
```
option DMRGEngine.max_N_for_ED: int
Maximum matrix dimension of the effective Hamiltonian up to which the 'default' diag_method uses ED instead of Lanczos.

option DMRGEngine.diag_method: str
One of the following strings:
- 'default' Same as 'lanczos' for large bond dimensions, but if the total dimension of the effective Hamiltonian does not exceed the DMRG parameter 'max_N_for_ED' it uses 'ED_block'.
- 'lanczos' lanczos() Default, the Lanczos implementation in TeNPy.
- 'arpack' lanczos_arpack() Based on scipy.linalg.sparse.eigsh(). Slower than 'lanczos', since it needs to convert the npc arrays to numpy arrays during each matvec, and possibly does many more iterations.
- 'ED_block' full_diag_effH() Contract the effective Hamiltonian to a (large!) matrix and diagonalize the block in the charge sector of the initial state. Preserves the charge sector of the explicitly conserved charges. However, if you don't preserve a charge explicitly, it can break it. For example if you use a SpinChain({'conserve': 'parity'}), it could change the total "Sz", but not the parity of 'Sz'.
- 'ED_all' full_diag_effH() Contract the effective Hamiltonian to a (large!) matrix and diagonalize it completely. Allows to change the charge sector even for explicitly conserved charges. For example if you use a SpinChain({'conserve': 'Sz'}), it can change the total "Sz".

Parameters theta_guess (Array) – Initial guess for the ground state of the effective Hamiltonian.

Returns
- E0 (float) – Energy of the found ground state.
- theta (Array) – Ground state of the effective Hamiltonian.
- N (int) – Number of Lanczos iterations used. -1 if unknown.
- ov_change (float) – Change in the wave function 1. - abs(<theta_guess|theta_diag>)

environment_sweeps (N_sweeps)
Perform N_sweeps sweeps without optimization to update the environment.

Parameters N_sweeps (int) – Number of sweeps to run without optimization

get_sweep_schedule()
Define the schedule of the sweep.

One ‘sweep’ is a full sequence from the leftmost site to the right and back. Only those LP and RP that can be used later should be updated.

Returns schedule – Schedule for the sweep. Each entry is (i0, move_right, (update_LP, update_RP)), where i0 is the leftmost of the self.EffectiveH.length sites to be updated in update_local(), move_right indicates whether the next i0 in the schedule is right (True) of the current one, and update_LP, update_RP indicate whether it is necessary to update the LP and RP. The latter are chosen such that the environment is growing for infinite systems, but we only keep the minimal number of environment tensors in memory.

Return type iterable of (int, bool, (bool, bool))

init_env (model=None)
(Re-)initialize the environment.

7.9. algorithms 173
This function is useful to (re-)start a Sweep with a slightly different model or different (engine) parameters. Note that we assume that we still have the same $\psi$. Calls `reset_stats()`.

**Parameters**

- **model** (`MPOModel`) – The model representing the Hamiltonian for which we want to find the ground state. If `None`, keep the model used before.

**Options**

Deprecated since version 0.6.0: Options `LP`, `LP_age`, `RP` and `RP_age` are now collected in a dictionary `init_env_data` with different keys `init_LP`, `init_RP`, `age_LP`, `age_RP`.

- **Sweep.init_env_data** (`dict`) – Dictionary as returned by `self.env.get_initialization_data()` from `get_initialization_data()`.

- **Sweep.orthogonal_to** (`list of MPS`) – List of other matrix product states to orthogonalize against. Works only for finite systems. This parameter can be used to find (a few) excited states as follows. First, run DMRG to find the ground state and then run DMRG again while orthogonalizing against the ground state, which yields the first excited state (in the same symmetry sector), and so on.

- **Sweep.start_env** (`int`) – Number of sweeps to be performed without optimization to update the environment.

**Raises** `ValueError` – If the engine is re-initialized with a new model, which legs are incompatible with those of the old model.

**make_eff_H()**

Create new instance of `self.EffectiveH` at `self.i0` and set it to `self.eff_H`.

**mixed_svd(theta)**

Get (truncated) $B$ from the new theta (as returned by `diag`).

The goal is to split theta and truncate it:

```
| -- theta -- ==> -- U -- S -- VH -- |
| | | | |
```

Without a mixer, this is done by a simple svd and truncation of Schmidt values.

With a mixer, the state is perturbed before the SVD. The details of the perturbation are defined by the `Mixer` class.

Note that the returned $S$ is a general (not diagonal) matrix, with labels 'vL', 'vR'.

**Parameters** `theta` (`Array`) – The optimized wave function, prepared for svd.

**Returns**

- **U** (`Array`) – Left-canonical part of `theta`. Labels 'vL.p0', 'vR'.
- **S** (`1D` `ndarray` | `2D` `Array`) – Without mixer just the singular values of the array; with mixer it might be a general matrix with labels 'vL', 'vR'; see comment above.
- **VH** (`Array`) – Right-canonical part of `theta`. Labels 'vL', '(p1.vR)'.
- **err** (`TruncationError`) – The truncation error introduced.

**mixer_activate()**

Set `self.mixer` to the class specified by `options['mixer']`. 
option TwoSiteDMRGEngine.mixer: str | class | bool
Chooses the Mixer to be used. A string stands for one of the mixers defined in this module, a class is used as custom mixer. Default (None) uses no mixer. True uses DensityMatrixMixer for the 2-site case and SingleSiteMixer for the 1-site case.

option TwoSiteDMRGEngine.mixer_params: dict
Mixer parameters as described in Mixer.

mixer_cleanup()
Cleanup the effects of a mixer.
A sweep() with an enabled Mixer leaves the MPS psi with 2D arrays in S. To recover the original form, this function simply performs one sweep with disabled mixer.

property n_optimize
the number of sites to be optimized over at once.
Indirectly set by the class attribute EffectiveH and it’s length. For example, TwoSiteDMRGEngine uses the TwoSiteH and hence has n_optimize=2, while the SingleSiteDMRGEngine has n_optimize=1.

plot_sweep_stats(axes=None, xaxis='time', yaxis='E', y_exact=None, **kwargs)
Plot sweep_stats to display the convergence with the sweeps.
Parameters
• axes(matplotlib.axes.Axes) – The axes to plot into. Defaults to matplotlib.pyplot.gca().
• xaxis (key of sweep_stats) – Key of sweep_stats to be used for the x-axis and y-axis of the plots.
• yaxis (key of sweep_stats) – Key of sweep_stats to be used for the x-axis and y-axis of the plots.
• y_exact (float) – Exact value for the quantity on the y-axis for comparison. If given, plot abs((y-y_exact)/y_exact) on a log-scale yaxis.
• **kwargs – Further keyword arguments given to axes.plot(...).

plot_update_stats(axes, xaxis='time', yaxis='E', y_exact=None, **kwargs)
Plot update_stats to display the convergence during the sweeps.
Parameters
• axes(matplotlib.axes.Axes) – The axes to plot into. Defaults to matplotlib.pyplot.gca().
• xaxis ('N_updates' | 'sweep' | keys of update_stats) – Key of update_stats to be used for the x-axis of the plots. 'N_updates' is just enumerating the number of bond updates, and 'sweep' corresponds to the sweep number (including environment sweeps).
• yaxis ('E' | keys of update_stats) – Key of update_stats to be used for the y-axis of the plots. For ‘E’, use the energy (per site for infinite systems).
• y_exact (float) – Exact value for the quantity on the y-axis for comparison. If given, plot abs((y-y_exact)/y_exact) on a log-scale yaxis.
• **kwargs – Further keyword arguments given to axes.plot(...).

post_update_local(update_data)
Perform post-update actions.
Compute truncation energy, remove LP/RP that are no longer needed and collect statistics.

**Parameters**

`update_data (dict)` — What was returned by `update_local()`.

`prepare_svd (theta)`

Transform theta into matrix for svd.

`prepare_update ()`

Prepare `self` for calling `update_local()` on sites `i0 : i0+n_optimize`.

**Returns**

`theta` — Current best guess for the ground state, which is to be optimized. Labels are 'vL', 'p0', 'p1', 'vR', or combined versions of it (if `self.combine`). For single-site DMRG, the 'p1' label is missing.

**Return type** `Array`

`reset_stats ()`

Reset the statistics, useful if you want to start a new sweep run.

**option**

`DMRGEngine.chi_list: dict | None`

A dictionary to gradually increase the `chi_max` parameter of `trunc_params`. The key defines starting from which sweep `chi_max` is set to the value, e.g. `{0: 50, 20: 100}` uses `chi_max=50` for the first 20 sweeps and `chi_max=100` afterwards. Overwrites `trunc_params['chi_list']`. By default (None) this feature is disabled.

**option**

`DMRGEngine.sweep_0: int`

The number of sweeps already performed. (Useful for re-start).

`run ()`

Run the DMRG simulation to find the ground state.

**Returns**

- `E (float)` — The energy of the resulting ground state MPS.
- `psi (MPS)` — The MPS representing the ground state after the simulation, i.e. just a reference to `psi`.

**Options**

**option**

`DMRGEngine.diag_method: str`

Method to be used for diagonalization, default 'default'. For possible arguments see `DMRGEngine.diag()`.

**option**

`DMRGEngine.E_tol_to_trunc: float`

It's reasonable to choose the Lanczos convergence criteria 'E_tol' not many magnitudes lower than the current truncation error. Therefore, if `E_tol_to_trunc` is not None, we update `E_tol` of `lanczos_params` to `max_E_trunc*E_tol_to_trunc`, restricted to the interval `[E_tol_min, E_tol_max]`, where `max_E_trunc` is the maximal energy difference due to truncation right after each Lanczos optimization during the sweeps.

**option**

`DMRGEngine.E_tol_max: float`

See `E_tol_to_trunc`

**option**

`DMRGEngine.E_tol_min: float`

See `E_tol_to_trunc`

**option**

`DMRGEngine.max_E_err: float`

Convergence if the change of the energy in each step satisfies `-Delta E / max(|E|, 1) < max_E_err`. Note that this is also satisfied if `Delta E > 0`, i.e., if the energy increases (due to truncation).
option DMRGEngine.max_hours: float
If the DMRG took longer (measured in wall-clock time), ‘shelve’ the simulation, i.e. stop and return with the flag shelve=True.

option DMRGEngine.max_S_err: float
Convergence if the relative change of the entropy in each step satisfies \(|\Delta S|/S < \text{max}_S\text{err}\).

option DMRGEngine.max_sweeps: int
Maximum number of sweeps to be performed.

option DMRGEngine.min_sweeps: int
Minimum number of sweeps to be performed. Defaults to 1.5*N_sweeps_check.

option DMRGEngine.N_sweeps_check: int
Number of sweeps to perform between checking convergence criteria and giving a status update.

option DMRGEngine.norm_tol: float
After the DMRG run, update the environment with at most norm_tol_iter sweeps until np.linalg.norm(psi.norm_err()) < norm_tol.

option DMRGEngine.norm_tol_iter: float
Perform at most norm_tol_iter*update_env sweeps to converge the norm error below norm_tol. If the state is not converged after that, call canonical_form() instead.

option DMRGEngine.P_tol_to_trunc: float
It's reasonable to choose the Lanczos convergence criteria 'P_tol' not many magnitudes lower than the current truncation error. Therefore, if \(P\text{tol}_\text{to}_\text{trunc}\) is not None, we update \(P\text{tol}\) of lanczos_params to max_trunc_err*\(P\text{tol}_\text{to}_\text{trunc}\), restricted to the interval \([P\text{tol}_\text{min}, P\text{tol}_\text{max}]\), where max_trunc_err is the maximal truncation error (discarded weight of the Schmidt values) due to truncation right after each Lanczos optimization during the sweeps.

option DMRGEngine.P_tol_max: float
See \(P\text{tol}_\text{to}_\text{trunc}\)

option DMRGEngine.P_tol_min: float
See \(P\text{tol}_\text{to}_\text{trunc}\)

option DMRGEngine.update_env: int
Number of sweeps without bond optimization to update the environment for infinite boundary conditions, performed every N_sweeps_check sweeps.

set_B(U, S, VH)
Update the MPS with the U, S, VH returned by self.mixed_svd.

Parameters
- \(U\) (Array) – Left and Right-canonical matrices as returned by the SVD.
- \(VH\) (Array) – Left and Right-canonical matrices as returned by the SVD.
- \(S\) (1D array | 2D Array) – The middle part returned by the SVD, \(\theta = USVH\). Without a mixer just the singular values, with enabled mixer a 2D array.

sweep(optimize=True, meas_E_trunc=False)
One ‘sweep’ of the algorithm.
Iterate over the bond which is optimized, to the right and then back to the left to the starting point.

Parameters
- optimize (bool, optional) – Whether we actually optimize to find the ground state of the effective Hamiltonian. (If False, just update the environments).
**meas_E_trunc**(bool, *optional*) – Whether to measure truncation energies.

**Returns**

- **max_trunc_err** (*float*) – Maximal truncation error introduced.
- **max_E_trunc** (*None | float*) – None if meas_E_trunc is False, else the maximal change of the energy due to the truncation.

**update_LP**(U)

Update left part of the environment.

We always update the environment at site i0 + 1: this environment then contains the site where we just performed a local update (when sweeping right).

**Parameters**

- **U** (*Array*) – The U as returned by the SVD, with combined legs, labels 'vL', 'p0', 'vR'.

**update_RP**(VH)

Update right part of the environment.

We always update the environment at site i0: this environment then contains the site where we just performed a local update (when sweeping left).

**Parameters**

- **VH** (*Array*) – The VH as returned by SVD, with combined legs, labels 'vL', '(vR.p1)'.

**update_local**(theta, optimize=True)

Perform site-update on the site i0.

**Parameters**

- **theta** (*Array*) – Initial guess for the ground state of the effective Hamiltonian.
- **optimize** (*bool*) – Whether we actually optimize to find the ground state of the effective Hamiltonian. (If False, just update the environments).

**Returns**

**update_data** – Data computed during the local update, as described in the following:

- **E0** (*float*) – Total energy, obtained before truncation (if optimize=True), or after truncation (if optimize=False) (but never None).
- **N** (*int*) – Dimension of the Krylov space used for optimization in the lanczos algorithm. 0 if optimize=False.
- **age** (*int*) – Current size of the DMRG simulation: number of physical sites involved into the contraction.

**U**, **VH**: *Array* U and VH returned by mixed_svd().

**ov_change**: *float* – Change in the wave function \(1 - \text{abs}(<\text{theta}_\text{guess}|\theta>)\) induced by diag(), not including the truncation!

**Return type** *dict*
EngineFracture

- full name: tenpy.algorithms.dmrg.EngineFracture
- parent module: tenpy.algorithms.dmrg
- type: class

Inheritance Diagram

```
DMRGEngine
   ▼
   |  TwoSiteDMRGEngine
   |  ▼
   |   EngineFracture
```

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<table>
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</tr>
<tr>
<td><code>EngineFracture.environment_sweeps(N_sweeps)</code></td>
<td>Perform $N_sweeps$ sweeps without optimization to update the environment.</td>
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<td>Define the schedule of the sweep.</td>
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<td>Set <code>self.mixer</code> to the class specified by <code>options['mixer']</code>.</td>
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<td>Cleanup the effects of a mixer.</td>
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</tr>
</tbody>
</table>

continues on next page
Table 20 – continued from previous page

<table>
<thead>
<tr>
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</thead>
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<td>One ‘sweep’ of a the algorithm.</td>
</tr>
<tr>
<td>EngineFracture.update_LP(U)</td>
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</tr>
<tr>
<td>EngineFracture.update_RP(VH)</td>
<td>Update right part of the environment.</td>
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<tr>
<td>EngineFracture.update_local(theta[, optimize])</td>
<td>Perform site-update on the site i0.</td>
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</tbody>
</table>

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<table>
<thead>
<tr>
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<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>EngineFracture.DMRG_params</td>
<td></td>
</tr>
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<td></td>
</tr>
<tr>
<td>EngineFracture.n_optimize</td>
<td>the number of sites to be optimized over at once.</td>
</tr>
</tbody>
</table>

class tenpy.algorithms.dmrq.EngineFracture(psi, model, DMRG_params)
Bases: tenpy.algorithms.dmrq.TwoSiteDMRGEngine

Engine which keeps the legs separate.

Due to a different contraction order in matvec(), this engine might be faster than EngineCombine, at least for large physical dimensions and if the MPO is sparse. One matvec() is $O(2\chi^3d^2W + 2\chi^2d^3W^2)$.

Deprecated since version 0.5.0: Directly use the TwoSiteDMRGEngine with the DMRG parameter combine=False.

DefaultMixer
 alias of DensityMatrixMixer

EffectiveH
 alias of tenpy.algorithms.mps_common.TwoSiteH

diag(theta_guess)
 Diagonalize the effective Hamiltonian represented by self.

option DMRGEngine.max_N_for_ED: int
 Maximum matrix dimension of the effective hamiltonian up to which the 'default' diag_method uses ED instead of Lanczos.

option DMRGEngine.diag_method: str
 One of the following strings:
 ‘default’ Same as 'lanczos' for large bond dimensions, but if the total dimension of the effective Hamiltonian does not exceed the DMRG parameter 'max_N_for_ED' it uses 'ED_block'.
 ‘lanczos’ lanczos() Default, the Lanczos implementation in TeNPy.
‘arpack’ *lanczos_arpack()* Based on *scipy.linalg.sparse.eigsh()*(). Slower than ‘lanczos’, since it needs to convert the *npc* arrays to *numpy* arrays during *each* matvec, and possibly does many more iterations.

‘ED_block’ *full_diag_effH()* Contract the effective Hamiltonian to a (large!) matrix and diagonalize the block in the charge sector of the initial state. Preserves the charge sector of the explicitly conserved charges. However, if you don’t preserve a charge explicitly, it can break it. For example if you use a *SpinChain*({‘conserve’: ’parity’}), it could change the total “Sz”, but not the parity of “Sz”.

‘ED_all’ *full_diag_effH()* Contract the effective Hamiltonian to a (large!) matrix and diagonalize it completely. Allows to change the charge sector *even for explicitly conserved charges*. For example if you use a *SpinChain*({‘conserve’: ’Sz’}), it *can* change the total “Sz”.

**Parameters**

**theta_guess** (*Array*) – Initial guess for the ground state of the effective Hamiltonian.

**Returns**

- **E0** (*float*) – Energy of the found ground state.
- **theta** (*Array*) – Ground state of the effective Hamiltonian.
- **N** (*int*) – Number of Lanczos iterations used. -1 if unknown.
- **ov_change** (*float*) – Change in the wave function 1. - abs(<theta_guess|theta_diag>)

**environment_sweeps** (*N_sweeps*)

Perform *N_sweeps* sweeps without optimization to update the environment.

**Parameters**

**N_sweeps** (*int*) – Number of sweeps to run without optimization

**get_sweep_schedule**()

Define the schedule of the sweep.

One ‘sweep’ is a full sequence from the leftmost site to the right and back. Only those *LP* and *RP* that can be used later should be updated.

**Returns**

**schedule** – Schedule for the sweep. Each entry is (*i0*, move_right, (update_LP, update_RP)), where *i0* is the leftmost of the self.EffectiveH. length sites to be updated in *update_local()*, move_right indicates whether the next *i0* in the schedule is rigth (*True*) of the current one, and *update_LP*, *update_RP* indicate whether it is necessary to update the *LP* and *RP*. The latter are chosen such that the environment is growing for infinite systems, but we only keep the minimal number of environment tensors in memory.

**Return type** iterable of (*int*, bool, (bool, bool))

**init_env** (*model=None*)

(Re-)initialize the environment.

This function is useful to (re-)start a Sweep with a slightly different model or different (engine) parameters. Note that we assume that we still have the same *psi*. Calls *reset_stats()*.

**Parameters**

**model** (*MPOModel*) – The model representing the Hamiltonian for which we want to find the ground state. If *None*, keep the model used before.
Options

Deprecated since version 0.6.0: Options LP, LP_age, RP and RP_age are now collected in a dictionary init_env_data with different keys init_LP, init_RP, age_LP, age_RP

option Sweep.init_env_data: dict
Dictionary as returned by self.env.get_initialization_data() from get_initialization_data().

option Sweep.orthogonal_to: list of MPS
List of other matrix product states to orthogonalize against. Works only for finite systems. This parameter can be used to find (a few) excited states as follows. First, run DMRG to find the ground state and then run DMRG again while orthogonalizing against the ground state, which yields the first excited state (in the same symmetry sector), and so on.

option Sweep.start_env: int
Number of sweeps to be performed without optimization to update the environment.

Raises ValueError – If the engine is re-initialized with a new model, which legs are incompatible with those of the old model.

make_eff_H()
Create new instance of self.EffectiveH at self.i0 and set it to self.eff_H.

mixed_svd(theta)
Get (truncated) B from the new theta (as returned by diag).

The goal is to split theta and truncate it:

| -- theta -- ==> -- U -- S -- VH -- |
| | | | | | | |

Without a mixer, this is done by a simple svd and truncation of Schmidt values.

With a mixer, the state is perturbed before the SVD. The details of the perturbation are defined by the Mixer class.

Note that the returned S is a general (not diagonal) matrix, with labels 'vL', 'vR'.

Parameters theta (Array) – The optimized wave function, prepared for svd.

Returns

• U (Array) – Left-canonical part of theta. Labels '(vL.p0)', 'vR'.

• S (1D ndarray | 2D Array) – Without mixer just the singular values of the array; with mixer it might be a general matrix with labels 'vL', 'vR'; see comment above.

• VH (Array) – Right-canonical part of theta. Labels 'vL', '(p1.vR)'.

• err (TruncationError) – The truncation error introduced.

mixer_activate()
Set self.mixer to the class specified by options['mixer'].

option TwoSiteDMRGEngine.mixer: str | class | bool
Chooses the Mixer to be used. A string stands for one of the mixers defined in this module, a class is used as custom mixer. Default (None) uses no mixer, True uses DensityMatrixMixer for the 2-site case and SingleSiteMixer for the 1-site case.

option TwoSiteDMRGEngine.mixer_params: dict
Mixer parameters as described in Mixer.
mixer_cleanup()
Cleanup the effects of a mixer.

A sweep() with an enabled Mixer leaves the MPS psi with 2D arrays in S. To recover the original form, this function simply performs one sweep with disabled mixer.

property n_optimize
the number of sites to be optimized over at once.

Indirectly set by the class attribute EffectiveH and its length. For example, TwoSiteDMRGEngine uses the TwoSiteH and hence has n_optimize=2, while the SingleSiteDMRGEngine has n_optimize=1.

plot_sweep_stats(axes=None, xaxis='time', yaxis='E', y_exact=None, **kwargs)
Plot sweep_stats to display the convergence with the sweeps.

Parameters
• axes (matplotlib.axes.Axes) – The axes to plot into. Defaults to matplotlib.pyplot.gca().
• xaxis (key of sweep_stats) – Key of sweep_stats to be used for the x-axis and y-axis of the plots.
• yaxis (key of sweep_stats) – Key of sweep_stats to be used for the x-axis and y-axis of the plots.
• y_exact (float) – Exact value for the quantity on the y-axis for comparison. If given, plot abs((y-y_exact)/y_exact) on a log-scale yaxis.
• **kwargs – Further keyword arguments given to axes.plot(...).

plot_update_stats(axes, xaxis='time', yaxis='E', y_exact=None, **kwargs)
Plot update_stats to display the convergence during the sweeps.

Parameters
• axes (matplotlib.axes.Axes) – The axes to plot into. Defaults to matplotlib.pyplot.gca().
• xaxis ('N_updates' | 'sweep' | keys of update_stats) – Key of update_stats to be used for the x-axis of the plots. 'N_updates' is just enumerating the number of bond updates, and 'sweep' corresponds to the sweep number (including environment sweeps).
• yaxis ('E' | keys of update_stats) – Key of update_stats to be used for the y-axis of the plots. For 'E', use the energy (per site for infinite systems).
• y_exact (float) – Exact value for the quantity on the y-axis for comparison. If given, plot abs((y-y_exact)/y_exact) on a log-scale yaxis.
• **kwargs – Further keyword arguments given to axes.plot(...).

post_update_local(update_data)
Perform post-update actions.

Compute truncation energy, remove LP/RP that are no longer needed and collect statistics.

Parameters update_data (dict) – What was returned by update_local().

prepare_svd(theta)
Transform theta into matrix for svd.

prepare_update()
Prepare self for calling update_local() on sites i0 : i0+n_optimize.
Returns **theta** – Current best guess for the ground state, which is to be optimized. Labels are 'vL', 'p0', 'p1', 'vR', or combined versions of it (if *self.combine*). For single-site DMRG, the 'p1' label is missing.

Return type *Array*

**reset_stats()**
Reset the statistics, useful if you want to start a new sweep run.

**option** DMRGEngine.chi_list: *dict | None*
A dictionary to gradually increase the *chi_max* parameter of *trunc_params*. The key defines starting from which sweep *chi_max* is set to the value, e.g. {0: 50, 20: 100} uses *chi_max*=50 for the first 20 sweeps and *chi_max*=100 afterwards. Overwrites *trunc_params['chi_list']*. By default (None) this feature is disabled.

**option** DMRGEngine.sweep_0: *int*
The number of sweeps already performed. (Useful for re-start).

**run()**
Run the DMRG simulation to find the ground state.

**Returns**

- **E** (*float*) – The energy of the resulting ground state MPS.
- **psi** (*MPS*) – The MPS representing the ground state after the simulation, i.e. just a reference to *psi*.

**Options**

**option** DMRGEngine.diag_method: *str*
Method to be used for diagonalization, default 'default'. For possible arguments see DMRGEngine.diag().

**option** DMRGEngine.E_tol_to_trunc: *float*
It's reasonable to choose the Lanczos convergence criteria 'E_tol' not many magnitudes lower than the current truncation error. Therefore, if *E_tol_to_trunc* is not None, we update *E_tol* of *lanczos_params* to max_E_trunc*E_tol_to_trunc*, restricted to the interval [E_tol_min, E_tol_max], where max_E_trunc is the maximal energy difference due to truncation right after each Lanczos optimization during the sweeps.

**option** DMRGEngine.E_tol_max: *float*
See *E_tol_to_trunc*

**option** DMRGEngine.E_tol_min: *float*
See *E_tol_to_trunc*

**option** DMRGEngine.max_E_err: *float*
Convergence if the change of the energy in each step satisfies - Delta E / max(|E|, 1) < max_E_err. Note that this is also satisfied if Delta E > 0, i.e., if the energy increases (due to truncation).

**option** DMRGEngine.max_hours: *float*
If the DMRG took longer (measured in wall-clock time), 'shelve' the simulation, i.e. stop and return with the flag *shelve=True*.

**option** DMRGEngine.max_S_err: *float*
Convergence if the relative change of the entropy in each step satisfies |Delta S|/S < max_S_err
option DMRGEngine.max_sweeps: int
Maximum number of sweeps to be performed.

option DMRGEngine.min_sweeps: int
Minimum number of sweeps to be performed. Defaults to 1.5*N_sweeps_check.

option DMRGEngine.N_sweeps_check: int
Number of sweeps to perform between checking convergence criteria and giving a status update.

option DMRGEngine.norm_tol: float
After the DMRG run, update the environment with at most norm_tol_iter sweeps until np.linalg.
norm(psi.norm_err()) < norm_tol.

option DMRGEngine.norm_tol_iter: float
Perform at most norm_tol_iter*update_env sweeps to converge the norm error below norm_tol. If
the state is not converged after that, call canonical_form() instead.

option DMRGEngine.P_tol_to_trunc: float
It's reasonable to choose the Lanczos convergence criteria 'P_tol' not many magnitudes lower
than the current truncation error. Therefore, if P_tol_to_trunc is not None, we update P_tol of
lanczos_params to max_trunc_err*P_tol_to_trunc, restricted to the interval [P_tol_min,
P_tol_max], where max_trunc_err is the maximal truncation error (discarded weight of the
Schmidt values) due to truncation right after each Lanczos optimization during the sweeps.

option DMRGEngine.P_tol_max: float
See P_tol_to_trunc

option DMRGEngine.P_tol_min: float
See P_tol_to_trunc

option DMRGEngine.update_env: int
Number of sweeps without bond optimization to update the environment for infinite boundary condi-
tions, performed every N_sweeps_check sweeps.

set_B(U, S, VH)
Update the MPS with the U, S, VH returned by self.mixed_svd.

Parameters

• U (Array) – Left and Right-canonical matrices as returned by the SVD.

• VH (Array) – Left and Right-canonical matrices as returned by the SVD.

• S (1D array | 2D Array) – The middle part returned by the SVD, theta = U S VH.
Without a mixer just the singular values, with enabled mixer a 2D array.

sweep(optimizer=True, meas_E_trunc=False)
One 'sweep' of a the algorithm.

Iterate over the bond which is optimized, to the right and then back to the left to the starting point.

Parameters

• optimize (bool, optional) – Whether we actually optimize to find the ground
state of the effective Hamiltonian. (If False, just update the environments).

• meas_E_trunc (bool, optional) – Whether to measure truncation energies.

Returns

• max_trunc_err (float) – Maximal truncation error introduced.

• max_E_trunc (None | float) – None if meas_E_trunc is False, else the maximal change
of the energy due to the truncation.
update_LP ($U$)
Update left part of the environment.

We always update the environment at site $i_0 + 1$: this environment then contains the site where we just performed a local update (when sweeping right).

**Parameters** $U$ (Array) – The $U$ as returned by the SVD, with combined legs, labels 'vL', 'p0', 'vR'.

update_RP ($VH$)
Update right part of the environment.

We always update the environment at site $i_0$: this environment then contains the site where we just performed a local update (when sweeping left).

**Parameters** $VH$ (Array) – The VH as returned by SVD, with combined legs, labels 'vL', '(vR.p1)'.

update_local ($theta$, optimize=True)
Perform site-update on the site $i_0$.

**Parameters**
- $theta$ (Array) – Initial guess for the ground state of the effective Hamiltonian.
- optimize (bool) – Whether we actually optimize to find the ground state of the effective Hamiltonian. (If False, just update the environments).

**Returns**

update_data – Data computed during the local update, as described in the following:

- $E_0$ [float] Total energy, obtained before truncation (if optimize=True), or after truncation (if optimize=False) but never None.
- $N$ [int] Dimension of the Krylov space used for optimization in the lanczos algorithm. 0 if optimize=False.
- $age$ [int] Current size of the DMRG simulation: number of physical sites involved into the contraction.

$U$, $VH$: Array $U$ and $VH$ returned by mixed_svd().

$ov_change$: float Change in the wave function $1. - abs(<theta_guess|theta>)$ induced by $diag()$, not including the truncation!

**Return type** dict

SingleSiteMixer

- full name: tenpy.algorithms.dmrg.SingleSiteMixer
- parent module: tenpy.algorithms.dmrg
- type: class
Inheritance Diagram

```
Mixer
↓
SingleSiteMixer
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>SingleSiteMixer.__init__(options)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>SingleSiteMixer.perturb_svd(engine, theta, ...)</code></td>
<td>Mix extra terms to theta and perform an SVD.</td>
</tr>
<tr>
<td><code>SingleSiteMixer.subspace_expand(engine, ...)</code></td>
<td>Expand the MPS subspace, to allow the bond dimension to increase.</td>
</tr>
<tr>
<td><code>SingleSiteMixer.update_amplitude(sweeps)</code></td>
<td>Update the amplitude, possibly disable the mixer.</td>
</tr>
</tbody>
</table>

```python
class tenpy.algorithms.dmrg.SingleSiteMixer( options )
    Bases: tenpy.algorithms.dmrg.Mixer
```

Mixer for single-site DMRG.

Performs a subspace expansion following [hubig2015].

**perturb_svd**(engine, theta, i0, move_right, next_B)
Mix extra terms to theta and perform an SVD.

We calculate the left and right reduced density matrix using the mixer (which might include applications of $H$). These density matrices are diagonalized and truncated such that we effectively perform a svd for the case mixer.amplitude=0.

**Parameters**

- **engine**(Engine) – The DMRG engine calling the mixer.
- **theta**(Array) – The optimized wave function, prepared for svd.
- **i0**(int) – The site index where theta lives.
- **move_right**(bool) – Whether we move to the right (True) or left (False).
- **next_B**(Array) – The subspace expansion requires to change the tensor on the next site as well. If move_right, it should correspond to engine.psi.get_B(i0+1, form='B'). If not move_right, it should correspond to engine.psi.get_B(i0-1, form='A').

**Returns**
• **U (Array)** – Left-canonical part of `tensordot(theta, next_B)`. Labels 'vL.p0', 'vR'.
• **S (1D ndarray)** – (Perturbed) singular values on the new bond (between `theta` and `next_B`).
• **VH (Array)** – Right-canonical part of `tensordot(theta, next_B)`. Labels 'vL', '(p1. vR)'.
• **err (TruncationError)** – The truncation error introduced.

**subspace_expand (engine, theta, i0, move_right, next_B)**
Expand the MPS subspace, to allow the bond dimension to increase.

This is the subspace expansion following [hubig2015].

**Parameters**

- **engine** *(SingleSiteDMRGEngine | TwoSiteDMRGEngine)* – ‘Engine’ for the DMRG algorithm
- **theta** *(Array)* – Optimized guess for the ground state of the effective local Hamiltonian.
- **i0** *(int)* – Site index at which the local update has taken place.
- **move_right** *(bool)* – Whether the next `i0` of the sweep will be right or left of the current one.
- **next_B** *(Array)* – The subspace expansion requires to change the tensor on the next site as well. If `move_right`, it should correspond to `engine.psi.get_B(i0+1, form='B')`. If not `move_right`, it should correspond to `engine.psi.get_B(i0-1, form='A')`.

**Returns**

- **theta** – Local MPS tensor at site `i0` after subspace expansion.
- **next_B** – MPS tensor at site `i0+1` or `i0-1` (depending on sweep direction) after subspace expansion.

**update_amplitude (sweeps)**
Update the amplitude, possibly disable the mixer.

**Parameters** **sweeps** *(int)* – The number of performed sweeps, to check if we need to disable the mixer.

**Returns** **mixer** – Returns `self` if we should continue mixing, or `None`, if the mixer should be disabled.

**Return type** **Mixer | None**

**TwoSiteMixer**

- full name: `tenpy.algorithms.dmrgr.TwoSiteMixer`
- parent module: `tenpy.algorithms.dmrgr`
- type: class
Inheritance Diagram

```
Mixer
  ↓
SingleSiteMixer
  ↓
TwoSiteMixer
```

Methods

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<tr>
<td><code>TwoSiteMixer.__init__(options)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>TwoSiteMixer.perturb_svd(engine, theta, i0, ...)</code></td>
<td>Mix extra terms to theta and perform an SVD.</td>
</tr>
<tr>
<td><code>TwoSiteMixer.subspace_expand(engine, theta, ...)</code></td>
<td>Expand the MPS subspace, to allow the bond dimension to increase.</td>
</tr>
<tr>
<td><code>TwoSiteMixer.update_amplitude(sweeps)</code></td>
<td>Update the amplitude, possibly disable the mixer.</td>
</tr>
</tbody>
</table>

```python
class tenpy.algorithms.dmrg.TwoSiteMixer(options)
    Bases: tenpy.algorithms.dmrg.SingleSiteMixer

    Mixer for two-site DMRG.

    This is the two-site version of the mixer described in [hubig2015]. Equivalent to the DensityMatrixMixer, but never construct the full density matrix.

    **perturb_svd** (engine, theta, i0, move_right)
    Mix extra terms to theta and perform an SVD.

    Parameters
    - **engine** *(Engine)* – The DMRG engine calling the mixer.
    - **theta** *(Array)* – The optimized wave function, prepared for svd.
    - **i0** *(int)* – Site index; theta lives on i0, i0+1.
    - **update_LP** *(bool)* – Whether to calculate the next env.LP[i0+1].
    - **update_RP** *(bool)* – Whether to calculate the next env.RP[i0].

    Returns
    - **U** *(Array)* – Left-canonical part of theta. Labels '(vL.p0)', 'vR'.
```
• \texttt{S} (1D \texttt{ndarray} | 2D \texttt{Array}) – Without mixer just the singular values of the array; with mixer it might be a general matrix; see comment above.

• \texttt{VH} (\texttt{Array}) – Right-canonical part of \textit{theta}. Labels 'vL', '(vR.p1)'.

• \texttt{err} (\texttt{TruncationError}) – The truncation error introduced.

\texttt{subspace\_expand} \texttt{(engine, theta, i0, move\_right, next\_B)}

Expand the MPS subspace, to allow the bond dimension to increase.

This is the subspace expansion following [hubig2015].

Parameters

• \texttt{engine} (\texttt{SingleSiteDMRGEngine} | \texttt{TwoSiteDMRGEngine}) – ‘Engine’ for the DMRG algorithm.

• \texttt{theta} (\texttt{Array}) – Optimized guess for the ground state of the effective local Hamiltonian.

• \texttt{i0} (\texttt{int}) – Site index at which the local update has taken place.

• \texttt{move\_right} (\texttt{bool}) – Whether the next \texttt{i0} of the sweep will be right or left of the current one.

• \texttt{next\_B} (\texttt{Array}) – The subspace expansion requires to change the tensor on the next site as well. If move\_right, it should correspond to \texttt{engine.psi.get\_B(i0+1, form='B')} . If not move\_right, it should correspond to \texttt{engine.psi.get\_B(i0-1, form='A')}. 

Returns

• \texttt{theta} – Local MPS tensor at site \texttt{i0} after subspace expansion.

• \texttt{next\_B} – MPS tensor at site \texttt{i0+1} or \texttt{i0-1} (depending on sweep direction) after subspace expansion.

\texttt{update\_amplitude(sweeps)}

Update the amplitude, possibly disable the mixer.

Parameters \texttt{sweeps} (\texttt{int}) – The number of performed sweeps, to check if we need to disable the mixer.

Returns \texttt{mixer} – Returns \texttt{self} if we should continue mixing, or \texttt{None}, if the mixer should be disabled.

Return type \texttt{Mixer} | \texttt{None}

\textbf{Functions}

\begin{itemize}
  \item \texttt{chi\_list(chi\_max[, dchi, nsweeps])} \: \: \text{Compute a ‘ramping-up’ chi\_list.}
  \item \texttt{full\_diag\_effH(effH, theta\_guess[, keep\_sector])} \: \: \text{Perform an exact diagonalization of effH.}
  \item \texttt{run(psi, model, options)} \: \: \text{Run the DMRG algorithm to find the ground state of the given model.}
\end{itemize}
chi_list

• full name: tenpy.algorithms.dmrg.chi_list
• parent module: tenpy.algorithms.dmrg
• type: function
tenpy.algorithms.dmrg.chi_list(chi_max, dchi=20, nsweeps=20)

Compute a ‘ramping-up’ chi_list.

The resulting chi_list allows to increases chi by dchi every nsweeps sweeps up to a given maximal chi_max.

Parameters

• chi_max (int) – Final value for the bond dimension.
• dchi (int) – Step size how to increase chi
• nsweeps (int) – Step size for sweeps

Returns chi_list – To be used as chi_list parameter for DMRG, see run(). Keys increase by nsweeps, values by dchi, until a maximum of chi_max is reached.

Return type dict

full_diag_effH

• full name: tenpy.algorithms.dmrg.full_diag_effH
• parent module: tenpy.algorithms.dmrg
• type: function
tenpy.algorithms.dmrg.full_diag_effH(effH, theta_guess, keep_sector=True)

Perform an exact diagonalization of effH.

This function offers an alternative to lanczos().

Parameters

• effH (EffectiveH) – The effective Hamiltonian.
• theta_guess (Array) – Current guess to select the charge sector. Labels as specified by effH.acts_on.

Module description

Density Matrix Renormalization Group (DMRG).

Although it was originally not formulated with tensor networks, the DMRG algorithm (invented by Steven White in 1992 [white1992]) opened the whole field with its enormous success in finding ground states in 1D.

We implement DMRG in the modern formulation of matrix product states [schollwoeck2011], both for finite systems ('finite' or 'segment' boundary conditions) and in the thermodynamic limit ('infinite' b.c.).

The function run() - well - runs one DMRG simulation. Internally, it generates an instance of an Sweep. This class implements the common functionality like defining a sweep, but leaves the details of the contractions to be performed to the derived classes.

Currently, there are two derived classes implementing the contractions: SingleSiteDMRGEngine and TwoSiteDMRGEngine. They differ (as their name implies) in the number of sites which are optimized simultaneously. They should both give the same results (up to rounding errors). However, if started from a product state,
SingleSiteDMRGEngine depends critically on the use of a Mixer, while TwoSiteDMRGEngine is in principle more computationally expensive to run and has occasionally displayed some convergence issues. Which one is preferred in the end is not obvious a priori and might depend on the used model. Just try both of them.

A Mixer should be used initially to avoid that the algorithm gets stuck in local energy minima, and then slowly turned off in the end. For SingleSiteDMRGEngine, using a mixer is crucial, as the one-site algorithm cannot increase the MPS bond dimension by itself.

A generic protocol for approaching a physics question using DMRG is given in Protocol for using (i)DMRG.

7.9.5 tdvp

- full name: tenpy.algorithms.tdvp
- parent module: tenpy.algorithms
- type: module

Classes

| Engine(psi, model, options[, environment]) | Time dependent variational principle ‘Engine’. |
| H0_mixed(Lp, Rp) | Class defining the zero site Hamiltonian for Lanczos. |
| H1_mixed(Lp, Rp, W) | Class defining the one site Hamiltonian for Lanczos. |
| H2_mixed(Lp, Rp, W0, W1) | Class defining the two sites Hamiltonian for Lanczos. |

H0_mixed

- full name: tenpy.algorithms.tdvp.H0_mixed
- parent module: tenpy.algorithms.tdvp
- type: class

Inheritance Diagram

H0_mixed
Methods

H0_mixed.__init__(Lp, Rp) Initialize self.
H0_mixed.matvec(x)

class tenpy.algorithms.tdvp.H0_mixed(Lp, Rp)
    Bases: object
    Class defining the zero site Hamiltonian for Lanczos.
    Parameters
    • Lp (tenpy.linalg.np_conserved.Array) – left part of the environment
    • Rp (tenpy.linalg.np_conserved.Array) – right part of the environment
    Lp  left part of the environment
    Type  tenpy.linalg.np_conserved.Array
    Rp  right part of the environment
    Type  tenpy.linalg.np_conserved.Array

H1_mixed

• full name: tenpy.algorithms.tdvp.H1_mixed
• parent module: tenpy.algorithms.tdvp
• type: class

Inheritance Diagram

Methods

H1_mixed.__init__(Lp, Rp, W) Initialize self.
H1_mixed.matvec(theta)

class tenpy.algorithms.tdvp.H1_mixed(Lp, Rp, W)
    Bases: object
    Class defining the one site Hamiltonian for Lanczos.

7.9. algorithms
Parameters

- \( L_p \) (\texttt{tenpy.linalg.np_conserved.Array}) – left part of the environment
- \( R_p \) (\texttt{tenpy.linalg.np_conserved.Array}) – right part of the environment
- \( M \) (\texttt{tenpy.linalg.np_conserved.Array}) – MPO which is applied to the ‘p’ leg of theta

\( L_p \)
left part of the environment

\text{Type} \ \texttt{tenpy.linalg.np_conserved.Array}

\( R_p \)
right part of the environment

\text{Type} \ \texttt{tenpy.linalg.np_conserved.Array}

\( W \)
MPO which is applied to the ‘p0’ leg of theta

\text{Type} \ \texttt{tenpy.linalg.np_conserved.Array}

**H2\_mixed**

- full name: \texttt{tenpy.algorithms.tdvp.H2\_mixed}
- parent module: \texttt{tenpy.algorithms.tdvp}
- type: class

**Inheritance Diagram**

```
H2_mixed
```

**Methods**

```python
H2_mixed.__init__ (Lp, Rp, W0, W1) Initialize self.
H2_mixed.matvec(theta)
```

**class** \texttt{tenpy.algorithms.tdvp.H2\_mixed}(\texttt{Lp, Rp, W0, W1})

Bases: \texttt{object}

Class defining the two sites Hamiltonian for Lanczos.

**Parameters**

- \( L_p \) (\texttt{tenpy.linalg.np_conserved.Array}) – left part of the environment
Module description

Time Dependant Variational Principle (TDVP) with MPS (finite version only).

The TDVP MPS algorithm was first proposed by [haegeman2011]. However the stability of the algorithm was later improved in [haegeman2016], that we are following in this implementation. The general idea of the algorithm is to project the quantum time evolution in the manifolds of MPS with a given bond dimension. Compared to e.g. TEBD, the algorithm has several advantages: e.g. it conserves the unitarity of the time evolution and the energy (for the single-site version), and it is suitable for time evolution of Hamiltonian with arbitrary long range in the form of MPOs. We have implemented the one-site formulation which does not allow for growth of the bond dimension, and the two-site algorithm which does allow the bond dimension to grow - but requires truncation as in the TEBD case.

Todo: This is still a beta version, use with care. The interface might still change.

Todo: long-term: Much of the code is similar as in DMRG. To avoid too much duplicated code, we should have a general way to sweep through an MPS and updated one or two sites, used in both cases.

7.9.6 purification

- full name: tenpy.algorithms.purification
- parent module: tenpy.algorithms
- type: module
Classes

```
NpcLinearOperator
  |      |
  |      |
EffectiveH
  |      |
  |      |
TwoSiteH
  |      |
PurificationTwoSiteU

Engine
  |      |
PurificationTEBD
  |      |
PurificationTEBD2
  |      |
PurificationTwoSiteU

Sweep
  |      |
VariationalCompression
  |      |
VariationalApplyMPO
  |      |
PurificationApplyMPO
```

### PurificationApplyMPO

- **full name:** `tenpy.algorithms.purification.PurificationApplyMPO`
- **parent module:** `tenpy.algorithms.purification`
- **type:** class

#### PurificationApplyMPO

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>PurificationApplyMPO(\psi, U_MPO, options)</code></td>
<td>Variant of <code>VariationalApplyMPO</code> suitable for purification.</td>
</tr>
<tr>
<td><code>PurificationTEBD(\psi, model, options)</code></td>
<td>Time evolving block decimation (TEBD) for purification MPS.</td>
</tr>
<tr>
<td><code>PurificationTEBD2(\psi, model, options)</code></td>
<td>Similar as PurificationTEBD, but perform sweeps instead of brickwall.</td>
</tr>
<tr>
<td><code>PurificationTwoSiteU(env, i0[, combine, ...])</code></td>
<td>Variant of <code>TwoSiteH</code> suitable for purification.</td>
</tr>
</tbody>
</table>
PurificationApplyMPO
VariationalApplyMPO
Sweep
VariationalCompression

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>__init__</code>(psi, U_MPO,...)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>environment_sweeps</code>(N_sweeps)</td>
<td>Perform $N_{sweeps}$ sweeps without optimization to update the environment.</td>
</tr>
<tr>
<td><code>get_sweep_schedule()</code></td>
<td>Define the schedule of the sweep.</td>
</tr>
<tr>
<td><code>init_env</code>(U_MPO)</td>
<td>Initialize the environment.</td>
</tr>
<tr>
<td><code>make_eff_H()</code></td>
<td>Create new instance of <code>self.EffectiveH</code> at <code>self.i0</code> and set it to <code>self.eff_H</code>.</td>
</tr>
<tr>
<td><code>post_update_local</code>(...)</td>
<td>Algorithm-specific actions to be taken after local update.</td>
</tr>
<tr>
<td><code>prepare_update()</code></td>
<td>Prepare everything algorithm-specific to perform a local update.</td>
</tr>
<tr>
<td><code>reset_stats()</code></td>
<td>Reset the statistics.</td>
</tr>
<tr>
<td><code>run()</code></td>
<td>Run the compression.</td>
</tr>
<tr>
<td><code>sweep</code>([optimize])</td>
<td>One ‘sweep’ of a sweeper algorithm.</td>
</tr>
<tr>
<td><code>update_LP()</code></td>
<td>Perform local update.</td>
</tr>
<tr>
<td><code>update_RP()</code></td>
<td></td>
</tr>
<tr>
<td><code>update_local</code>([, optimize])</td>
<td></td>
</tr>
<tr>
<td><code>update_new_psi</code>(theta)</td>
<td></td>
</tr>
</tbody>
</table>

7.9. algorithms
Class Attributes and Properties

| PurificationApplyMPO.engine_params | the number of sites to be optimized over at once. |

```python
class tenpy.algorithms.purification.PurificationApplyMPO(psi, U_MPO, options)
    Bases: tenpy.algorithms.mps_common.VariationalApplyMPO

    Variant of VariationalApplyMPO suitable for purification.

    EffectiveH
        alias of PurificationTwoSiteU

    update_local(_, optimize=True)
        Perform local update.

        This simply contracts the environments and theta from the ket to get an updated theta for the bra self.psi (to be changed in place).

    environment_sweeps(N_sweeps)
        Perform N_sweeps sweeps without optimization to update the environment.

        Parameters
            N_sweeps (int) – Number of sweeps to run without optimization

    get_sweep_schedule()
        Define the schedule of the sweep.

        One ‘sweep’ is a full sequence from the leftmost site to the right and back. Only those LP and RP that can be used later should be updated.

        Returns
            schedule – Schedule for the sweep. Each entry is (i0, move_right, (update_LP, update_RP)), where i0 is the leftmost of the self.EffectiveH.

            length sites to be updated in update_local(), move_right indicates whether the next i0 in the schedule is right (True) of the current one, and update_LP, update_RP indicate whether it is necessary to update the LP and RP. The latter are chosen such that the environment is growing for infinite systems, but we only keep the minimal number of environment tensors in memory.

            Return type
                iterable of (int, bool, (bool, bool))

    init_env(U_MPO)
        Initialize the environment.

        Parameters
            U_MPO (MPO) – The MPO to be applied to the sate.

    make_eff_H()
        Create new instance of self.EffectiveH at self.i0 and set it to self.eff_H.

    property n_optimize
        the number of sites to be optimized over at once.

        Indirectly set by the class attribute EffectiveH and it’s length. For example, TwoSiteDMRGEngine uses the TwoSiteH and hence has n_optimize=2, while the SingleSiteDMRGEngine has n_optimize=1.

    post_update_local(update_data)
        Algorithm-specific actions to be taken after local update.

        An example would be to collect statistics.

    prepare_update()
        Prepare everything algorithm-specific to perform a local update.
```

198 Chapter 7. License
**reset_stats()**
Reset the statistics. Useful if you want to start a new Sweep run.

This method is expected to be overwritten by subclass, and should then define self.update_stats and self.sweep_stats dicts consistent with the statistics generated by the algorithm particular to that subclass.

**option Sweep.sweep_0: int**
Number of sweeps that have already been performed.

**run()**
Run the compression.

The state \(\psi\) is compressed in place.

**Returns** \(\text{max_trunc_err}\) – The maximal truncation error of a two-site wave function.

**Return type** \(\text{TruncationError}\)

**sweep (optimize=True)**
One ‘sweep’ of a sweeper algorithm.

Iterate over the bond which is optimized, to the right and then back to the left to the starting point. If optimize=False, don’t actually diagonalize the effective hamiltonian, but only update the environment.

**Parameters**
- \(\text{optimize (bool, optional)}\) – Whether we actually optimize to find the ground state of the effective Hamiltonian. (If False, just update the environments).

**Returns** \(\text{max_trunc_err}\) – Maximal truncation error introduced.

**Return type** \(\text{float}\)

**PurificationTEBD**

- full name: tenpy.algorithms.purification.PurificationTEBD
- parent module: tenpy.algorithms.purification
- type: class

**Inheritance Diagram**

```
Engine
↓
PurificationTEBD
```
Methods

<table>
<thead>
<tr>
<th>Method Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PurificationTEBD.<strong>init</strong>(psi, model, options)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>PurificationTEBD.calc_U(order, delta_t[, ...])</td>
<td>See calc_U()</td>
</tr>
<tr>
<td>PurificationTEBD.disentangle(theta)</td>
<td>Disentangle theta before splitting with svd.</td>
</tr>
<tr>
<td>PurificationTEBD.disentangle_global([pair])</td>
<td>Try global disentangling by determining the maximally entangled pairs of sites.</td>
</tr>
<tr>
<td>PurificationTEBD.disentangle_global_nsite([n])</td>
<td>Perform a sweep through the system and disentangle with disentangle_n_site().</td>
</tr>
<tr>
<td>PurificationTEBD.disentangle_n_site(i, n, theta)</td>
<td>Generalization of disentangle() to n sites.</td>
</tr>
<tr>
<td>PurificationTEBD.run()</td>
<td>(Real-)time evolution with TEBD (time evolving block decimation).</td>
</tr>
<tr>
<td>PurificationTEBD.run_GS()</td>
<td>TEBD algorithm in imaginary time to find the ground state.</td>
</tr>
<tr>
<td>PurificationTEBD.run_imaginary(beta)</td>
<td>Run imaginary time evolution to cool down to the given beta.</td>
</tr>
<tr>
<td>PurificationTEBD.suzuki_trotter_decomposition(...)</td>
<td>Returns list of necessary steps for the suzuki trotter decomposition.</td>
</tr>
<tr>
<td>PurificationTEBD.suzuki_trotter_time_steps(order)</td>
<td>Return time steps of U for the Suzuki Trotter decomposition of desired order.</td>
</tr>
<tr>
<td>PurificationTEBD.update(N_steps)</td>
<td>Evolve by N_steps * U_param['dt'].</td>
</tr>
<tr>
<td>PurificationTEBD.update_bond(i, U_bond)</td>
<td>Updates the B matrices on a given bond.</td>
</tr>
<tr>
<td>PurificationTEBD.update_bond_imag(i, U_bond)</td>
<td>Update a bond with a (possibly non-unitary) U_bond.</td>
</tr>
<tr>
<td>PurificationTEBD.update_img(N_steps)</td>
<td>Perform an update suitable for imaginary time evolution.</td>
</tr>
<tr>
<td>PurificationTEBD.update_step(U_idx_dt, odd)</td>
<td>Updates either even or odd bonds in unit cell.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PurificationTEBD.TEBD_params</td>
<td>For each bond the total number of iterations performed in any Disentangler.</td>
</tr>
<tr>
<td>PurificationTEBD.disent_iterations</td>
<td>Truncation error introduced on each non-trivial bond.</td>
</tr>
<tr>
<td>PurificationTEBD.trunc_err_bonds</td>
<td></td>
</tr>
</tbody>
</table>

```python
class tenpy.algorithms.purification.PurificationTEBD(psi, model, options)
    Bases: tenpy.algorithms.tebd.Engine

Time evolving block decimation (TEBD) for purification MPS.

Deprecated since version 0.6.0: Renamed parameter/attribute TEBD_params to options.

Parameters

- psi (PurificationMPS) – Initial state to be time evolved. Modified in place.
- model (NearestNeighborModel) – The model representing the Hamiltonian for which we want to find the ground state.
- options (dict) – Further optional parameters as described in the following table. Use
```
verbose=1 to print the used parameters during runtime. See \texttt{run()} and \texttt{run\_GS()} for more details.

\textbf{used\_disentangler}

The disentangler to be used on the auxiliar indices. Chosen by \texttt{get\_disentangler()}, called with the TEBD parameter 'disentangle'. Defaults to the trivial disentangler for \texttt{options['disentangle']=None}.

\begin{itemize}
  \item \textbf{Type} Disentangler
\end{itemize}

\textbf{\_disent\_iterations}

Number of iterations performed on all bonds, including trivial bonds; length $L$.

\begin{itemize}
  \item \textbf{Type} 1D ndarray
\end{itemize}

\textbf{\_guess\_U\_disent}

Same index structure as \texttt{self\_U}: for each two-site $U$ of the physical time evolution the disentangler from the last application. Initialized to identities.

\begin{itemize}
  \item \textbf{Type} list of list of npc.Array
\end{itemize}

\textbf{run\_imaginary(beta)}

Run imaginary time evolution to cool down to the given $beta$.

Note that we don’t change the \texttt{norm} attribute of the MPS, i.e. normalization is preserved.

\begin{itemize}
  \item \textbf{Parameters} $beta$ (float) – The inverse temperature $beta = 1/T$, by which we should cool down. We evolve to the closest multiple of \texttt{options['dt']}, see also \texttt{evolved\_time}.
\end{itemize}

\textbf{property disent\_iterations}

For each bond the total number of iterations performed in any Disentangler.

\textbf{calc\_U(order, delta\_t, type\_evo='real', E\_offset=None)}

see \texttt{calc\_U()}

\textbf{update\_bond(i, U\_bond)}

Updates the B matrices on a given bond.

Function that updates the B matrices, the bond matrix $s$ between and the bond dimension $\chi$ for bond $i$. This would look something like:

\begin{verbatim}
| | | |
| ... - B1 - s - B2 - ... |
| | | |
| ----------- |
| | U |
| ----------- |
| | |
\end{verbatim}

\begin{itemize}
  \item \textbf{Parameters}
    \begin{itemize}
      \item i (int) – Bond index; we update the matrices at sites $i-1$, $i$.
      \item U\_bond (Array) – The bond operator which we apply to the wave function. We expect labels 'p0', 'p1', 'p0*', 'p1*' for \texttt{U\_bond}.
    \end{itemize}
  \end{itemize}

\textbf{Returns} trunc\_err – The error of the represented state which is introduced by the truncation during this update step.

\textbf{Return type} TruncationError
update_bond_imag \( (i, U_{\text{bond}}) \)

Update a bond with a (possibly non-unitary) \( U_{\text{bond}} \).

Similar as \( \text{update_bond()} \); but after the SVD just keep the \( A, S, B \) canonical form. In that way, one can sweep left or right without using old singular values, thus preserving the canonical form during imaginary time evolution.

**Parameters**

- \( i (\text{int}) \) – Bond index; we update the matrices at sites \( i-1, i \).
- \( U_{\text{bond}} (\text{Array}) \) – The bond operator which we apply to the wave function. We expect labels 'p0', 'p1', 'p0*', 'p1*'.

**Returns** \( \text{trunc_err} \) – The error of the represented state which is introduced by the truncation during this update step.

**Return type** \( \text{TruncationError} \)

disentangle \( (\theta) \)

Disentangle \( \theta \) before splitting with svd.

For the purification we write \( \rho_P = Tr_Q |\psi_{P,Q}><\psi_{P,Q}| \). Thus, we can actually apply any unitary to the auxiliar \( Q \) space of \( |\psi> \) without changing the result.

**Note:** We have to apply the same unitary to the ‘bra’ and ‘ket’ used for expectation values/correlation functions!

The behaviour of this function is set by \( \text{used_disentangler} \), which in turn is obtained from \( \text{get_disentangler(options['disentangle'])} \), see \( \text{get_disentangler()} \) for details on the syntax.

**Parameters** \( \theta (\text{Array}) \) – Wave function to disentangle, with legs 'vL', 'vR', 'p0', 'p1', 'q0', 'q1'.

**Returns**

- \( \theta_{\text{disentangled}} (\text{Array}) \) – Disentangled \( \theta \); \( \text{npc.tensordot}(U, \theta, \text{axes}=[[\text{'q0*'}, \text{'q1*'}], [\text{'q0'}, \text{'q1'}]]) \).
- \( U (\text{Array}) \) – The unitary used to disentangle \( \theta \), with labels 'q0', 'q1', 'q0*', 'q1*'. If no unitary was found/applied, it might also be None.

disentangle_global \( (\text{pair=None}) \)

Try global disentangling by determining the maximally entangled pairs of sites.

Caculate the mutual information (in the auxiliar space) between two sites and determine where it is maximal. Disentangle these two sites with \( \text{disentangle()} \)

disentangle_global_nsite \( (n=2) \)

Perform a sweep through the system and disentangle with \( \text{disentangle_n_site()} \). 

**Parameters** \( n (\text{int}) \) – maximal number of sites to disentangle at once.

disentangle_n_site \( (i, n, \theta) \)

Generalization of \( \text{disentangle()} \) to \( n \) sites.

Simply group left and right \( n/2 \) physical legs, adjust labels, and apply \( \text{disentangle()} \) to disentangle the central bond. Recursively proceed to disentangle left and right parts afterwards. Scales (for even \( n \)) as \( O(\chi^3 d^n d^{n/2}) \).
run()
(Real-)time evolution with TEBD (time evolving block decimation).

option TEBD.dt: float
Time step.

option TEBD.N_steps: int
Number of time steps \( dt \) to evolve. The Trotter decompositions of order > 1 are slightly more efficient if more than one step is performed at once.

option TEBD.order: int
Order of the algorithm. The total error scales as \( O(t^\cdot dt^{\cdot order}) \).

run_GS()
TEBD algorithm in imaginary time to find the ground state.

Note: It is almost always more efficient (and hence advisable) to use DMRG. This algorithms can nonetheless be used quite well as a benchmark and for comparison.

option TEBD.delta_tau_list: list
A list of floats: the timesteps to be used. Choosing a large timestep \( delta\_tau \) introduces large (Trotter) errors, but a too small time step requires a lot of steps to reach \( \exp(-\tau H) \rightarrow |\psi0><\psi0| \). Therefore, we start with fairly large time steps for a quick time evolution until convergence, and the gradually decrease the time step.

option TEBD.order: int
Order of the Suzuki-Trotter decomposition.

option TEBD.N_steps: int
Number of steps before measurement can be performed

static suzuki_trotter_decomposition(order, N_steps)
Returns list of necessary steps for the suzuki trotter decomposition.

We split the Hamiltonian as \( H = H_{even} + H_{odd} = H[0] + H[1] \). The Suzuki-Trotter decomposition is an approximation \( \exp(tH) \approx \prod_{(j,k) \in ST} \exp(d[j]tH[k]) + O(t^{\cdot order+1}) \).

Parameters

- order (1, 2, 4, '4_opt') – The desired order of the Suzuki-Trotter decomposition. Order 1 approximation is simply \( e^Ae^B \). Order 2 is the “leapfrog” \( e^{[A/2]}e^Be^{[A/2]} \). Order 4 is the fourth-order from [suzuki1991] (also referenced in [schollwoeck2011]), and '4_opt' gives the optimized version of Equ. (30a) in [barthel2020].

Returns ST_decomposition – Indices \( j, k \) of the time-steps \( d \) = suzuki_trotter_time_step(order) and the decomposition of \( H \). They are chosen such that a subsequent application of \( \exp(d[j] t H[k]) \) to a given state \( |\psi> \) yields \( \exp(N_{\cdot steps} t H[k]) + O(N_{\cdot steps} t^{\cdot (order+1)})|\psi> \).

Return type list of (int, int)

static suzuki_trotter_time_steps(order)
Return time steps of \( U \) for the Suzuki Trotter decomposition of desired order.

See suzuki_trotter_decomposition() for details.

Parameters

- order (int) – The desired order of the Suzuki-Trotter decomposition.

Returns time_steps – We need \( U = \exp(-i \cdot H_{\cdot (even/odd)} \cdot delta_t \cdot dt) \) for the \( dt \) returned in this list.

Return type list of float
property trunc_err_bonds
truncation error introduced on each non-trivial bond.

update (N_steps)
Evolve by N_steps * U_param['dt'].

Parameters N_steps (int) – The number of steps for which the whole lattice should be updated.

Returns trunc_err – The error of the represented state which is introduced due to the truncation during this sequence of update steps.

Return type TruncationError

update_imag (N_steps)
Perform an update suitable for imaginary time evolution.

Instead of the even/odd brick structure used for ordinary TEBD, we ‘sweep’ from left to right and right to left, similar as DMRG. Thanks to that, we are actually able to preserve the canonical form.

Parameters N_steps (int) – The number of steps for which the whole lattice should be updated.

Returns trunc_err – The error of the represented state which is introduced due to the truncation during this sequence of update steps.

Return type TruncationError

update_step (U_idx_dt, odd)
Updates either even or odd bonds in unit cell.

Depending on the choice of p, this function updates all even (E, odd=False,0) or odd (O) (odd=True,1) bonds:

```
| - B0 - B1 - B2 - B3 - B4 - B5 - B6 - |
| | | | | | | |
| | ---- | ---- | ---- | |
| | | E | | E | | E |
| | ---- | ---- | ---- | |
| ---- | ---- | ---- | ---- | |
| O | O | O | |
| ---- | ---- | ---- | |
```

Note that finite boundary conditions are taken care of by having Us[0] = None.

Parameters
• U_idx_dt (int) – Time step index in self._U, evolve with Us[i] = self._U[U_idx_dt][i] at bond (i-1,i).

• odd (bool/int) – Indication of whether to update even (odd=False,0) or even (odd=True,1) sites

Returns trunc_err – The error of the represented state which is introduced due to the truncation during this sequence of update steps.

Return type TruncationError
PurificationTEBD2

- full name: tenpy.algorithms.purification.PurificationTEBD2
- parent module: tenpy.algorithms.purification
- type: class

Inheritance Diagram

![Inheritance Diagram]

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PurificationTEBD2.<strong>init</strong>(psi, model, options)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>PurificationTEBD2.calc_U(order, delta_t[, ...])</td>
<td>see calc_U()</td>
</tr>
<tr>
<td>PurificationTEBD2.disentangle(theta)</td>
<td>Disentangle theta before splitting with svd.</td>
</tr>
<tr>
<td>PurificationTEBD2.disentangle_global([pair])</td>
<td>Try global disentangling by determining the maximally entangled pairs of sites.</td>
</tr>
<tr>
<td>PurificationTEBD2.disentangle_global_nsite(n)</td>
<td>Perform a sweep through the system and disentangle with disentangle_n_site().</td>
</tr>
<tr>
<td>PurificationTEBD2.disentangle_n_site(i, n, theta)</td>
<td>Generalization of disentangle() to n sites.</td>
</tr>
<tr>
<td>PurificationTEBD2.run()</td>
<td>(Real-)time evolution with TEBD (time evolving block decimation).</td>
</tr>
<tr>
<td>PurificationTEBD2.run_GS()</td>
<td>TEBD algorithm in imaginary time to find the ground state.</td>
</tr>
<tr>
<td>PurificationTEBD2.run_imaginary(beta)</td>
<td>Run imaginary time evolution to cool down to the given beta.</td>
</tr>
<tr>
<td>PurificationTEBD2.suzuki_trotter_decomposition(...)</td>
<td>Returns list of necessary steps for the suzuki trotter decomposition.</td>
</tr>
<tr>
<td>PurificationTEBD2.suzuki_trotter_time_steps(order)</td>
<td>Return time steps of U for the Suzuki Trotter decomposition of desired order.</td>
</tr>
</tbody>
</table>
Table 34 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PurificationTEBD2.update(N_steps)</td>
<td>Evolve by N_steps * U_param['dt'].</td>
</tr>
<tr>
<td>PurificationTEBD2.update_bond(i, U_bond)</td>
<td>Updates the B matrices on a given bond.</td>
</tr>
<tr>
<td>PurificationTEBD2.update_bond_imag(i, U_bond)</td>
<td>Update a bond with a (possibly non-unitary) U_bond.</td>
</tr>
<tr>
<td>PurificationTEBD2.update_imag(N_steps)</td>
<td>Perform an update suitable for imaginary time evolution.</td>
</tr>
<tr>
<td>PurificationTEBD2.update_step(U_idx_dt, odd)</td>
<td>Updates bonds in unit cell.</td>
</tr>
</tbody>
</table>

**Class Attributes and Properties**

- `PurificationTEBD2.TEBD_params`
- `PurificationTEBD2.disent_iterations` - For each bond the total number of iterations performed in any Disentangler.
- `PurificationTEBD2.trunc_err_bonds` - truncation error introduced on each non-trivial bond.

```python
class tenpy.algorithms.purification.PurificationTEBD2(psi, model, options):
    Bases: tenpy.algorithms.purification.PurificationTEBD

    Similar as PurificationTEBD, but perform sweeps instead of brickwall.
    Instead of the A-B pattern of even/odd bonds used in TEBD, perform sweeps similar as in DMRG for real-time evolution (similar as update_imag() does for imaginary time evolution).

    **update(N_steps)**
    Evolve by N_steps * U_param['dt'].

    Parameters
    - `N_steps (int)` - The number of steps for which the whole lattice should be updated.

    Returns
    - `trunc_err` - The error of the represented state which is introduced due to the truncation during this sequence of update steps.

    Return type
    - `TruncationError`

    **update_step(U_idx_dt, odd)**
    Updates bonds in unit cell.

    Depending on the choice of `odd`, perform a sweep to the left or right, updating once per site with a time step given by U_idx_dt.

    Parameters
    - `U_idx_dt (int)` - Time step index in self._U, evolve with Us[i] = self._U[U_idx_dt][i] at bond (i-1,i).
    - `odd (bool/int)` - Indication of whether to update even (odd=False,0) or even (odd=True,1) sites

    Returns
    - `trunc_err` - The error of the represented state which is introduced due to the truncation during this sequence of update steps.

    Return type
    - `TruncationError`

    **calc_U(order, delta_t, type_evo='real', E_offset=None)**
    see calc_U()```
property disent_iterations
For each bond the total number of iterations performed in any Disentangler.

disentangle (theta)
Disentangle theta before splitting with svd.
For the purification we write $\rho_P = Tr_Q |\psi_{P,Q}><\psi_{P,Q}|$. Thus, we can actually apply any unitary to the auxiliar $Q$ space of $|\psi>$ without changing the result.

Note: We have to apply the same unitary to the `bra' and `ket' used for expectation values / correlation functions!

The behaviour of this function is set by used_disentangler, which in turn is obtained from get_disentangler(options['disentangle']), see get_disentangler() for details on the syntax.

Parameters theta (Array) – Wave function to disentangle, with legs 'vL', 'vR', 'p0', 'p1', 'q0', 'q1'.

Returns

• theta_disentangled (Array) – Disentangled theta; npc.tensordot(U, theta, axes=[[\'q0\*', \'q1\*\'], [\'q0\', \'q1\']]).
• U (Array) – The unitary used to disentangle theta, with labels 'q0', 'q1', 'q0*', 'q1*'. If no unitary was found/applied, it might also be None.

disentangle_global (pair=None)
Try global disentangling by determining the maximally entangled pairs of sites. Calculate the mutual information (in the auxiliar space) between two sites and determine where it is maximal. Disentangle these two sites with disentangle()

disentangle_global_nsite (n=2)
Perform a sweep through the system and disentangle with disentangle_n_site().

Parameters n (int) – maximal number of sites to disentangle at once.

disentangle_n_site (i, n, theta)
Generalization of disentangle() to $n$ sites.
Simply group left and right $n/2$ physical legs, adjust labels, and apply disentangle() to disentangle the central bond. Recursively proceed to disentangle left and right parts afterwards. Scales (for even $n$) as $O(\chi^3 d^n d^{n/2})$.

run ()
(Real-)time evolution with TEBD (time evolving block decimation).

option TEBD.dt: float
Time step.

option TEBD.N_steps: int
Number of time steps $dt$ to evolve. The Trotter decompositions of order $>1$ are slightly more efficient if more than one step is performed at once.

option TEBD.order: int
Order of the algorithm. The total error scales as $O(t^* dt^\text{order})$.

run_GS ()
TEBD algorithm in imaginary time to find the ground state.
**Note:** It is almost always more efficient (and hence advisable) to use DMRG. This algorithm can nonetheless be used quite well as a benchmark and for comparison.

**option TEBD.delta_tau_list: list**
A list of floats: the timesteps to be used. Choosing a large timestep delta_tau introduces large (Trotter) errors, but a too small time step requires a lot of steps to reach $\exp(-\tau H) \rightarrow |\psi_0><\psi_0|$. Therefore, we start with fairly large time steps for a quick time evolution until convergence, and the gradually decrease the time step.

**option TEBD.order: int**
Order of the Suzuki-Trotter decomposition.

**option TEBD.N_steps: int**
Number of steps before measurement can be performed

**run_imaginary(beta)**
Run imaginary time evolution to cool down to the given beta.

Note that we don’t change the norm attribute of the MPS, i.e. normalization is preserved.

**Parameters beta (float) – The inverse temperature beta = 1/T, by which we should cool down. We evolve to the closest multiple of options['dt'], see also evolved_time.**

**static suzuki_trotter_decomposition(order,N_steps)**
Returns list of necessary steps for the suzuki trotter decomposition.

We split the Hamiltonian as $H = H_{even} + H_{odd} = H[0] + H[1]$. The Suzuki-Trotter decomposition is an approximation $\exp(tH) \approx \prod_{(j,k) \in ST} \exp(d[j]tH[k]) + O(t^{order+1})$.

**Parameters order (1, 2, 4, '4_opt') – The desired order of the Suzuki-Trotter decomposition. Order 1 approximation is simply $e^{A/2}e^Be^{A/2}$. Order 2 is the “leapfrog” $e^{iA/2}e^{iB}e^{iA/2}$. Order 4 is the fourth-order from [suzuki1991] (also referenced in [schollwoeck2011]), and '4_opt' gives the optimized version of Eq. (30a) in [barthel2020].**

Returns ST_decomposition – Indices j, k of the time-steps $d =$ suzuki_trotter_time_step(order) and the decomposition of $H$. They are chosen such that a subsequent application of $\exp(d[j] t H[k])$ to a given state $|\psi\rangle$ yields $(\exp(N_{steps} t H[k]) + O(N_{steps} t^{order+1})))|\psi\rangle$.

**Return type** list of (int, int)

**static suzuki_trotter_time_steps(order)**
Return time steps of U for the Suzuki Trotter decomposition of desired order.

See suzuki_trotter_decomposition() for details.

**Parameters order (int) – The desired order of the Suzuki-Trotter decomposition.**

**Returns time_steps – We need $U = \exp(-i H_{(even/odd)} \delta_{t} \ast dt)$ for the dt returned in this list.**

**Return type** list of float

**property trunc_err_bonds**
truncation error introduced on each non-trivial bond.

**update_bond(i, U_bond)**
Updates the B matrices on a given bond.
Function that updates the B matrices, the bond matrix s between and the bond dimension chi for bond i. This would look something like:

\[
\begin{array}{cccc}
| & | & | & \\
| ... - B1 - s - B2 - ... & \\
| | | \\
| | | \\
| | ------------- \\
| | U \\
| | ------------- \\
| | \\
\end{array}
\]

**Parameters**

- **i** (*int*) – Bond index; we update the matrices at sites \(i-1, i\).
- **U\_bond** (*Array*) – The bond operator which we apply to the wave function. We expect labels `'p0'`, `'p1'`, `'p0*'`, `'p1*` for `U\_bond`.

**Returns**

- **trunc\_err** – The error of the represented state which is introduced by the truncation during this update step.

**Return type** *TruncationError*

**update\_bond\_imag(i, U\_bond)**

Update a bond with a (possibly non-unitary) \(U\_bond\).

Similar as **update\_bond()**; but after the SVD just keep the \(A, S, B\) canonical form. In that way, one can sweep left or right without using old singular values, thus preserving the canonical form during imaginary time evolution.

**Parameters**

- **i** (*int*) – Bond index; we update the matrices at sites \(i-1, i\).
- **U\_bond** (*Array*) – The bond operator which we apply to the wave function. We expect labels `'p0'`, `'p1'`, `'p0*'`, `'p1*`.

**Returns**

- **trunc\_err** – The error of the represented state which is introduced by the truncation during this update step.

**Return type** *TruncationError*

**update\_imag(N\_steps)**

Perform an update suitable for imaginary time evolution.

Instead of the even/odd brick structure used for ordinary TEBD, we ‘sweep’ from left to right and right to left, similar as DMRG. Thanks to that, we are actually able to preserve the canonical form.

**Parameters**

- **N\_steps** (*int*) – The number of steps for which the whole lattice should be updated.

**Returns**

- **trunc\_err** – The error of the represented state which is introduced due to the truncation during this sequence of update steps.

**Return type** *TruncationError*
PurificationTwoSiteU

- full name: tenpy.algorithms.purification.PurificationTwoSiteU
- parent module: tenpy.algorithms.purification
- type: class

Inheritance Diagram

```
NpcLinearOperator
  ↓
  EffectiveH
  ↓
  TwoSiteH
  ↓
PurificationTwoSiteU
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PurificationTwoSiteU.<strong>init</strong>(env, i0[, ...])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>PurificationTwoSiteU.adjoint()</td>
<td>Return the hermitian conjugate of self.</td>
</tr>
<tr>
<td>PurificationTwoSiteU.combine_Heff()</td>
<td>Combine LP and RP with W to form LHeff and RHeff.</td>
</tr>
<tr>
<td>PurificationTwoSiteU.combine_theta(theta)</td>
<td>Combine the legs of theta, such that it fits to how we combined the legs of self.</td>
</tr>
<tr>
<td>PurificationTwoSiteU.matvec(theta)</td>
<td>Apply the effective Hamiltonian to theta.</td>
</tr>
<tr>
<td>PurificationTwoSiteU.to_matrix()</td>
<td>Contract self to a matrix.</td>
</tr>
</tbody>
</table>
**Class Attributes and Properties**

- `acts_on`
- `length`

```python
class tenpy.algorithms.purification.PurificationTwoSiteU(env, i0, combine=False, move_right=True):
    Bases: tenpy.algorithms.mps_common.TwoSiteH
    Variant of TwoSiteH suitable for purification.
    The MPO gets only applied to the physical legs p0, p1, the ancillla legs q0, q1 of theta are ignored.

    combine_Heff()
    Combine LP and RP with W to form LHeff and RHeff.
    Combine LP with W0 and RP with W1 to get the effective parts of the Hamiltonian with piped legs.

    adjoint()
    Return the hermitian conjugate of self.

    combine_theta(theta)
    Combine the legs of theta, such that it fits to how we combined the legs of self.
    Parameters theta (Array) – Wave function with labels 'vL', 'p0', 'p1', 'vR'
    Returns theta – Wave function with labels 'vL', 'p0', 'p1', 'vR'
    Return type Array

    matvec(theta)
    Apply the effective Hamiltonian to theta.
    Parameters theta (Array) – Labels: vL, p0, p1, vR if combine=False, (vL,p0), (p1,vR) if True
    Returns Product of theta and the effective Hamiltonian.
    Return type theta Array

    to_matrix()
    Contract self to a matrix.
```

**Module description**

Algorithms for using Purification.

### 7.9.7 mpo_evolution

- full name: tenpy.algorithms.mpo_evolution
- parent module: tenpy.algorithms
- type: module
Classes

**ExpMPOEvolution**

```
ExpMPOEvolution(psi, model, options) Time evolution of an MPS using the W_I or W_II approximation for \( \exp(H \, dt) \).
```

**Module description**

Time evolution using the WI or WII approximation of the time evolution operator.

### 7.9.8 network_contractor

- **full name:** tenpy.algorithms.network_contractor
- **parent module:** tenpy.algorithms
- **type:** module

**Functions**

```
contract(tensor_list[, tensor_names, ...]) Contract a network of tensors.
ncon(tensor_list, leg_links, sequence) Implementation of ncon.m for TeNPy Arrays.
```

**contract**

- **full name:** tenpy.algorithms.network_contractor.contract
- **parent module:** tenpy.algorithms.network_contractor
- **type:** function

```python

tenpy.algorithms.network_contractor.contract(tensor_list, tensor_names=None, leg_contractions=None, open_legs=None, sequence=None)
```

Contract a network of tensors.

Based on the MatLab function ncon.m as described in arXiv:1402.0939.

**Parameters**

- **tensor_list** (list of Array) – The tensors to be contracted.
- **leg_contractions** (list of \([n1, l1, n2, l2]\)) – A list of contraction instructions. An entry of leg_contractions has the form \([n1, l1, n2, l2]\), where \(n1, n2\) are entries of tensor_names and each identify an Array in tensor_list. \(l1, l2\) are leg labels of
the corresponding `Array`. The instruction implies to contract leg 11 of tensor \( n_1 \) with leg 12 of tensor \( n_2 \).

- **open_legs** (list of [\( n_1, \, 11, \, 1 \)]) – A list of instructions for “open” (uncontracted) legs. [\( n_1, \, 11, \, 1 \)] implies that leg 11 of tensor \( n_1 \) is not contracted and is labelled 1 in the result.

- **tensor_names** (list of str) – A list of names for each tensor, to be used in `leg_contractions` and `open_legs`. The default value is list(range(len(tensor_list))), so that the tensor “names” are 0, 1, 2, ... .

- **sequence** (list of int) – The order in which the leg_contractions are to be performed. An entry of network_contractor.outer_product indicates performing an outer product. This corresponds to the zero-in-sequence convention of arXiv:1304.6112

Returns **result** – The number or tensor resulting from the contraction.

Return type `Array` | complex

**ncon**

- full name: tenpy.algorithms.network_contractor.ncon
- parent module: tenpy.algorithms.network_contractor
- type: function

`tenpy.algorithms.network_contractor.ncon(tensor_list, leg_links, sequence)`

Implementation of ncon.m for TeNPy Arrays.

This function is a python implementation of ncon.m (arXiv:1304.6112) for tenpy `Array`. `contract()` is a wrapper that translates from a more python/tenpy input style

Parameters

- **tensor_list** (list of :class:`Array`) – Tensors to be contracted.

- **leg_links** (list of list of int) – Each entry of leg_links describes the connectivity of the corresponding tensor in tensor_list. Each entry is a list that has an entry for each leg of the corresponding tensor. Values 0,1,2,... are labels of contracted legs and should appear exactly twice in leg_links. Values -1,-2,-3,... are labels of uncontracted legs and indicate the final ordering (-1 is first axis).

- **sequence** (list of int) – The order in which the contractions are to be performed. An entry of network_contractor.outer_product indicates performing an outer product. This corresponds to the zero-in-sequence convention of arXiv:1304.6112

Returns **result** – The number or tensor resulting from the contraction.

Return type `Array` | complex
Module description

Network Contractor.

A tool to contract a network of multiple tensors.

This is an implementation of ‘NCON: A tensor network contractor for MATLAB’ by Robert N. C. Pfeifer, Glen Evenbly, Sukhwinder Singh, Guifre Vidal, see arXiv:1402.0939

\[ \text{tenpy.algorithms.network_contractor.outer_product} = -66666666 \]

a constant that represents an outer product in the sequence of ncon

Todo:

- implement or wrap netcon.m, a function to find optimal contractionn sequences (arXiv:1304.6112)
- improve helpfulness of Warnings
- \_do_trace: trace over all pairs of legs at once. need the correspondingnpc function first.

7.9.9 exact_diag

- full name: tenpy.algorithms.exact_diag
- parent module: tenpy.algorithms
- type: module

Classes

**ExactDiag**

\[ \text{ExactDiag(model[, charge_sector, sparse,...])} \]  
(Full) exact diagonalization of the Hamiltonian.

**ExactDiag**

- full name: tenpy.algorithms.exact_diag.ExactDiag
- parent module: tenpy.algorithms.exact_diag
- type: class
Inheritance Diagram

Methods

```python
ExactDiag.__init__(model[, charge_sector, ...])
Initialize self.

ExactDiag.build_full_H_from_bonds()
Calculate self.full_H from self.mpo.

ExactDiag.build_full_H_from_mpo()
Calculate self.full_H from self.mpo.

ExactDiag.exp_H(dt)
Return \( U(dt) := \exp(-i \ H \ dt) \).

ExactDiag.from_H_mpo(H_MPO, *args, **kwargs)
Wrapper taking directly an MPO instead of a Model.

ExactDiag.full_diagonalization(*args, **kwargs)
Full diagonalization to obtain all eigenvalues and eigenvectors.

ExactDiag.full_to_mps(psi[, canonical_form])
Convert a full state (with a single leg) to an MPS.

ExactDiag.groundstate([charge_sector])
Pick the ground state energy and ground state from self.V.

ExactDiag.matvec(psi)
Allow to use self as LinearOperator for lanczos.

ExactDiag.mps_to_full(mps)
Contract an MPS along the virtual bonds and combine its legs.

ExactDiag.sparse_diag(k, *args, **kwargs)
Call speigs().
```

class tenpy.algorithms.exact_diag.ExactDiag(model, charge_sector=None, sparse=False, max_size=2000000.0)

Bases: object

(Full) exact diagonalization of the Hamiltonian.

Parameters

- **model** (MPOModel|CouplingModel) – The model which is to be diagonalized.
- **charge_sector** (None | charges) – If not None, project onto the given charge sector.
- **sparse** (bool) – If True, don’t sort/bunch the LegPipe used to combine the physical legs. This results in array blocks with just one entry, requires much more charge data, and is not what np_conserved was designed for, so it’s not recommended.
- **max_size** (int) – The build_H_* functions will do nothing (but emit a warning) if the total size of the Hamiltonian would be larger than this.

model
The model which is to be diagonalized.

Type MPOModel|CouplingModel

chinfo
The nature of the charge (which is the same for all sites).
```
Type `ChargeInfo`

**charge_sector**
If not `None`, we project onto the given charge sector.

Type `None | charges`

**max_size**
The `build_H_`* functions will do nothing (but emit a warning) if the total size of the Hamiltonian would be larger than this.

Type `int`

**full_H**
The full Hamiltonian to be diagonalized with legs `'(p0,p1,...)'`, `'(p0*,p1*...)'` (in that order). `None` if the `build_H_`* functions haven’t been called yet, or if `max_size` would have been exceeded.

Type `Array | None`

**E**
1D array of eigenvalues.

Type `ndarray | None`

**V**
Eigenvectors. First leg `'ps'` are physical legs, the second leg `'ps*'` corresponds to the eigenvalues.

Type `Array | None`

**_sites**
The sites in the given order.

Type `list of Site`

**_labels_p**
The labels use for the physical legs; just `['p0', 'p1', ...., 'p{L-1}']`.

Type `list or str`

**_labels_pconj**
Just each of `_labels_p` with an `*`.

Type `list or str`

**_pipe**
The pipe from the single physical legs to the full combined leg.

Type `LegPipe`

**_pipe_conj**
Just `_pipe.conj()`.

Type `LegPipe`

**_mask**
Bool mask, which of the indices of the pipe are in the desired `charge_sector`.

Type `1D bool ndarray | None`

```python
classmethod from_H_mpo(H_MPO, *args, **kwargs)
```
Wrapper taking directly an MPO instead of a Model.

Parameters

* `H_MPO (MPO)` – The MPO representing the Hamiltonian.
• `*args` – Further keyword arguments as for the `__init__` of the class.
• `**kwargs` – Further keyword arguments as for the `__init__` of the class.

`build_full_H_from_mpo()`  
Calculate `self.full_H` from `self.mpo`.

`build_full_H_from_bonds()`  
Calculate `self.full_H` from `self.mpo`.

`full_diagonalization(*args, **kwargs)`  
Full diagonalization to obtain all eigenvalues and eigenvectors.
  
Arguments are given to `eigh`.

`groundstate(charge_sector=None)`  
Pick the ground state energy and ground state from `self.V`.
  
Parameters `charge_sector` (None | 1D ndarray) – By default (None), consider all charge sectors. Alternatively, give the `qtotal` which the returned state should have.
  
Returns
  
• `E0` (float) – Ground state energy (possibly in the given sector).
• `psi0` (Array) – Ground state (possibly in the given sector).

`exp_H(dt)`  
Return $U(dt) := \exp(-i \ H \ dt)$.

`mps_to_full(mps)`  
Contract an MPS along the virtual bonds and combine its legs.
  
Parameters `mps` (MPS) – The MPS to be contracted.
  
Returns `psi` – The MPO contracted along the virtual bonds.
  
Return type Array

`full_to_mps(psi, canonical_form='B')`  
Convert a full state (with a single leg) to an MPS.
  
Parameters
  
• `psi` (Array) – The state (with a single leg) which should be splitted into an MPS.
• `canonical_form` (Array) – The form in which the MPS will be afterwards.
  
Returns `mps` – An normalized MPS representation in canonical form.
  
Return type MPS

`matvec(psi)`  
Allow to use `self` as LinearOperator for lanczos.
  
Just applies `full_H` to (the first axis of) the given `psi`.

`sparse_diag(k, *args, **kwargs)`  
Call `speigs()`.
Module description

Full diagonalization (ED) of the Hamiltonian.

The full diagonalization of a small system is a simple approach to test other algorithms. In case you need the full spectrum, a full diagonalization is often the only way. This module provides functionality to quickly diagonalize the Hamiltonian of a given model. This might be used to obtain the spectrum, the ground state or highly excited states.

Note: Good use of symmetries is crucial to increase the treatable system size. While we can simply use the defined LegCharge of a model, we don’t make use of any other symmetries like translation symmetry, SU(2) symmetry or inversion symmetries. In other words, this code does not aim to provide state-of-the-art exact diagonalization, but just the ability to diagonalize the defined models for small system sizes without additional extra work.

7.10 linalg

- full name: tenpy.linalg
- parent module: tenpy
- type: module

Module description

Linear-algebra tools for tensor networks.

Most notably is the module np_conserved, which contains everything needed to make use of charge conservation in the context of tensor networks.

Relevant contents of charges are imported to np_conserved, so you probably won’t need to import charges directly.

Submodules

<table>
<thead>
<tr>
<th>np_conserved</th>
<th>A module to handle charge conservation in tensor networks.</th>
</tr>
</thead>
<tbody>
<tr>
<td>charges</td>
<td>Basic definitions of a charge.</td>
</tr>
<tr>
<td>svd_robust</td>
<td>(More) robust version of singular value decomposition.</td>
</tr>
<tr>
<td>random_matrix</td>
<td>Provide some random matrix ensembles for numpy.</td>
</tr>
<tr>
<td>sparse</td>
<td>Providing support for sparse algorithms (using matrix-vector products only).</td>
</tr>
<tr>
<td>lanczos</td>
<td>Lanczos algorithm for np_conserved arrays.</td>
</tr>
</tbody>
</table>
7.10.1 np_conserved

- full name: tenpy.linalg.np_conserved
- parent module: tenpy.linalg
- type: module

**Classes**

Array

Array(legcharges[, dtype, qtotal, labels]) A multidimensional array (=tensor) for using charge conservation.

**Methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Array.<strong>init</strong>(legcharges[, dtype, qtotal, ...])</td>
<td>see help(self)</td>
</tr>
<tr>
<td>Array.add_charge(add_legs[, chinfo, qtotal])</td>
<td>Add charges.</td>
</tr>
<tr>
<td>Array.add_leg(leg, i[, axis, label])</td>
<td>Add a leg to self, setting the current array as slice for a given index.</td>
</tr>
<tr>
<td>Array.add_trivial_leg([axis, label, qconj])</td>
<td>Add a trivial leg (with just one entry) to self.</td>
</tr>
</tbody>
</table>

continues on next page
<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>Array.as_completely_blocked()</code></td>
<td>Gives a version of self which is completely blocked by charges.</td>
</tr>
<tr>
<td><code>Array.astype(dtype[, copy])</code></td>
<td>Return copy with new dtype, upcasting all blocks in <code>._data</code>.</td>
</tr>
<tr>
<td><code>Array.binary_blockwise(func, other, *args, ...)</code></td>
<td>Roughly return <code>func(self, other)</code>, block-wise.</td>
</tr>
<tr>
<td><code>Array.change_charge(charge, new_qmod[, ...])</code></td>
<td>Change the <code>qmod</code> of one charge in <code>chinfo</code>.</td>
</tr>
<tr>
<td><code>Array.combine_legs(combine_legs[, new_axes, ...])</code></td>
<td>Reshape: combine multiple legs into multiple pipes.</td>
</tr>
<tr>
<td><code>Array.complex_conj()</code></td>
<td>Return copy which is complex conjugated without conjugating the charge data.</td>
</tr>
<tr>
<td><code>Array.conj([complex_conj, inplace])</code></td>
<td>Conjugate: complex conjugate data, conjugate charge data.</td>
</tr>
<tr>
<td><code>Array.copy([deep])</code></td>
<td>Return a (deep or shallow) copy of self.</td>
</tr>
<tr>
<td><code>Array.drop_charge([charge, chinfo])</code></td>
<td>Drop (one of) the charges.</td>
</tr>
<tr>
<td><code>Array.extend(axis, extra)</code></td>
<td>Increase the dimension of a given axis, filling the values with zeros.</td>
</tr>
<tr>
<td><code>Array.from_func(func, legcharges[, dtype, ...])</code></td>
<td>Create an Array from a numpy func.</td>
</tr>
<tr>
<td><code>Array.from_func_square(func, leg[, dtype, ...])</code></td>
<td>Create an Array from a (numpy) function.</td>
</tr>
<tr>
<td><code>Array.from_hdf5(hdf5_loader, h5gr, subpath)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>Array.from_ndarray(data_flat, legcharges[, ...])</code></td>
<td>Convert a flat (numpy) ndarray to an Array.</td>
</tr>
<tr>
<td><code>Array.from_ndarray_trivial(data_flat[, ...])</code></td>
<td>Convert a flat numpy ndarray to an Array with trivial charge conservation.</td>
</tr>
<tr>
<td><code>Array.gauge_total_charge(axis[, newqtotal, ...])</code></td>
<td>Changes the total charge by adjusting the charge on a certain leg.</td>
</tr>
<tr>
<td><code>Array.get_block(qindices[, insert])</code></td>
<td>Return the ndarray in <code>_data</code> representing the block corresponding to <code>qindices</code>.</td>
</tr>
<tr>
<td><code>Array.get_leg(label)</code></td>
<td>Return <code>self.legs[self.get_leg_index(label)]</code>.</td>
</tr>
<tr>
<td><code>Array.get_leg_index(label)</code></td>
<td>Translate a leg-index or leg-label to a leg-index.</td>
</tr>
<tr>
<td><code>Array.get_leg_indices(labels)</code></td>
<td>Translate a list of leg-indices or leg-labels to leg indices.</td>
</tr>
<tr>
<td><code>Array.get_leg_labels()</code></td>
<td>Return list of the leg labels, with <code>None</code> for anonymous legs.</td>
</tr>
<tr>
<td><code>Array.has_label(label)</code></td>
<td>Check whether a given label exists.</td>
</tr>
<tr>
<td><code>Array.iadd_prefactor_other(prefactor, other)</code></td>
<td>Self += prefactor * other for scalar prefactor and Array other.</td>
</tr>
<tr>
<td><code>Array.ibinary_blockwise(func, other, *args, ...)</code></td>
<td>Roughly self = func(self, other), block-wise; in place.</td>
</tr>
<tr>
<td><code>Array.iconj([complex_conj])</code></td>
<td>Wrapper around self.conj() with inplace=True.</td>
</tr>
<tr>
<td><code>Array.idrop_labels([old_labels])</code></td>
<td>Remove leg labels from self; in place.</td>
</tr>
<tr>
<td><code>Array.iproject(mask, axes)</code></td>
<td>Applying masks to one or multiple axes; in place.</td>
</tr>
<tr>
<td><code>Array.ipurge_zeros([cutoff, norm_order])</code></td>
<td>Removes self._data blocks with norm less than cutoff; in place.</td>
</tr>
<tr>
<td><code>Array.ireplace_label(old_label, new_label)</code></td>
<td>Replace the leg label <code>old_label</code> with <code>new_label</code>; in place.</td>
</tr>
<tr>
<td><code>Array.ireplace_labels(old_labels, new_labels)</code></td>
<td>Replace leg label <code>old_labels[i]</code> with <code>new_labels[i]</code>; in place.</td>
</tr>
<tr>
<td><code>Array.is_completely_blocked()</code></td>
<td>Return bool whether all legs are blocked by charge.</td>
</tr>
<tr>
<td><code>Array.iscale_axis(s[, axis])</code></td>
<td>Scale with varying values along an axis; in place.</td>
</tr>
<tr>
<td><code>Array.iscale_prefactor(prefactor)</code></td>
<td>Self *= prefactor for scalar prefactor.</td>
</tr>
</tbody>
</table>

continues on next page
Array.iset_leg_labels(labels) Set labels for the different axes/legs; in place.
Array.isort_qdata() (Lexiographically) sort self._qdata; in place.
Array.iswapaxes(axis1, axis2) Similar as np.swapaxes; in place.
Array.itranspose(axes) Transpose axes like np.transpose; in place.
Array.iunary_blockwise(func, *args, **kwargs) Roughly self = f(self), block-wise; in place.
Array.make_pipe(axes, **kwargs) Generates a LegPipe for specified axes.
Array.matvec(other) This function is used by the Lanczos algorithm needed for DMRG.
Array.norm([ord, convert_to_float]) Norm of flattened data.
Array.permute(perm, axis) Apply a permutation in the indices of an axis.
Array.replace_label(old_label, new_label) Return a shallow copy with the leg label old_label replaced by new_label.
Array.replace_labels(old_labels, new_labels) Return a shallow copy with old_labels[i] replaced by new_labels[i].
Array.save_hdf5(hdf5_saver, h5gr, subpath) Export self into a HDF5 file.
Array.scale_axis(s[, axis]) Same as iscale_axis(), but return a (deep) copy.
Array.sort_legcharge([sort, bunch]) Return a copy with one or all legs sorted by charges.
Array.sparse_stats() Returns a string detailing the sparse statistics.
Array.split_legs([axes, cutoff]) Reshape: opposite of combine_legs: split (some) legs which are LegPipes.
Array.squeeze(axes) Like np.squeeze.
Array.take_slice(indices, axes) Return a copy of self fixing indices along one or multiple axes.
Array.test_sanity() Sanity check.
Array.to_ndarray() Convert self to a dense numpy ndarray.
Array.transpose([axes]) Like itranspose(), but on a deep copy.
Array.unary_blockwise(func, *args, **kwargs) Roughly return func(self), block-wise.
Array.zeros_like() Return a copy of self with only zeros as entries, containing no_data.

Class Attributes and Properties

Array.labels
Array.ndim Alias for rank or len(self.shape).
Array.size The number of dtype-objects stored.
Array.stored_blocks The number of (non-zero) blocks stored in _data.

class tenpy.linalg.np_conserved.Array(legcharges, dtype=<class 'numpy.float64'>, qto-
tal=None, labels=None)

Bases: object

A multidimensional array (=tensor) for using charge conservation.

An Array represents a multi-dimensional tensor, together with the charge structure of its legs (for abelian charges). Further information can be found in Charge conservation with np_conserved.

The default __init__() (i.e. Array(...)) does not insert any data, and thus yields an Array ‘full’ of zeros, equivalent to zeros(). Further, new arrays can be created with one of from_ndarray_trivial(), from_ndarray(), or from_func(), and of course by copying/tensordot/svd etc.

In-place methods are indicated by a name starting with i. (But is_completely_blocked is not inplace...)
Parameters

- **legcharges** (list of *LegCharge*) – The leg charges for each of the legs. The ChargeInfo is read out from it.
- **dtype** *(type or string)* – The data type of the array entries. Defaults to np.float64.
- **qtotal** *(1D array of QTYPE)* – The total charge of the array. Defaults to 0.
- **labels** *(list of {str | None})* – Labels associated to each leg, None for non-named labels.

**rank**

The rank or “number of dimensions”, equivalent to `len(shape)`.

Type int

**shape**

The number of indices for each of the legs.

Type tuple(int)

**dtype**

The data type of the entries.

Type np.dtype

**chinfo**

The nature of the charge.

Type ChargeInfo

**qtotal**

The total charge of the tensor.

Type 1D array

**legs**

The leg charges for each of the legs.

Type list of *LegCharge*

**_labels**

Labels for the different legs, None for non-labeled legs.

Type list of {str | None}

**_data**

The actual entries of the tensor.

Type list of arrays

**_qdata**

For each of the _data entries the qindices of the different legs.

Type 2D array (len(_data), rank), dtype np.intp

**_qdata_sorted**

Whether self._qdata is lexsorted. Defaults to True, but must be set to False by algorithms changing _qdata.

Type Bool

**test_sanity**()

Sanity check.

 Raises ValueErrors, if something is wrong.
copy (deep=True)
    Return a (deep or shallow) copy of self.

Both deep and shallow copies will share chinfo and the Leg Charges in legs.

In contrast to a deep copy, the shallow copy will also share the tensor entries, namely the same instances of _qdata and _data and labels (and other ‘immutable’ properties like the shape or dtype).

Note: Shallow copies are not recommended unless you know the consequences! See the following examples illustrating some of the pitfalls.

Examples

Be very careful when making non-deep copies: In the following example, the original a is changed if and only if the corresponding block existed in a before.

```python
>>> a = npc.Array.from_ndarray_trivial(np.arange(6.).reshape(2, 3))
>>> print(a.to_ndarray())
[[0. 1. 2.]
 [3. 4. 5.]]
>>> b = a.copy(deep=False)  # shallow copy
>>> b[1, 2] = 8.
>>> a[1, 2]  # changed!
8.0
```

Other inplace operations might* have no effect at all (although we don’t guarantee that):

```python
>>> a *= 2  # has no effect on `b`
>>> b.iconj()  # nor does this change `a`
```

save_hdf5 (hdf5_saver, h5gr, subpath)
    Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5().

Specifically, it saves chinfo, legs, dtype under these names, qtotal as "total_charge", _data as "blocks", _qdata as :block inds", the labels in the list-form (as returned by get_leg_labels()). Moreover, it saves rank, shape and _qdata_sorted (under the name "block inds sorted") as HDF5 attributes.

Parameters

• hdf5_saver (Hdf5Saver) – Instance of the saving engine.
• h5gr (:class:`Group`) – HDF5 group which is supposed to represent self.
• subpath (str) – The name of h5gr with a '/' in the end.

classmethod from_hdf5 (hdf5_loader, h5gr, subpath)
    Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

Parameters

• hdf5_loader (Hdf5Loader) – Instance of the loading engine.
• h5gr (Group) – HDF5 group which is represent the object to be constructed.
• subpath (str) – The name of h5gr with a '/' in the end.
classmethod `from_ndarray_trivial` *(data_flat, dtype=None, labels=None)*

convert a flat numpy ndarray to an Array with trivial charge conservation.

**Parameters**

- `data_flat` *(array_like)* – The data to be converted to a Array.
- `dtype` *(np.dtype)* – The data type of the array entries. Defaults to dtype of `data_flat`.
- `labels` *(list of {str | None})* – Labels associated to each leg, None for non-named labels.

**Returns** `res` – An Array with data of `data_flat`.

**Return type** `Array`

classmethod `from_ndarray` *(data_flat, legcharges, dtype=None, qtotal=None, cutoff=None, labels=None, raise_wrong_sector=True)*

convert a flat (numpy) ndarray to an Array.

**Parameters**

- `data_flat` *(array_like)* – The flat ndarray which should be converted to a npc Array. The shape has to be compatible with `legcharges`.
- `legcharges` (list of `LegCharge`) – The leg charges for each of the legs. The `ChargeInfo` is read out from it.
- `dtype` *(np.dtype)* – The data type of the array entries. Defaults to dtype of `data_flat`.
- `qtotal` *(None | charges)* – The total charge of the new array.
- `cutoff` *(float)* – Blocks with `np.max(np.abs(block)) > cutoff` are considered as zero. Defaults to `QCUTOFF`.
- `labels` *(list of {str | None})* – Labels associated to each leg, None for non-named labels.
- `raise_wrong_sector` *(bool)* – If True, raise a ValueError in case of non-zero entries (larger than `cutoff`) in the wrong blocks of `data_flat`. If `False`, just raise a warning.

**Returns** `res` – An Array with data of `data_flat`.

**Return type** `Array`

See also:

`detect_qtotal` used to detect `qtotal` if not given.

classmethod `from_func` *(func, legcharges, dtype=None, qtotal=None, func_args=(), func_kwars={}, shape_kw=None, labels=None)*

Create an Array from a numpy func.

This function creates an array and fills the blocks *compatible* with the charges using `func`, where `func` is a function returning a `array_like` when given a shape, e.g. one of `np.ones` or `np.random.standard_normal`.

**Parameters**

- `func` *(callable)* – A function-like object which is called to generate the data blocks. We expect that `func` returns a flat array of the given `shape` convertible to `dtype`. If no `shape_kw` is given, it is called as `func(shape, *func_args, *func_kwars)`. 
**func_kwargs), otherwise as func(*func_args, `shape_kw`=shape,**func_kwars). shape is a tuple of int.

- legcharges (list of LegCharge) – The leg charges for each of the legs. The ChargeInfo is read out from it.

- dtype (None | type | string) – The data type of the output entries. Defaults to np.float64. Defaults to None: obtain it from the return value of the function. Note that this argument is not given to func, but rather a type conversion is performed afterwards. You might want to set a dtype in func_kwars as well.

- qtotal (None | charges) – The total charge of the new array. Defaults to charge 0.

- func_args (iterable) – Additional arguments given to func.

- func_kwars (dict) – Additional keyword arguments given to func.

- shape_kw (None | str) – If given, the keyword with which shape is given to func.

- labels (list of {str | None}) – Labels associated to each leg, None for non-named labels.

Returns res – An Array with blocks filled using func.

Return type Array

classmethod from_func_square (func, leg, dtype=None, func_args=(), func_kwars={}, shape_kw=None, labels=None)

Create an Array from a (numpy) function.

This function creates an array and fills the blocks compatible with the charges using func, where func is a function returning a array_like when given a shape, e.g. one of np.ones or np.random.standard_normal or the functions defined in random_matrix.

Parameters

- func (callable) – A function-like object which is called to generate the data blocks. We expect that func returns a flat array of the given shape convertible to dtype. If no shape_kw is given, it is called like func(shape, *fargs, **fkwargs), otherwise as func(*fargs, `shape_kw`=shape,**fkwargs). shape is a tuple of int.

- leg (LegCharge) – The leg charges for the first leg; the second leg is set to leg.conj(). The ChargeInfo is read out from it.

- dtype (None | type | string) – The data type of the output entries. Defaults to None: obtain it from the return value of the function. Note that this argument is not given to func, but rather a type conversion is performed afterwards. You might want to set a dtype in func_kwars as well.

- func_args (iterable) – Additional arguments given to func.

- func_kwars (dict) – Additional keyword arguments given to func.

- shape_kw (None | str) – If given, the keyword with which shape is given to func.

- labels (list of {str | None}) – Labels associated to each leg, None for non-named labels.

Returns res – An Array with blocks filled using func.

Return type Array

zeros_like ()

Return a copy of self with only zeros as entries, containing no _data.
**property size**
The number of dtype-objects stored.

**property stored_blocks**
The number of (non-zero) blocks stored in `_data`.

**property ndim**
Alias for `rank` or `len(self.shape)`.

**get_leg_index**(label)
translate a leg-index or leg-label to a leg-index.

    Parameters label (int | string) – The leg-index directly or a label (string) set before.
    Returns leg_index – The index of the label.
    Return type int

See also:

`get_leg_indices` calls `get_leg_index` for a list of labels.

`iset_leg_labels` set the labels of different legs.

**get_leg_indices**(labels)
Translate a list of leg-indices or leg-labels to leg indices.

    Parameters labels (iterable of string/int) – The leg-labels (or directly indices) to be translated in leg-indices.
    Returns leg_indices – The translated labels.
    Return type list of int

See also:

`get_leg_index` used to translate each of the single entries.

`iset_leg_labels` set the labels of different legs.

**iset_leg_labels**(labels)
Set labels for the different axes/legs; in place.

Introduction to leg labeling can be found in *Charge conservation with np_conserved*.

    Parameters labels (iterable (strings | None), len=self.rank) – One label for each of the legs. An entry can be None for an anonymous leg.

See also:

`get_leg` translate the labels to indices.

**get_leg_labels**()
Return list of the leg labels, with None for anonymous legs.

**has_label**(label)
Check whether a given label exists.

**get_leg**(label)
Return self.legs[self.get_leg_index(label)].

Convenient function returning the leg corresponding to a leg label/index.
replace_label (old_label, new_label)
    Replace the leg label old_label with new_label; in place.

replace_labels (old_labels, new_labels)
    Return a shallow copy with the leg label old_label replaced by new_label.

irreplace_labels (old_labels, new_labels)
    Replace leg label old_labels[i] with new_labels[i]; in place.

ireplace_labels (old_labels, new_labels)
    Return a shallow copy with old_labels[i] replaced by new_labels[i].

idrop_labels (old_labels=None)
    Remove leg labels from self; in place.

    Parameters
    old_labels (list of str/int) -- The leg labels/indices for which the label
    should be removed. By default (None), remove all labels.

sparse_stats ()
    Returns a string detailing the sparse statistics.

to_ndarray ()
    Convert self to a dense numpy ndarray.

get_block (qindices, insert=False)
    Return the ndarray in _data representing the block corresponding to qindices.

    Parameters
    qindices (1D array of np.intp) -- The qindices, for which we need to look in
    qdata.
    insert (bool) -- If True, insert a new (zero) block, if qindices is not existent in self.
    _data. Otherwise just return None.

    Returns block -- The block in _data corresponding to qindices. If insert=False and there is
    not block with qindices, return None.

    Return type ndarray | None

    Raises IndexError -- If qindices are incompatible with charge and raise_incomp_q.

take_slice (indices, axes)
    Return a copy of self fixing indices along one or multiple axes.

    For a rank-4 Array A.take_slice([i, j], [1,2]) is equivalent to A[:, i, j, :].

    Parameters
    indices ((iterable of) int) -- The (flat) index for each of the legs specified by
    axes.
    axes ((iterable of) str/int) -- Leg labels or indices to specify the legs for
    which the indices are given.

    Returns sliced_self -- A copy of self, equivalent to taking slices with indices inserted in axes.

    Return type Array

    See also:

    add_leg opposite action of inserting a new leg.

add_trivial_leg (axis=0, label=None, qconj=1)
    Add a trivial leg (with just one entry) to self.
Parameters

- **axis** (*int*) – The new leg is inserted before index axis.
- **label** (*str | None*) – If not None, use it as label for the new leg.
- **qconj** (*+1 | -1*) – The direction of the new leg.

Returns extended – A (possibly) shallow copy of self with an additional leg of ind_len 1 and charge 0.

Return type *Array*

**add_leg**(*leg, i, axis=0, label=None*)

Add a leg to self, setting the current array as slice for a given index.

Parameters

- **leg** (*LegCharge*) – The charge data of the leg to be added.
- **i** (*int*) – Index within the leg for which the data of self should be set.
- **axis** (*axis*) – The new leg is inserted before this current axis.
- **label** (*str | None*) – If not None, use it as label for the new leg.

Returns extended – A copy of self with the new leg at axis, such that extended. take_slice(i, axis) returns a copy of self.

Return type *Array*

See also:

**take_slice** opposite action reducing the number of legs.

**extend**(*axis, extra*)

Increase the dimension of a given axis, filling the values with zeros.

Parameters

- **axis** (*int | str*) – The axis (or axis-label) to be extended.
- **extra** (*LegCharge | int*) – By what to extend, i.e. the charges to be appended to the leg of axis. An int stands for extending the length of the array by a single new block of that size with zero charges.

Returns extended – A copy of self with the specified axis increased.

Return type *Array*

**gauge_total_charge**(*axis, newqtotal=None, new_qconj=None*)

Changes the total charge by adjusting the charge on a certain leg.

The total charge is given by finding a nonzero entry [i1, i2, ...] and calculating:

```python
gtotal = self.chinfo.make_valid(
    np.sum([l.get_charge(l.get_qindex(qi))[0]
             for i, l in zip([i1,i2,...], self.legs)], axis=0))
```

Thus, the total charge can be changed by redefining (= shifting) the LegCharge of a single given leg. This is exactly what this function does.

Parameters

- **axis** (*int or string*) – The new leg (index or label), for which the charge is changed.
• **newqtotal** (*charge values, defaults to 0*) – The new total charge.

• **new_qconj** (*(+1, -1, None]*) – Whether the new LegCharge points inward (+1) or outward (-1) afterwards. By default (None) use the previous `self.legs[leg].qconj`.

**Returns** **copy** – A shallow copy of self with `copy.qtotal == newqtotal` and `new copy.legs[leg]`. The new leg will be a `class LegCharge`, even if the old leg was a LegPipe.

**Return type** `Array`

### add_charge

#### Description
Add charges.

#### Parameters
- **add_legs** (*iterable of LegCharge*) – One `LegCharge` for each axis of `self`, to be added to the one in `legs`.

- **chargeinfo** (*ChargeInfo*) – The ChargeInfo for all charges; create new if None.

- **qtotal** (*None / charges*) – The total charge with respect to `add_legs`. If None, derive it from non-zero entries of `self`.

**Returns** **charges_added** – A copy of `self`, where the LegCharges `add_legs` where added to `self.legs`. Note that the LegCharges are neither bunched or sorted; you might want to use `sort_legcharge()`.

**Return type** `Array`

### drop_charge

#### Description
Drop (one of) the charges.

#### Parameters
- **charge** (*int / str*) – Number or name of the charge (within `chargeinfo`) which is to be dropped. None means dropping all charges.

- **chargeinfo** (*ChargeInfo*) – The ChargeInfo with `charge` dropped; create a new one if None.

**Returns** **dropped** – A copy of `self`, where the specified `charge` has been removed. Note that the LegCharges are neither bunched or sorted; you might want to use `sort_legcharge()`.

**Return type** `Array`

### change_charge

#### Description
Change the `qmod` of one charge in `chargeinfo`.

#### Parameters
- **charge** (*int / str*) – Number or name of the charge (within `chargeinfo`) which is to be changed. None means dropping all charges.

- **new_qmod** (*int*) – The new `qmod` to be set.

- **new_name** (*str*) – The new name of the charge.

- **chargeinfo** (*ChargeInfo*) – The ChargeInfo with `qmod` of `charge` changed; create a new one if None.

**Returns** **changed** – A copy of `self`, where the `qmod` of the specified `charge` has been changed. Note that the LegCharges are neither bunched or sorted; you might want to use `sort_legcharge()`.
Return type **Array**

**is_completely_blocked()**
Return bool whether all legs are blocked by charge.

**sort_legcharge**(sort=True, bunch=True)
Return a copy with one or all legs sorted by charges.

Sort/bunch one or multiple of the LegCharges. Legs which are sorted *and* bunched are guaranteed to be blocked by charge.

**Parameters**

- **sort** (**True** | **False** | **list of** (**True**, **False**, **perm**)) – A single bool holds for all legs, default=**True**. Else, **sort** should contain one entry for each leg, with a bool for sort/don’t sort, or a 1D array perm for a given permutation to apply to a leg.

- **bunch** (**True** | **False** | **list of** (**True**, **False**)) – A single bool holds for all legs, default=**True**. Whether or not to bunch at each leg, i.e. combine contiguous blocks with equal charges.

**Returns**

- **perm** (**tuple of 1D arrays**) – The permutation applied to each of the legs, such that cp.
to_ndarray() = self.to_ndarray()[np.ix_(*perm)].

- **result** (**Array**) – A shallow copy of self, with legs sorted/bunched.

**isort_qdata()**
(Lexiographically) sort self._qdata; in place.

Lexsort self._qdata and self._data and set self._qdata_sorted = True.

**make_pipe**(axes, **kwargs)
Generates a LegPipe for specified axes.

**Parameters**

- **axes** (**iterable of str|int**) – The leg labels for the axes which should be combined. Order matters!

- **kwargs** – Additional keyword arguments given to LegPipe.

**Returns** pipe – A pipe of the legs specified by axes.

**Return type** LegPipe

**combine_legs**(combine_legs, new_axes=None, pipes=None, qconj=None)
Reshape: combine multiple legs into multiple pipes. If necessary, transpose before.

**Parameters**

- **combine_legs** (**(iterable of) iterable of {str|int}**) – Bundles of leg indices or labels, which should be combined into a new output pipes. If multiple pipes should be created, use a list fore each new pipe.

- **new_axes** (**None** | (**iterable of**) **int**) – The leg-indices, at which the combined legs should appear in the resulting array. Default: for each pipe the position of its first pipe in the original array, (taking into account that some axes are ‘removed’ by combining). Thus no transposition is perfomed if combine_legs contains only contiguous ranges.

- **pipes** (**None** | (**iterable of**) **(LegPipes | None)**) – Optional: provide one or multiple of the resulting LegPipes to avoid overhead of computing new leg pipes for the same legs.
multiple times. The LegPipes are conjugated, if that is necessary for compatibility with the legs.

- **qconj**: *(iterable of) (+1, -1)* – Specify whether new created pipes point inward or outward. Defaults to +1. Ignored for given pipes, which are not newly calculated.

**Returns reshaped** – A copy of self, with some legs combined into pipes as specified by the arguments.

**Return type** *Array*

See also:

**split_legs** inverse reshaping splitting LegPipes.

**Notes**

Labels are inherited from self. New pipe labels are generated as `'(' + ' '.join(*leglabels) + ')'`. For these new labels, previously unlabeled legs are replaced by '()?#', where # is the leg-index in the original tensor `self`.

**Examples**

```python
c1 = orig_array.combine_legs([1, 2], qconj=-1) # only single output pipe
print(c1.get_leg_labels())
print(c1.shape)
```

Indices of `combine_legs` refer to the original array. If transposing is necessary, it is performed automatically:

```python
c2 = orig_array.combine_legs([[0, 3], [4, 1]], qconj=[+1, -1]) # two
output pipes
print(c2.get_leg_labels())
print(c2.shape)
c3 = orig_array.combine_legs([[a', 'd'], ['e', 'b']], new_axes=[2, 1],
... pipes=[c2.legs[0], c2.legs[2]])
```

**split_legs** *(axes=None, cutoff=0.0)*

Reshape: opposite of `combine_legs`: split (some) legs which are LegPipes.

Reverts `combine_legs()` (except a possibly performed `transpose`). The split legs are replacing the LegPipes at their position, see the examples below. Labels are split reverting what was done in `combine_legs()`. '?'#' labels are replaced with None.

**Parameters**
• **axes** ((iterable of) int|str) – Leg labels or indices determining the axes to split. The corresponding entries in self.legs must be LegPipe instances. Defaults to all legs, which are LegPipe instances.

• **cutoff** (float) – Splitted data blocks with \( \text{np.max(np.abs(block))} > \text{cutoff} \) are considered as zero. Defaults to 0.

Returns **reshaped** – A copy of self where the specified legs are splitted.

Return type **Array**

See also:

* **combine_legs** this is reversed by split_legs.

Examples

Given a rank-5 Array `orig_array`, you can combine it and split it again:

```python
>>> orig_array = npc.Array.from_ndarray_trivial(np.arange(60).reshape([2, 3, 2, 1, 5]), ...
...       labels=['a', 'b', 'c', 'd', 'e'])
>>> orig_array.shape
(2, 3, 2, 1, 5)
>>> comb_array = orig_array.combine_legs([['a', 'd'], ['c', 'e']])
>>> comb_array.get_leg_labels()
['(a,d)', 'b', '(c,e)']
>>> comb_array.shape
(2, 3, 10)
>>> split_array = comb_array.split_legs()
>>> split_array.get_leg_labels()
['a', 'd', 'b', 'c', 'e']
>>> npc.norm(split_array.transpose(orig_array.get_leg_labels()) - orig_array)
0.0
```

as_completely_blocked()

Gives a version of self which is completely blocked by charges.

Functions like `svd()` or `eigh()` require a complete blocking by charges. This can be achieved by encapsulating each leg which is not completely blocked into a LegPipe (containing only that single leg). The LegPipe will then contain all necessary information to revert the blocking.

Returns

• **encapsulated_axes** (list of int) – The leg indices which have been encapsulated into Pipes.

• **blocked_self** (Array) – Self (if `len(encapsulated_axes) = 0`) or a copy of self, which is completely blocked.

squeeze(**axes=None**)

Like `np.squeeze`.

If a squeezed leg has non-zero charge, this charge is added to `qtotal`.

Parameters **axes** (None | (iterable of) (int|str)) – Labels or indices of the legs which should be 'squeezed', i.e. the legs removed. The corresponding legs must be trivial, i.e., have `ind_len` 1.
Returns `squeezed` – A scalar of `self.dtype`, if all axes were squeezed. Else a copy of `self` with reduced rank as specified by `axes`.

Return type: `class:Array | scalar`

`astype` *(dtype, copy=True)*

Return copy with new dtype, upcasting all blocks in `_data`.

Parameters

- `dtype` *(convertible to a np.dtype)* – The new data type. If None, deduce the new dtype as common type of `self._data`.
- `copy` *(bool)* – Whether to make a copy of the blocks even if the type didn’t change.

Returns `copy` – Deep copy of self with new dtype.

Return type: `Array`

`ipurge_zeros` *(cutoff=2.220446049250313e-15, norm_order=None)*

Removes `self._data` blocks with norm less than cutoff; in place.

Parameters

- `cutoff` *(float)* – Blocks with norm <= cutoff are removed. defaults to `QCUTOFF`.
- `norm_order` – A valid ord argument for `np.linalg.norm`. Default None gives the Frobenius norm/2-norm for matrices/everything else. Note that this differs from other methods, e.g. `from_ndarray()`, which use the maximum norm.

`iproject` *(mask, axes)*

Applying masks to one or multiple axes; in place.

This function is similar as `np.compress` with boolean arrays For each specified axis, a boolean 1D array `mask` can be given, which chooses the indices to keep.

**Warning:** Although it is possible to use an 1D int array as a mask, the order is ignored! If you need to permute an axis, use `permute()` or `sort_legcharge()`.

Parameters

- `mask` *(list of 1D array (bool|int))* – For each axis specified by `axes` a mask, which indices of the axes should be kept. If `mask` is a bool array, keep the indices where `mask` is True. If `mask` is an int array, keep the indices listed in the mask, ignoring the order or multiplicity.
- `axes` *(list of int | string)* – The i’th entry in this list specifies the axis for the i’th entry of `mask`, either as an int, or with a leg label. If axes is just a single int/string, specify just a single mask.

Returns

- `map_qind` *(list of 1D arrays)* – The mapping of qindices for each of the specified axes.
- `block_masks` *(list of lists of 1D bool arrays)* – `block_masks[a][qind]` is a boolean mask which indices to keep in block qindex of axes[a].

`permute` *(perm, axis)*

Apply a permutation in the indices of an axis.

Similar as np.take with a 1D array. Roughly equivalent to `res[ :, ...] = self[perm, ...]` for the corresponding axis. Note: This function is quite slow, and usually not needed!
Parameters

- **perm** (*array_like 1D int*) – The permutation which should be applied to the leg given by *axis*.

- **axis** (*str | int*) – A leg label or index specifying on which leg to take the permutation.

Returns **res** – A copy of self with leg *axis* permuted, such that \( \text{res}[i, ...] = \text{self}[\text{perm}[i], ...] \) for \( i \) along *axis*.

Return type **Array**

See also:

- **sort_legcharge** can also be used to perform a general permutation. Preferable, since it is faster for permutations which don’t mix charge blocks.

- **itranspose** (*axes=None*)
  Transpose axes like *np.transpose*; in place.

  Parameters **axes** (iterable (int|string), len rank | None) – The new order of the axes. By default (None), reverse axes.

- **transpose** (*axes=None*)
  Like *itranspose()* , but on a deep copy.

- **iswapaxes** (*axis1, axis2*)
  Similar as *np.swapaxes*; in place.

- **iscale_axis** (*s, axis=-1*)
  Scale with varying values along an axis; in place.

  Rescale to \( \text{new_self}[i1, ..., i\_axis, ...] = s[i\_axis] \times \text{self}[i1, ..., i\_axis, ...] \).

  Parameters

  - **s** (*1D array, len=self.shape[axis]*) – The vector with which the axis should be scaled.

  - **axis** (*str|int*) – The leg label or index for the axis which should be scaled.

  See also:

- **iproject** can be used to discard indices for which *s* is zero.

- **scale_axis** (*s, axis=-1*)
  Same as **iscale_axis()**, but return a (deep) copy.

- **iunary_blockwise** (**func**, *args**, **kwargs**)
  Roughly \( \text{self} = f(\text{self}) \), block-wise; in place.

  Applies an unary function *func* to the non-zero blocks in *self._data*.

  **Note:** Assumes implicitly that *func(np.zeros(...), *args, **kwargs)* gives 0, since we don’t let *func* act on zero blocks!
• **func** (*function*) – A function acting on flat arrays, returning flat arrays. It is called like `new_block = func(block, *args, **kwargs)`.

• ***args** – Additional arguments given to function after the block.

• ****kwargs** – Keyword arguments given to the function.

### Examples

```python
>>> a = npc.Array.from_ndarray_trivial([1., 2.j])
>>> a.iunary_blockwise(np.conj).to_ndarray()  # same data as a.iconj(), but doesn’t charge conjugate.
array([1.-0.j, 0.-2.j])
>>> a.iunary_blockwise(np.real).to_ndarray()  # get real part.
array([1., 0.])
```

```python
unary_blockwise(func, *args, **kwargs)
Same as iunary_blockwise(), but makes a shallow copy first.
```

```python
conj(complex_conj=True, inplace=False)
Conjugate: complex conjugate data, conjugate charge data.
Conjugate all legs, set negative qtotal.
Labeling: takes ‘a’ -> ‘a*’, ‘a’-> ‘a’ and ‘(a,(b*,c))’ -> ‘(a*, (b, c*))’

Parameters

• complex_conj (bool) – Whether the data should be complex conjugated.

• inplace (bool) – Whether to apply changes to self, or to return a deep copy.
```

```python
complex_conj()  
Return copy which is complex conjugated without conjugating the charge data.
```

```python
norm(ord=None, convert_to_float=True)
Norm of flattened data.
See norm() for details.
```

```python
ibinary_blockwise(func, other, *args, **kwargs)
Roughly self = func(self, other), block-wise; in place.
Applies a binary function ‘block-wise’ to the non-zero blocks of self._data and other._data, storing result in place. Assumes that other is an Array as well, with the same shape and compatible legs. If leg labels of other and self are same up to permutations, other gets transposed accordingly before the action.

Note: Assumes implicitly that func(np.zeros(...), np.zeros(...), *args, **kwargs) gives 0, since we don’t let func act on zero blocks!

Parameters
```
• **func** (*function*) – Binary function, called as `new_block = func(block_self, block_other, *args, **kwargs)` for blocks (=NumPy arrays) of equal shape.

• **other** (*Array*) – Other Array from which to take blocks. Should have the same leg structure as self.

• **args** – Extra arguments given to `func`.

• **kwargs** – Extra keyword arguments given to `func`.

### Examples
```python
>>> a = npc.Array.from_ndarray_trivial([1., 3.])
>>> b = npc.Array.from_ndarray_trivial([4., 2.])
>>> a.ibinary_blockwise(np.maximum, b).to_ndarray()  # a = max(a, b)
array([4., 3.])
>>> a.ibinary_blockwise(np.add, b).to_ndarray()  # roughly `a += b`
array([8., 5.])
```

### Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>concatenate(arrays[, axis, copy])</code></td>
<td>Stack arrays along a given axis, similar as np.concatenate.</td>
</tr>
<tr>
<td><code>detect_grid_outer_legcharge(grid, grid_legs)</code></td>
<td>Derive a LegCharge for a grid used for <code>grid_outer()</code>.</td>
</tr>
<tr>
<td><code>detect_legcharge(flat_array, chargeinfo, . . .)</code></td>
<td>Calculate a missing LegCharge by looking for nonzero entries of a flat array.</td>
</tr>
<tr>
<td><code>detect_qtotal(flat_array, legcharges[, cutoff])</code></td>
<td>Returns the total charge (w.r.t legs) of first non-zero sector found in <code>flat_array</code>.</td>
</tr>
<tr>
<td><code>diag(s, leg[, dtype, labels])</code></td>
<td>Returns a square, diagonal matrix of entries <code>s</code>.</td>
</tr>
<tr>
<td><code>eig(a[, sort])</code></td>
<td>Calculate eigenvalues and eigenvectors for a non-hermitian matrix.</td>
</tr>
</tbody>
</table>
Table 46 – continued from previous page

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>eigh(a[, UPLO, sort])</code></td>
<td>Calculate eigenvalues and eigenvectors for a hermitian matrix.</td>
</tr>
<tr>
<td><code>eigvals(a[, sort])</code></td>
<td>Calculate eigenvalues for a hermitian matrix.</td>
</tr>
<tr>
<td><code>eigvalsh(a[, sort])</code></td>
<td>Calculate eigenvalues for a hermitian matrix.</td>
</tr>
<tr>
<td><code>expm(a)</code></td>
<td>Use scipy.linalg.expm to calculate the matrix exponential of a square matrix.</td>
</tr>
<tr>
<td><code>eye_like(a[, axis, labels])</code></td>
<td>Return an identity matrix contractible with the leg <code>axis</code> of the Array <code>a</code>.</td>
</tr>
<tr>
<td><code>grid_concat(grid, axes[, copy])</code></td>
<td>Given an np.array of npc.Arrays, performs a multi-dimensional concatenation along ‘axes’.</td>
</tr>
<tr>
<td><code>grid_outer(grid, grid_legs[, qtotal, ...])</code></td>
<td>Given an np.array of npc.Arrays, return the corresponding higher-dimensional Array.</td>
</tr>
<tr>
<td><code>inner(a, b[, axes, do_conj])</code></td>
<td>Contract all legs in <code>a</code> and <code>b</code>, return scalar.</td>
</tr>
<tr>
<td><code>norm(a[, ord, convert_to_float])</code></td>
<td>Norm of flattened data.</td>
</tr>
<tr>
<td><code>ones(legcharges[, dtype, qtotal, labels])</code></td>
<td>Short-hand for <code>Array.from_func()</code> with function <code>numpy.ones()</code>.</td>
</tr>
<tr>
<td><code>outer(a, b)</code></td>
<td>Forms the outer tensor product, equivalent to <code>tensordot(a, b, axes=0)</code>.</td>
</tr>
<tr>
<td><code>pinv(a[, cutoff])</code></td>
<td>Compute the (Moore-Penrose) pseudo-inverse of a matrix.</td>
</tr>
<tr>
<td><code>qr(a[, mode, inner_labels, cutoff])</code></td>
<td>Q-R decomposition of a matrix.</td>
</tr>
<tr>
<td><code>speigs(a, charge_sector, k, *args, **kwargs)</code></td>
<td>Sparse eigenvalue decomposition ( \lambda, \ v ) of square <code>a</code> in a given charge sector.</td>
</tr>
<tr>
<td><code>svd(a[, full_matrices, compute_uv, cutoff, ...])</code></td>
<td>Singular value decomposition of an Array <code>a</code>.</td>
</tr>
<tr>
<td><code>tensordot(a, b[, axes])</code></td>
<td>Similar as <code>np.tensordot</code> but for <code>Array</code>.</td>
</tr>
<tr>
<td><code>to_iterable_arrays(array_list)</code></td>
<td>Similar as <code>to_iterable()</code>, but also enclose npc Arrays in a list.</td>
</tr>
<tr>
<td><code>trace(a[, leg1, leg2])</code></td>
<td>Trace of <code>a</code>, summing over leg <code>1</code> and leg <code>2</code>.</td>
</tr>
<tr>
<td><code>zeros(legcharges[, dtype, qtotal, labels])</code></td>
<td>Create a npc array full of zeros (with no _data).</td>
</tr>
</tbody>
</table>

**concatenate**

- full name: tenpy.linalg.np_conserved.concatenate
- parent module: tenpy.linalg.np_conserved
- type: function

```python
tenpy.linalg.np_conserved.concatenate(arrays, axis=0, copy=True)
```

Stack arrays along a given axis, similar as `np.concatenate`.

Stacks the qind of the array, without sorting/blocking. Labels are inherited from the first array only.

**Parameters**

- `arrays` (iterable of `Array`) – The arrays to be stacked. They must have the same shape and charge data except on the specified axis.
- `axis` (`int` | `str`) – Leg index or label of the first array. Defines the axis along which the arrays are stacked.
- `copy` (`bool`) – Whether to copy the data blocks.

**Returns** stacked – Concatenation of the given `arrays` along the specified axis.

**Return type** `Array`
See also:

**Array.sort_legcharge** can be used to block by charges along the axis.

### detect_grid_outer_legcharge

- **full name**: tenpy.linalg.np_conserved.detect_grid_outer_legcharge
- **parent module**: tenpy.linalg.np_conserved
- **type**: function

```python

tenpy.linalg.np_conserved.detect_grid_outer_legcharge(grid, grid_legs, qtotal=None, qconj=1, bunch=False)
```

Derive a LegCharge for a grid used for `grid_outer()`.

Note: The resulting LegCharge is *not* bunched.

**Parameters**

- `grid` (array_like of {Array | None}) – The grid as it will be given to `grid_outer()`.
- `grid_legs` (list of {LegCharge | None}) – One LegCharge for each dimension of the grid, except for one entry which is None. This missing entry is to be calculated.
- `qtotal` (charge) – The desired total charge of the array. Defaults to 0.

**Returns** `new_grid_legs` – A copy of the given `grid_legs` with the `None` replaced by a compatible LegCharge. The new LegCharge is neither bunched nor sorted!

**Return type** list of LegCharge

See also:

**detect_legcharge** similar functionality for a flat numpy array instead of a grid.

### detect_legcharge

- **full name**: tenpy.linalg.np_conserved.detect_legcharge
- **parent module**: tenpy.linalg.np_conserved
- **type**: function

```python

tenpy.linalg.np_conserved.detect_legcharge(flat_array, chargeinfo, legcharges, qtotal=None, qconj=1, cutoff=None)
```

Calculate a missing LegCharge by looking for nonzero entries of a flat array.

**Parameters**

- `flat_array` (ndarray) – A flat array, in which we look for non-zero entries.
- `chargeinfo` (ChargeInfo) – The nature of the charge.
- `legcharges` (list of LegCharge) – One LegCharge for each dimension of flat_array, except for one entry which is None. This missing entry is to be calculated.
- `qconj` ((+1, -1)) – `qconj` for the new calculated LegCharge.
- `qtotal` (charges) – Desired total charge of the array. Defaults to zeros.
- `cutoff` (float) – Blocks with `np.max(np.abs(block)) > cutoff` are considered as zero. Defaults to QCUTOFF.
Returns `new_legcharges` – A copy of the given `legcharges` with the `None` replaced by a compatible `LegCharge`. The new legcharge is ‘bunched’, but not sorted!

Return type list of `LegCharge`

See also:

- `detect_grid_outer_legcharge` similar functionality if the flat array is given by a ‘grid’.
- `detect_qtotal` detects the total charge, if all legs are known.

**detect_qtotal**

- full name: `tenpy.linalg.np_conserved.detect_qtotal`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
tenpy.linalg.np_conserved.detect_qtotal(flat_array, legcharges, cutoff=None)
```

Returns the total charge (w.r.t legs) of first non-zero sector found in `flat_array`.

Parameters

- `flat_array` (array) – The flat numpy array from which you want to detect the charges.
- `legcharges` (list of `LegCharge`) – For each leg the `LegCharge`.
- `cutoff` (float) – Blocks with `np.max(np.abs(block)) > cutoff` are considered as zero. Defaults to `QCUTOFF`.

Returns `qtotal` – The total charge for the first non-zero (i.e. > cutoff) charge block.

Return type charge

See also:

- `detect_legcharge` detects the charges of one missing `LegCharge` if `qtotal` is known.
- `detect_grid_outer_legcharge` similar functionality if the flat array is given by a ‘grid’.

**diag**

- full name: `tenpy.linalg.np_conserved.diag`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
tenpy.linalg.np_conserved.diag(s, leg, dtype=None, labels=None)
```

Returns a square, diagonal matrix of entries `s`.

The resulting matrix has legs `(leg, leg.conj())` and charge 0.

Parameters

- `s` (scalar / 1D array) – The entries to put on the diagonal. If scalar, all diagonal entries are the same.
- `leg` (`LegCharge`) – The first leg of the resulting matrix.
- `dtype` (None / type) – The data type to be used for the result. By default, use `dtype of s`.
• **labels** *(list of (str | None)) – Labels associated to each leg, None for non-named labels.*

Returns diagonal – A square matrix with diagonal entries \(s\).

Return type *Array*

See also:

* **Array.scale_axis** similar as `tenpy.linalg.np_conserved.tensordot(diag(s), ...)`, but faster.

### eig

• full name: `tenpy.linalg.np_conserved.eig`

• parent module: *tenpy.linalg.np_conserved*

• type: function

```
tenpy.linalg.np_conserved.eig(a, sort=None)
```

Calculate eigenvalues and eigenvectors for a non-hermitian matrix.

\[W, V = \text{eig}(a) \text{ yields } aV = V\text{diag}(w).\]

Parameters

• **a** *(Array) – The hermitian square matrix to be diagonalized.*

• **sort** *(\{’m>’, ’m<’, ’>’, ’<’, None\}) – How the eigenvalues should are sorted within each charge block. Defaults to None, which is same as ’<’. See `argsort()` for details.*

Returns

• **W** *(1D ndarray) – The eigenvalues, sorted within the same charge blocks according to sort.*

• **V** *(Array) – Unitary matrix; \(V[:, i]\) is normalized eigenvector with eigenvalue \(W[i]\).*

   The first label is inherited from \(A\), the second label is ’eig’.

Notes

Requires the legs to be contractible. If \(a\) is not blocked by charge, a blocked copy is made via a permutation \(P\), :math:`a' = P a P = V' W' (V')^\dagger`. The eigenvectors \(V\) are then obtained by the reverse permutation, \(V = P^{-1} V'\) such that \(A = V W V^\dagger`.

### eigh

• full name: `tenpy.linalg.np_conserved.eigh`

• parent module: *tenpy.linalg.np_conserved*

• type: function

```
tenpy.linalg.np_conserved.eigh(a, UPLO='L', sort=None)
```

Calculate eigenvalues and eigenvectors for a hermitian matrix.

\[W, V = \text{eigh}(a) \text{ yields } a = V\text{diag}(w)V^\dagger.\] **Assumes** that \(a\) is hermitian, \(a.conj().transpose() == a\).

Parameters

• **a** *(Array) – The hermitian square matrix to be diagonalized.*
• **UPLO** (\{'L', 'U'\}) – Whether to take the lower ('L', default) or upper ('U') triangular part of a.

• **sort** (\{'m>', 'm<', '>', '<', None\}) – How the eigenvalues should be sorted within each charge block. Defaults to None, which is same as ‘<’. See argsort() for details.

**Returns**

• **W** (1D ndarray) – The eigenvalues, sorted within the same charge blocks according to sort.

• **V** (Array) – Unitary matrix; \(V[:, i]\) is normalized eigenvector with eigenvalue \(W[i]\). The first label is inherited from \(A\), the second label is ‘eig’.

**Notes**

Requires the legs to be contractible. If \(a\) is not blocked by charge, a blocked copy is made via a permutation \(P\), \[a' = P a P = V' W' (V')^{dagger}\]. The eigenvectors \(V\) are then obtained by the reverse permutation, \(V = P^{-1} V'\) such that \(A = V W V^{dagger}\).

eigvals

• full name: tenpy.linalg.np_conserved.eigvals

• parent module: tenpy.linalg.np_conserved

• type: function

`tenpy.linalg.np_conserved.eigvals(a, sort=None)`

Calculate eigenvalues for a hermitian matrix.

**Parameters**

• **a** (Array) – The hermitian square matrix to be diagonalized.

• **sort** (\{'m>', 'm<', '>', '<', None\}) – How the eigenvalues should be sorted within each charge block. Defaults to None, which is same as ‘<’. See argsort() for details.

**Returns** **W** – The eigenvalues, sorted within the same charge blocks according to sort.

**Return type** 1D ndarray

**Notes**

The eigenvalues are sorted within blocks of the completely blocked legs.

eigvalsh

• full name: tenpy.linalg.np_conserved.eigvalsh

• parent module: tenpy.linalg.np_conserved

• type: function

`tenpy.linalg.np_conserved.eigvalsh(a, UPLO='L', sort=None)`

Calculate eigenvalues for a hermitian matrix.

**Assumes** that \(a\) is hermitian, \(a.conj().transpose() == a\).

**Parameters**
• **a** (*Array*) – The hermitian square matrix to be diagonalized.

• **UPLO** ([‘L’, ‘U’]) – Whether to take the lower (‘L’, default) or upper (‘U’) triangular part of \( a \).

• **sort** ([‘m>’, ‘m<’, ‘>’, ‘<’, None]) – How the eigenvalues should be sorted *within* each charge block. Defaults to None, which is same as ‘<’. See argsort() for details.

**Returns**

\( W \) – The eigenvalues, sorted within the same charge blocks according to *sort*.

**Return type**

1D ndarray

**Notes**

The eigenvalues are sorted within blocks of the completely blocked legs.

### expm

• full name: tenpy.linalg.np_conserved.expm

• parent module: tenpy.linalg.np_conserved

• type: function
tenpy.linalg.np_conserved.expm(\( a \))

Use scipy.linalg.expm to calculate the matrix exponential of a square matrix.

**Parameters**

\( a \) (*Array*) – A square matrix to be exponentiated.

**Returns**

\( \exp_a \) – The matrix exponential \( \expm(a) \), calculated using scipy.linalg.expm. Same legs/labels as \( a \).

**Return type**

*Array*

### eye_like

• full name: tenpy.linalg.np_conserved.eye_like

• parent module: tenpy.linalg.np_conserved

• type: function
tenpy.linalg.np_conserved.eye_like(\( a \), axis=0, labels=None)

Return an identity matrix contractible with the leg *axis* of the *Array* \( a \).

### grid_concat

• full name: tenpy.linalg.np_conserved.grid_concat

• parent module: tenpy.linalg.np_conserved

• type: function
tenpy.linalg.np_conserved.grid_concat(\( grid \), *axes*, copy=True)

Given an np.array of npc.Arrays, performs a multi-dimensional concatenation along ‘axes’.

Similar to numpy.block(), but only for uniform blocking.

Stacks the qind of the array, *without* sorting/blocking.

**Parameters**
• **grid** (array_like of *Array*) – The grid of arrays.

• **axes** (list of int) – The axes along which to concatenate the arrays, same len as the dimension of the grid. Concatenate arrays of the *i*’th axis of the grid along the axis `axes[i]`

• **copy** (bool) – Whether the _data_ blocks are copied.

---

### Examples

Assume we have prepared rank 2 Arrays A, B, C, D sharing the legs of equal sizes and looking like this:

```python
>>> print(A.to_ndarray())
[[0 1]]
>>> print(B.to_ndarray())
[[10 11 12 13]]
>>> print(C.to_ndarray())
[[20 21]
  [22 23]
  [24 25]]
>>> print(D.to_ndarray())
[[30 31 32 33]
  [34 35 36 37]
  [38 39 40 41]]
```

Then the following grid will result in a (1+3, 2+4) shaped array:

```python
>>> g = npc.grid_concat([[A, B],
...                       [C, D]], axes=[0, 1])
>>> g.shape
(4, 6)
>>> print(g.to_ndarray())
[[ 0  1 10 11 12 13]
 [20 21 30 31 32 33]
 [22 23 34 35 36 37]
 [24 25 38 39 40 41]]
```

If A, B, C, D were rank 4 arrays, with the first and last leg as before, and sharing *common* legs 1 and 2 of dimensions 1, 2, then you would get a rank-4 array:

```python
>>> g = grid_concat([[A, B], [C, D]], axes=[0, 3])
>>> g.shape
(4, 1, 2, 6)
```

---

See also:

*Array.sort_legcharge* can be used to block by charges.
grid_outer

- full name: tenpy.linalg.np_conserved.grid_outer
- parent module: tenpy.linalg.np_conserved
- type: function

\texttt{tenpy.linalg.np_conserved.grid_outer}(grid, grid_legs, qtotal=None, grid_labels=None)

Given an np.array of npc.Arrays, return the corresponding higher-dimensional Array.

**Parameters**

- \texttt{grid} (array_like of \{Array | None\}) – The grid gives the first part of the axes of the resulting array. Entries have to have all the same shape and charge-data, giving the remaining axes. None entries in the grid are interpreted as zeros.

- \texttt{grid_legs} (list of LegCharge) – One LegCharge for each dimension of the grid along the grid.

- \texttt{qtotal} (charge) – The total charge of the Array. By default (None), derive it out from a non-trivial entry of the grid.

- \texttt{grid_labels} (list of \{str | None\}) – One label associated to each of the grid axes. None for non-named labels.

**Returns res** – An Array with shape \texttt{grid.shape + nontrivial_grid_entry.shape}. Constructed such that \texttt{res[idx] == grid[idx]} for any index \texttt{idx} of the \texttt{grid} the \texttt{grid} entry is not trivial (None).

**Return type** \texttt{Array}

See also:

\texttt{detect_grid_outer_legcharge} can calculate one missing LegCharge of the grid.

**Examples**

A typical use-case for this function is the generation of an MPO. Say you have npc.Arrays \texttt{Splus, Sminus, Sz, Id}, each with legs \{\texttt{phys.conj()}, \texttt{phys}\}. Further, you have to define appropriate LegCharges \texttt{l.left} and \texttt{l.right}. Then one ‘matrix’ of the MPO for a nearest neighbour Heisenberg Hamiltonian could look like:

```python
>>> s = tenpy.networks.site.SpinHalfSite(conserve='Sz')
>>> Id, Splus, Sminus, Sz = s.Id, s.Sp, s.Sm, s.Sz
>>> J = 1.
>>> leg_wR = npc.LegCharge.from_qflat(s.leg.chinfo,
...     [op.qtotal for op in [Id, Splus, Sminus, Sz,
...        Id]],
...     qconj=-1)
>>> W_mpo = npc.grid_outer([[Id, Splus, Sminus, Sz, None],
...             [None, None, None, None, J*0.5*Sminus],
...             [None, None, None, None, J*0.5*Splus],
...             [None, None, None, None, J*Sz],
...             [None, None, None, None, Id]],
...             grid_legs=[leg_wR.conj(), leg_wR],
...             grid_labels=['wL', 'wR'])
>>> W_mpo.shape
(5, 5, 2, 2)
>>> W_mpo.get_leg_labels()
['wL', 'wR', 'p', 'p*']
```
inner

- full name: `tenpy.linalg.np_conserved.inner`
- parent module: `tenpy.linalg.np_conserved`
- type: function

`tenpy.linalg.np_conserved.inner(a, b, axes=None, do_conj=False)`

Contract all legs in `a` and `b`, return scalar.

Parameters

- `a` (class: `Array`) – The arrays for which to calculate the product. Must have same rank, and compatible LegCharges.
- `b` (class: `Array`) – The arrays for which to calculate the product. Must have same rank, and compatible LegCharges.
- `axes ((axes_a, axes_b) | 'range', 'labels')` – `axes_a` and `axes_b` specify the legs of `a` and `b`, respectively, which should be contracted. Legs can be specified with leg labels or indices. We contract leg `axes_a[i]` of `a` with leg `axes_b[i]` of `b`. The default `axes='range'` is equivalent to `(range(rank), range(rank)).axes='labels'` is equivalent to either `(a.get_leg_labels(), a.get_leg_labels())` for `do_conj=True`, or to `(a.get_leg_labels(), conj_labels(a.get_leg_labels()))` for `do_conj=False`. In other words, `axes='labels'` requires `a` and `b` to have the same/conjugated labels up to a possible transposition, which is then reverted.
- `do_conj (bool)` – If `False` (Default), ignore it. if `True`, conjugate `a` before, i.e., return `inner(a.conj(), b, axes)`

Returns: `inner_product` – A scalar (of common dtype of `a` and `b`) giving the full contraction of `a` and `b`.

Return type: `dtype`

norm

- full name: `tenpy.linalg.np_conserved.norm`
- parent module: `tenpy.linalg.np_conserved`
- type: function

`tenpy.linalg.np_conserved.norm(a, ord=None, convert_to_float=True)`

Norm of flattened data.

Equivalent to `np.linalg.norm(a.to_ndarray().flatten(), ord)`.

In contrast to numpy, we don’t distinguish between matrices and vectors, but simply calculate the norm for the flat (block) data. The usual `ord`-norm is defined as `(\sum_i |a_i|^ord) ^ {1/ord}`.
### Parameters

- **a** *(Array | np.ndarray)* – The array of which the norm should be calculated.
- **ord** – The order of the norm. See table above.
- **convert_to_float** – Convert integer to float before calculating the norm, avoiding int overflow.

**Returns** norm – The norm over the flat data of the array.

**Return type** float

### ones

- **full name**: tenpy.linalg.np_conserved.ones
- **parent module**: tenpy.linalg.np_conserved
- **type**: function

```python
tenpy.linalg.np_conserved.ones(legcharges, dtype=<class 'numpy.float64'>, qtotal=None, labels=None)
```

Short-hand for `Array.from_func()` with function `numpy.ones()`.

**Warning:** For non-trivial charges, only blocks with compatible charges are filled with ones!

### outer

- **full name**: tenpy.linalg.np_conserved.outer
- **parent module**: tenpy.linalg.np_conserved
- **type**: function

```python
tenpy.linalg.np_conserved.outer(a, b)
```

Forms the outer tensor product, equivalent to `tensordot(a, b, axes=0)`.

Labels are inherited from *a* and *b*. In case of a collision (same label in both *a* and *b*), they are both dropped.

**Parameters**

- **a** *(Array)* – The arrays for which to form the product.
- **b** *(Array)* – The arrays for which to form the product.

**Returns**

- **c** – Array of rank *a.rank + b.rank* such that (*Ra = a.rank; Rb = b.rank*):

#### Table: norm values

<table>
<thead>
<tr>
<th>ord</th>
<th>norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>None/’fro’</td>
<td>Frobenius norm (same as 2-norm)</td>
</tr>
<tr>
<td>np.inf</td>
<td>max(abs(x))</td>
</tr>
<tr>
<td>-np.inf</td>
<td>min(abs(x))</td>
</tr>
<tr>
<td>0</td>
<td>sum(a != 0) == np.count_nonzero(x)</td>
</tr>
<tr>
<td>other</td>
<td>usual ord-norm</td>
</tr>
</tbody>
</table>
\[ c[i₁, \ldots, i_{Ra}, j₁, \ldots j_R] = a[i₁, \ldots, i_{Ra}] \ast b[j₁, \ldots, j_\rightarrow rank_b] \]

**Return type** *Array*

**pinv**

- full name: `tenpy.linalg.np_conserved.pinv`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
import tenpy.linalg.np_conserved

def pinv(a, cutoff=1e-15):
    # Compute the (Moore-Penrose) pseudo-inverse of a matrix.
    Equivalent to the following procedure: Perform a SVD, \( U, S, VH = \text{svd}(a, \text{cutoff}=\text{cutoff}) \) with a \( \text{cutoff} > 0 \), calculate \( P = U \ast \text{diag}(1/S) \ast VH \) (with \( \ast \) denoting tensordot) and return \( P.\text{conj. transpose()} \).

    Parameters
    - *a* ((M, N) *Array*) – Matrix to be pseudo-inverted.
    - *cutoff* (float) – Cutoff for small singular values, as given to \( \text{svd()} \). (Note: different convention than numpy.)

    Returns *B* – The pseudo-inverse of *a*.

    **Return type** *(N, M) Array*
```

**qr**

- full name: `tenpy.linalg.np_conserved.qr`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
import tenpy.linalg.np_conserved

def qr(a, mode='reduced', inner_labels=[None, None], cutoff=None):
    # Q-R decomposition of a matrix.
    Decomposition such that \( A = \text{npc.tensordot}(q, r, axes=1) \) up to numerical rounding errors.

    Parameters
    - *a* (Array) – A square matrix to be exponentiated, shape (M, N).
    - *mode* ('reduced', 'complete') – 'reduced': return q and r with shapes (M,K) and (K,N), where K=min(M,N) 'complete': return q with shape (M,M).
    - *inner_labels* ([{str|None}, {str|None}]) – The first label is used for Q.legs[1], the second for R.legs[0].
    - *cutoff* (None or float) – If not None, discard linearly dependent vectors to given precision, which might reduce K of the ‘reduced’ mode even further.

    Returns
    - *q* (Array) – If mode is ‘complete’, a unitary matrix. For mode ‘reduced’ such that otherwise such that \( q_j^* q_{j,k} = \delta_{k,k} \)
• **r** (*Array*) – Upper triangular matrix if both legs of A are sorted by charges; Otherwise a simple transposition (performed when sorting by charges) brings it to upper triangular form.

**speigs**

- full name: `tenpy.linalg.np_conserved.speigs`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
tenpy.linalg.np_conserved.speigs(a, charge_sector, k, *args, **kwargs)
```

Sparse eigenvalue decomposition $w, v$ of square `a` in a given charge sector.

Finds $k$ right eigenvectors (chosen by `kwargs['which']`) in a given charge sector, $\text{tensordot}(A, V[i], \text{axes}=1) = W[i] * V[i]$.

**Parameters**

- `a` (*Array*) – A square array with contractible legs and vanishing total charge.
- `charge_sector` (*charges*) – `ndim` charges to select the block.
- `k` (*int*) – How many eigenvalues/vectors should be calculated. If the block of `charge_sector` is smaller than `k`, `k` may be reduced accordingly.
- `*args` – Additional arguments given to `scipy.sparse.linalg.eigs`.
- `**kwargs` – Additional keyword arguments given to `scipy.sparse.linalg.eigs`.

**Returns**

- `W` (*ndarray*) – $k$ (or less) eigenvalues
- `V` (list of *Array*) – $k$ (or less) right eigenvectors of `A` with total charge `charge_sector`. Note that when interpreted as a matrix, this is the transpose of what `np.eigs` normally gives.

**svd**

- full name: `tenpy.linalg.np_conserved.svd`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
tenpy.linalg.np_conserved.svd(a, full_matrices=False, compute_uv=True, cutoff=None, qtotal_LR=[None, None], inner_labels=[None, None], inner_qconj=1)
```

Singular value decomposition of an Array `a`.

Factorizes $U, S, VH = \text{svd}(a)$, such that $a = U * \text{diag}(S) * VH$ (where $*$ stands for a `tensordot` and `diag` creates an correctly shaped Array with $S$ on the diagonal). For a non-zero `cutoff` this holds only approximately.

There is a gauge freedom regarding the charges, see also `Array.gauge_total_charge()`. We ensure contractibility by setting $U.legs[1] = VH.legs[0].\text{conj}()$. Further, we gauge the LegCharge such that $U$ and $V$ have the desired `qtotal_LR`.

**Parameters**

- `a` (*Array*, shape `(M, N)*) – The matrix to be decomposed.
• `full_matrices (bool)` – If False (default), \(U\) and \(V\) have shapes \((M, K)\) and \((K, N)\), where \(K = \text{len}(S)\). If True, \(U\) and \(V\) are full square unitary matrices with shapes \((M, M)\) and \((N, N)\). Note that the arrays are not directly contractible in that case; \(\text{diag}(S)\) would need to be a rectangular \((M, N)\) matrix.

• `compute_uv (bool)` – Whether to compute and return \(U\) and \(V\).

• `cutoff (None | float)` – Keep only singular values which are (strictly) greater than `cutoff`. (Then the factorization holds only approximately). If None (default), ignored.

• `qtotal_LR ([(charges|None), (charges|None)])` – The desired `qtotal` for \(U\) and \(VH\), respectively. \([\text{None, None}]\) (Default) is equivalent to \([\text{None, a.qtotal}]\). A single `None` entry is replaced the unique charge satisfying the requirement \(U.\text{qtotal} + VH.\text{qtotal} = a.\text{qtotal} \mod \text{qmod}\).

• `inner_labels_LR ([(str|None), (str|None)])` – The first label corresponds to \(U.\text{legs}[1]\), the second to \(VH.\text{legs}[0]\).

• `inner_qconj (+1, -1)` – Direction of the charges for the new leg. Default +1. The new `LegCharge` is constructed such that \(VH.\text{legs}[0].\text{qconj} = \text{qconj}\).

Returns

• `U (Array)` – Matrix with left singular vectors as columns. Shape \((M, M)\) or \((M, K)\) depending on `full_matrices`.

• `S (1D ndarray)` – The singular values of the array. If no `cutoff` is given, it has length \(\min(M, N)\).

• `VH (Array)` – Matrix with right singular vectors as rows. Shape \((N, N)\) or \((K, N)\) depending on `full_matrices`.

tensordot

• full name: `tenpy.linalg.np_conserved.tensordot`

• parent module: `tenpy.linalg.np_conserved`

• type: function

`tenpy.linalg.np_conserved.tensordot(a, b, axes=2)`

Similar as `np.tensordot` but for `Array`.

Builds the tensor product of \(a\) and \(b\) and sums over the specified axes. Does not require complete blocking of the charges.

Labels are inherited from \(a\) and \(b\). In case of a collision (= the same label would be inherited from \(a\) and \(b\) after the contraction), both labels are dropped.

Detailed implementation notes are available in the doc-string of `_tensordot_worker()`.

Parameters

• `a (Array)` – The first and second npc Array for which axes are to be contracted.

• `b (Array)` – The first and second npc Array for which axes are to be contracted.

• `axes ((axes_a, axes_b) | int)` – A single integer is equivalent to \((\text{range}(-\text{axes}, 0), \text{range}(*\text{axes}))\). Alternatively, `axes_a` and `axes_b` specify the legs of \(a\) and \(b\), respectively, which should be contracted. Legs can be specified with leg labels or indices. Contract leg `axes_a[i]` of \(a\) with leg `axes_b[i]` of \(b\).
Returns `a_dot_b` – The tensor product of `a` and `b`, summed over the specified axes. Returns a scalar in case of a full contraction.

Return type *Array*

to_iterable_arrays

- full name: `tenpy.linalg.np_conserved.to_iterable_arrays`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
tenpy.linalg.np_conserved.to_iterable_arrays(array_list)
```

Similar as `to_iterable()`, but also enclose npc Arrays in a list.

trace

- full name: `tenpy.linalg.np_conserved.trace`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
tenpy.linalg.np_conserved.trace(a, leg1=0, leg2=1)
```

Trace of `a`, summing over `leg1` and `leg2`.

Requires that the contracted legs are contractible (i.e. have opposite charges). Labels are inherited from `a`.

Parameters

- `leg1 (str|int)` – The leg label or index for the two legs which should be contracted (i.e. summed over).
- `leg2 (str|int)` – The leg label or index for the two legs which should be contracted (i.e. summed over).

Returns `traced` – A scalar if `a.rank == 2`, else an *Array* of rank `a.rank - 2`. Equivalent to `sum([a.take_slice([i, i], [leg1, leg2]) for i in range(a.shape[leg1])])`.

Return type *Array|a.dtype*

zeros

- full name: `tenpy.linalg.np_conserved.zeros`
- parent module: `tenpy.linalg.np_conserved`
- type: function

```python
tenpy.linalg.np_conserved.zeros(legcharges, dtype=<class 'numpy.float64'>, qtotal=None, labels=None)
```

Create a npc array full of zeros (with no _data).

This is just a wrapper around `Array(...)`, detailed documentation can be found in the class doc-string of `Array`. 
**Module description**

A module to handle charge conservation in tensor networks.

A detailed introduction to this module (including notations) can be found in *Charge conservation with np_conserved*.

This module *np_conserved* implements a class *Array* designed to make use of charge conservation in tensor networks. The idea is that the *Array* class is used in a fashion very similar to the *numpy.ndarray*, e.g. you can call the functions `tensordot()` or `svd()` (of this module) on them. The structure of the algorithms (as DMRG) is thus the same as with basic numpy ndarrays.

Internally, an *Array* saves charge meta data to keep track of blocks which are nonzero. All possible operations (e.g. `tensordot`, `svd`, ...) on such arrays preserve the total charge structure. In addition, these operations make use of the charges to figure out which of the blocks it has to use/combine - this is the basis for the speed-up.

```python
tenpy.linalg.np_conserved.QCUTOFF = 2.220446049250313e-15
```

A cutoff to ignore machine precision rounding errors when determining charges

```python
tenpy.linalg.np_conserved.QTYPE = <class 'numpy.int64'>
```

The type used for charges

**Overview**

**Classes**

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Array</em> ([legcharges[, dtype, qtotal, labels]])</td>
<td>A multidimensional array (=tensor) for using charge conservation.</td>
</tr>
<tr>
<td><em>ChargeInfo</em> ([mod, names])</td>
<td>Meta-data about the charge of a tensor.</td>
</tr>
<tr>
<td><em>LegCharge</em> ([chargeinfo, slices, charges[, qconj]])</td>
<td>Save the charge data associated to a leg of a tensor.</td>
</tr>
<tr>
<td><em>LegPipe</em> ([legs[, qconj, sort, bunch]])</td>
<td>A <em>LegPipe</em> combines multiple legs of a tensor to one.</td>
</tr>
</tbody>
</table>

**Array creation**

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Array.from_ndarray_trivial</em> ([data_flat[,...]])</td>
<td>Convert a flat numpy ndarray to an Array with trivial charge conservation.</td>
</tr>
<tr>
<td><em>Array.from_ndarray</em> ([data_flat, legcharges[...]]))</td>
<td>Convert a flat (numpy) ndarray to an Array.</td>
</tr>
<tr>
<td><em>Array.from_func</em> ([func, legcharges[, dtype,...]])</td>
<td>Create an Array from a numpy func.</td>
</tr>
<tr>
<td><em>Array.from_func_square</em> ([func, leg[, dtype,...]])</td>
<td>Create an Array from a (numpy) function.</td>
</tr>
<tr>
<td><em>zeros</em> ([legcharges[, dtype, qtotal, labels]])</td>
<td>Create a npc array full of zeros (with no _data).</td>
</tr>
<tr>
<td><em>eye_like</em> ([a[, axis, labels]])</td>
<td>Return an identity matrix contractible with the leg axis of the <em>Array</em> <em>a</em></td>
</tr>
<tr>
<td><em>diag</em> ([s, leg[, dtype, labels]])</td>
<td>Returns a square, diagonal matrix of entries <em>s</em>.</td>
</tr>
</tbody>
</table>
### Concatenation

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>concatenate</code></td>
<td>Stack arrays along a given axis, similar as <code>np.concatenate</code>.</td>
</tr>
<tr>
<td><code>grid_concat</code></td>
<td>Given an <code>np.array</code> of <code>npc.Arrays</code>, performs a multi-dimensional concatenation along ‘axes’.</td>
</tr>
<tr>
<td><code>grid_outer</code></td>
<td>Given an <code>np.array</code> of <code>npc.Arrays</code>, return the corresponding higher-dimensional <code>Array</code>.</td>
</tr>
</tbody>
</table>

### Detecting charges of flat arrays

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>detect_qtotal</code></td>
<td>Returns the total charge (w.r.t legs) of first non-zero sector found in <code>flat_array</code>.</td>
</tr>
<tr>
<td><code>detect_legcharge</code></td>
<td>Calculate a missing <code>LegCharge</code> by looking for nonzero entries of a flat array.</td>
</tr>
<tr>
<td><code>detect_grid_outer_legcharge</code></td>
<td>Derive a <code>LegCharge</code> for a grid used for <code>grid_outer()</code>.</td>
</tr>
</tbody>
</table>

### Contraction of some legs

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>tensordot</code></td>
<td>Similar as <code>np.tensordot</code> but for <code>Array</code>.</td>
</tr>
<tr>
<td><code>outer</code></td>
<td>Forms the outer tensor product, equivalent to <code>tensordot(a, b, axes=0)</code>.</td>
</tr>
<tr>
<td><code>inner</code></td>
<td>Contract all legs in <code>a</code> and <code>b</code>, return scalar.</td>
</tr>
<tr>
<td><code>trace</code></td>
<td>Trace of <code>a</code>, summing over leg <code>l</code> and leg <code>2</code>.</td>
</tr>
</tbody>
</table>

### Linear algebra

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>svd</code></td>
<td>Singualar value decomposition of an <code>Array</code> <code>a</code>.</td>
</tr>
<tr>
<td><code>pinv</code></td>
<td>Compute the (Moore-Penrose) pseudo-inverse of a matrix.</td>
</tr>
<tr>
<td><code>norm</code></td>
<td>Norm of flattened data.</td>
</tr>
<tr>
<td><code>qr</code></td>
<td>Q-R decomposition of a matrix.</td>
</tr>
<tr>
<td><code>expm</code></td>
<td>Use <code>scipy.linalg.expm</code> to calculate the matrix exponential of a square matrix.</td>
</tr>
</tbody>
</table>

### Eigen systems

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>eigh</code></td>
<td>Calculate eigenvalues and eigenvectors for a hermitian matrix.</td>
</tr>
<tr>
<td><code>eig</code></td>
<td>Calculate eigenvalues and eigenvectors for a non-hermitian matrix.</td>
</tr>
<tr>
<td><code>eigvals</code></td>
<td>Calculate eigenvalues for a hermitian matrix.</td>
</tr>
<tr>
<td><code>eigvals</code></td>
<td>Calculate eigenvalues for a hermitian matrix.</td>
</tr>
</tbody>
</table>
Table 53 – continued from previous page

\[ \text{speigs}(a, \text{charge\_sector}, k, *\text{args}, **\text{kwargs}) \] Sparse eigenvalue decomposition \( w, v \) of square \( a \) in a given charge sector.

7.10.2 charges

- full name: tenpy.linalg.charges
- parent module: tenpy.linalg
- type: module

Classes

<table>
<thead>
<tr>
<th>ChargeInfo</th>
<th>LegCharge</th>
</tr>
</thead>
</table>

ChargeInfo([mod, names]) Meta-data about the charge of a tensor.

LegCharge(chargeinfo, slices, charges[, qconj]) Save the charge data associated to a leg of a tensor.

LegPipe(legs[, qconj, sort, bunch]) A LegPipe combines multiple legs of a tensor to one.

ChargeInfo

- full name: tenpy.linalg.charges.ChargeInfo
- parent module: tenpy.linalg.charges
- type: class

Inheritance Diagram
Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ChargeInfo.<strong>init</strong>((mod, names))</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>ChargeInfo.add(chinfos)</td>
<td>Create a ChargeInfo combining multiple charges.</td>
</tr>
<tr>
<td>ChargeInfo.change(chinfo, charge, new_qmod)</td>
<td>Change the qmod of a given charge.</td>
</tr>
<tr>
<td>ChargeInfo.check_valid(charges)</td>
<td>Check, if charges has all entries as expected from self.mod.</td>
</tr>
<tr>
<td>ChargeInfo.drop(chinfo[, charge])</td>
<td>Remove a charge from a ChargeInfo.</td>
</tr>
<tr>
<td>ChargeInfo.from_hdf5(hdf5_loader, h5gr, subpath)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>ChargeInfo.make_valid([charges])</td>
<td>Take charges modulo self.mod.</td>
</tr>
<tr>
<td>ChargeInfo.save_hdf5(hdf5_saver, h5gr, subpath)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>ChargeInfo.test_sanity()</td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ChargeInfo.mod</td>
<td>Modulo how much each of the charges is taken.</td>
</tr>
<tr>
<td>ChargeInfo.qnumber</td>
<td>The number of charges.</td>
</tr>
</tbody>
</table>

class tenpy.linalg.charges.ChargeInfo(mod=[], names=None)

Bases: object

Meta-data about the charge of a tensor.

Saves info about the nature of the charge of a tensor. Provides make_valid() for taking modulo m.

(This class is implemented in tenpy.linalg.charges but also imported in tenpy.linalg
np_conserved for convenience.)

Parameters

- **mod** (iterable of QTYPE) – The len gives the number of charges, qnumber. Each entry is a positive integer, where 1 implies a $U(1)$ charge and $N>1$ implies a $Z_N$ symmetry. Defaults to “trivial”, i.e., no charge.

- **names** (list of str) – Descriptive names for the charges. Defaults to ['',]*qnumber.

  names
  A descriptive name for each of the charges. May have ‘’ entries.

  Type  list of strings

  _mask
  mask (mod == 1), to speed up make_valid in pure python.

  Type  1D array bool

  _mod_masked
  Equivalent to self.mod[self._maks_mod1]

  Type  1D array QTYPE

  _qnumber, _mod
  Storage of qnumber and mod.
Notes

Instances of this class can (should) be shared between different LegCharge and Array's.

**save_hdf5** *(hdf5_saver, h5gr, subpath)*

Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5().

It stores the names under the path "names", and mod as dataset "U1_ZN".

Parameters

- **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.
- **h5gr** (:class:`Group`) – HDF5 group which is supposed to represent self.
- **subpath** (*str*) – The name of h5gr with a '/' in the end.

**classmethod from_hdf5** *(hdf5_loader, h5gr, subpath)*

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

The "U1_ZN" dataset is mandatory, 'names' are optional.

Parameters

- **hdf5_loader** (*Hdf5Loader*) – Instance of the loading engine.
- **h5gr** (*Group*) – HDF5 group which is represent the object to be constructed.
- **subpath** (*str*) – The name of h5gr with a '/' in the end.

Returns **obj** – Newly generated class instance containing the required data.

Return type **cls**

**classmethod add**(chinfos)

Create a ChargeInfo combining multiple charges.

Parameters **chinfos** (iterable of ChargeInfo) – ChargeInfo instances to be combined into a single one (in the given order).

Returns **chinfo** – ChargeInfo combining all the given charges.

Return type **ChargeInfo**

**classmethod drop**(chinfo, charge=None)

Remove a charge from a ChargeInfo.

Parameters

- **chinfo** (ChargeInfo) – The ChargeInfo from where to drop/remove a charge.
- **charge** (int | str) – Number or name of the charge (within chinfo) which is to be dropped. None means dropping all charges.

Returns **chinfo** – ChargeInfo where the specified charge is dropped.

Return type **ChargeInfo**

**classmethod change**(chinfo, charge, new_qmod, new_name='')

Change the qmod of a given charge.

Parameters

- **chinfo** (ChargeInfo) – The ChargeInfo for which qmod of charge should be changed.
• **new_qmod** (*int*) – The new *qmod* to be set.
• **new_name** (*str*) – The new name of the charge.

**Returns**  
`chinfo` – ChargeInfo where *qmod* of the specified charge was changed.

**Return type**  
`ChargeInfo`

test_sanity()  
Sanity check, raises ValueError, if something is wrong.

**property qnumber**  
The number of charges.

**property mod**  
Modulo how much each of the charges is taken.
Entries are 1 for a *U*(1) charge, and *N* for a *Z*_*N* symmetry.

**make_valid** (*charges=None*)  
Take charges modulo self.mod.

**Parameters**  
*charges* (*array_like* or *None*) – 1D or 2D array of charges, last dimension `self.qnumber` None defaults to trivial charges `np.zeros(qnumber, dtype=QTYPE)`.

**Returns**  
A copy of `charges` taken modulo `mod`, but with `x % 1 := x`

**Return type**  
`charges`  

**check_valid** (*charges*)  
Check, if `charges` has all entries as expected from self.mod.

**Parameters**  
*charges* (*2D ndarray* *QTYPE_t*) – Charge values to be checked.

**Returns**  
`res` – True, if all 0 <= `charges` <= self.mod (wherever self.mod != 1)

**Return type**  
`bool`

**LegCharge**

• full name: `tenpy.linalg.charges.LegCharge`
• parent module: `tenpy.linalg.charges`
• type: class

**Inheritance Diagram**

![Inheritance Diagram](image)
## Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>LegCharge.__init__(chargeinfo, slices, charges)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>LegCharge.bunch()</code></td>
<td>Return a copy with bunched self.charges: form blocks for contiguous equal charges.</td>
</tr>
<tr>
<td><code>LegCharge.charge_sectors()</code></td>
<td>Return unique rows of self.charges.</td>
</tr>
<tr>
<td><code>LegCharge.conj()</code></td>
<td>Return a (shallow) copy with opposite self.qconj.</td>
</tr>
<tr>
<td><code>LegCharge.copy()</code></td>
<td>Return a (shallow) copy of self.</td>
</tr>
<tr>
<td><code>LegCharge.extend(extra)</code></td>
<td>Return a new LegCharge, which extends self with further charges.</td>
</tr>
<tr>
<td><code>LegCharge.flip_charges_qconj()</code></td>
<td>Return a copy with both negative qconj and charges.</td>
</tr>
<tr>
<td><code>LegCharge.from_add_charge(legs[, charge-info])</code></td>
<td>Add the (independent) charges of two or more legs to get larger qnumber.</td>
</tr>
<tr>
<td><code>LegCharge.from_change_charge(leg, charge, ...)</code></td>
<td>Remove a charge from a LegCharge.</td>
</tr>
<tr>
<td><code>LegCharge.from_drop_charge(leg[, charge, ...])</code></td>
<td>Remove a charge from a LegCharge.</td>
</tr>
<tr>
<td><code>LegCharge.from_hdf5(hdf5_loader, h5gr, sub-path)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>LegCharge.from_qdict(chargeinfo, qdict[, qconj])</code></td>
<td>Create a LegCharge from qdict form.</td>
</tr>
<tr>
<td><code>LegCharge.from_qflat(chargeinfo, qflat[, qconj])</code></td>
<td>Create a LegCharge from qflat form.</td>
</tr>
<tr>
<td><code>LegCharge.from_qind(chargeinfo, slices, charges)</code></td>
<td>Just a wrapper around self.<strong>init</strong>(), see class docstring for parameters.</td>
</tr>
<tr>
<td><code>LegCharge.from_trivial(ind_len[, ...])</code></td>
<td>Create trivial (qnumber=0) LegCharge for given len of indices ind_len.</td>
</tr>
<tr>
<td><code>LegCharge.get_block_sizes()</code></td>
<td>Return the sizes of the individual blocks.</td>
</tr>
<tr>
<td><code>LegCharge.get_charge(qindex)</code></td>
<td>Return charge self.charges[qindex] * self.qconj for a given qindex.</td>
</tr>
<tr>
<td><code>LegCharge.get_qindex(flat_index)</code></td>
<td>Find qindex containing a flat index.</td>
</tr>
<tr>
<td><code>LegCharge.get_qindex_of_charges(charges)</code></td>
<td>Return the slice selecting the block for given charge values.</td>
</tr>
<tr>
<td><code>LegCharge.get_slice(qindex)</code></td>
<td>Return slice selecting the block for a given qindex.</td>
</tr>
<tr>
<td><code>LegCharge.is_blocked()</code></td>
<td>Returns whether self is blocked, i.e. qindex map 1:1 to charge values.</td>
</tr>
<tr>
<td><code>LegCharge.is_bunched()</code></td>
<td>Checks whether bunch() would change something.</td>
</tr>
<tr>
<td><code>LegCharge.is_sorted()</code></td>
<td>Returns whether self.charges is sorted lexiographically.</td>
</tr>
<tr>
<td><code>LegCharge.perm_flat_from_perm_qind(perm_qind)</code></td>
<td>Convert a permutation of qind (acting on self) into a flat permutation.</td>
</tr>
<tr>
<td><code>LegCharge.perm_qind_from_perm_flat(perm)</code></td>
<td>Convert flat permutation into qind permutation.</td>
</tr>
<tr>
<td><code>LegCharge.project(mask)</code></td>
<td>Return copy keeping only the indices specified by mask.</td>
</tr>
<tr>
<td><code>LegCharge.save_hdf5(hdf5_saver, h5gr, sub-path)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>LegCharge.sort([bunch])</code></td>
<td>Return a copy of self sorted by charges (but maybe not bunched).</td>
</tr>
<tr>
<td><code>LegCharge.test_contractible(other)</code></td>
<td>Raises a ValueError if charges are incompatible for contraction with other.</td>
</tr>
<tr>
<td><code>LegCharge.test_equal(other)</code></td>
<td>Test if charges are equal including qconj.</td>
</tr>
<tr>
<td><code>LegCharge.test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td><code>LegCharge.to_qdict()</code></td>
<td>Return charges in qdict form.</td>
</tr>
</tbody>
</table>

continues on next page
Table 57 – continued from previous page

| `LegCharge.to_qflat()` | Return charges in `qflat` form. |

```python
class tenpy.linalg.charges.LegCharge(chargeinfo, slices, charges, qconj=1):
    Bases: object

    Save the charge data associated to a leg of a tensor.

    This class is more or less a wrapper around a 2D numpy array `charges` and a 1D array `slices`. See `Charge conservation with np_conserved` for more details.

    (This class is implemented in `tenpy.linalg.charges` but also imported in `tenpy.linalg.np_conserved` for convenience.)

    Parameters
    • `chargeinfo` (ChargeInfo) – The nature of the charge.
    • `slices` (1D array_like, len(block_number+1)) – A block with ‘qindex’ `qi` corresponds to the leg indices in slice(slices[qi], slices[qi+1]).
    • `charges` (2D array_like, shape(block_number, chargeinfo.qnumber)) – `charges[qi]` gives the charges for a block with ‘qindex’ `qi`.
    • `qconj` ({+1, -1}) – A flag telling whether the charge points inwards (+1, default) or outwards (-1).
```

```python
ind_len
    The number of indices for this leg.
    
    Type int

block_number
    The number of blocks, i.e., a ‘qindex’ for this leg is in range(block_number).

chargeinfo
    The nature of the charge. Can be shared between LegCharges.
    
    Type ChargeInfo instance

slices
    A block with ‘qindex’ `qi` corresponds to the leg indices in slice(self.slices[qi], self.slices[qi+1]). See `get_slice()`.
    
    Type ndarray[np.intp_t,ndim=1] (block_number+1)

charges
    `charges[qi]` gives the charges for a block with ‘qindex’ `qi`. Note: the sign might be changed by `qconj`. See also `get_charge()`.
    
    Type ndarray[QTYPE_t,ndim=1] (block_number, chargeinfo.qnumber)

qconj
    A flag telling whether the charge points inwards (+1) or outwards (-1). Whenever charges are added, they should be multiplied with their `qconj` value.
    
    Type {-1, 1}

sorted
    Whether the charges are guaranteed to be sorted.
    
    Type bool

bunched
    Whether the charges are guaranteed to be bunched.
```
Type: bool

Notes

Instances of this class can be shared between different npc.Array. Thus, functions changing self.slices or self.charges must always make copies. Further they must set sorted and bunched to False (if they might not preserve them).

copy()
Return a (shallow) copy of self.

save_hdf5(hdf5_saver, h5gr, subpath)
Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5().
Checks format for an output format key "LegCharge". Possible choices are:

"blocks" (default) Store slices and charges directly as datasets, and block_number, sorted, bunched as further attributes.

"compact" A single array np.hstack([self.slices[:-1], self.slices[1:], self.charges]) as dataset "blockcharges", and block_number, sorted, bunched as further attributes.

"flat" Insufficient (!) to recover the exact blocks; saves only the array returned by to_flat() as dataset 'charges'.

The ind_len, qconj, and the format parameter are saved as group attributes under the same names. chinfo is always saved as subgroup.

Parameters

• hdf5_saver (Hdf5Saver) – Instance of the saving engine.
• h5gr (:class `Group`) – HDF5 group which is supposed to represent self.
• subpath (str) – The name of h5gr with a '/' in the end.

classmethod from_hdf5(hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

Parameters

• hdf5_loader (Hdf5Loader) – Instance of the loading engine.
• h5gr (Group) – HDF5 group which is represent the object to be constructed.
• subpath (str) – The name of h5gr with a '/' in the end.

Returns obj – Newly generated class instance containing the required data.

Return type cls

classmethod from_trivial(ind_len, chargeinfo=None, qconj=1)
Create trivial (qnumber=0) LegCharge for given len of indices ind_len.

classmethod from_qflat(chargeinfo, qflat, qconj=1)
Create a LegCharge from qflat form.

Does neither bunch nor sort. We recommend to sort (and bunch) afterwards, if you expect that tensors using the LegCharge have entries at all positions compatible with the charges.
Parameters

- **chargeinfo** (*ChargeInfo*) – The nature of the charge.
- **qflat** *(array_like (ind_len, qnumber)) – qnumber charges for each index of the leg on entry.*
- **qconj** *({-1, 1}) – A flag telling whether the charge points inwards (+1) or outwards (-1).*

See also:

- **sort** sorts by charges
- **bunch** bunches contiguous blocks of the same charge.

```python
classmethod from_qind(chargeinfo, slices, charges, qconj=1)
```
Just a wrapper around self.__init__(), see class doc-string for parameters.

See also:

- **sort** sorts by charges
- **bunch** bunches contiguous blocks of the same charge.

```python
classmethod from_qdict(chargeinfo, qdict, qconj=1)
```
Create a LegCharge from qdict form.

Parameters

- **chargeinfo** (*ChargeInfo*) – The nature of the charge.
- **qdict** *(dict)* – A dictionary mapping a tuple of charges to slices.

```python
classmethod from_add_charge(legs, chargeinfo=None)
```
Add the (independent) charges of two or more legs to get larger qnumber.

Parameters

- **legs** *(iterable of LegCharge)* – The legs for which the charges are to be combined/added.
- **chargeinfo** (*ChargeInfo*) – The ChargeInfo for all charges; create new if None.

Returns **combined** – A LegCharge with the charges of both legs. Is neither sorted nor bunched!

Return type **LegCharge**

```python
classmethod from_drop_charge(leg, charge=None, chargeinfo=None)
```
Remove a charge from a LegCharge.

Parameters

- **leg** *(LegCharge)* – The leg from which to drop/remove a charge.
- **charge** *(int | str)* – Number or name of the charge (within chinfo) which is to be dropped. None means dropping all charges.
- **chargeinfo** (*ChargeInfo*) – The ChargeInfo with charge dropped; create new if None.

Returns **dropped** – A LegCharge with the specified charge dropped. Is neither sorted nor bunched!

Return type **LegCharge**
classmethod from_change_charge(leg, charge, new_qmod, new_name='', chargeinfo=None)
    Remove a charge from a LegCharge.

    Parameters
    • leg (LegCharge) – The leg from which to drop/remove a charge.
    • charge (int | str) – Number or name of the charge (within chargeinfo) for which mod
      is to be changed.
    • new_qmod (int) – The new mod to be set for charge in the ChargeInfo.
    • new_name (str) – The new name for charge.
    • chargeinfo (ChargeInfo) – The ChargeInfo with charge changed; create new if None.

    Returns leg – A LegCharge with the specified charge changed. Is neither sorted nor bunched!

    Return type LegCharge

test_sanity()
    Sanity check, raises ValueErrors, if something is wrong.

conj()
    Return a (shallow) copy with opposite self.qconj.

    Returns conjugated – Shallow copy of self with flipped qconj. test_contractible() of
    self with conjugated will not raise an error.

    Return type LegCharge

flip_charges_qconj()
    Return a copy with both negative qconj and charges.

    Returns conj_charges – (Shallow) copy of self with negative qconj and charges, thus represen-
    ting the very same charges. test_equal() of self with conj_charges will not raise an
    error.

    Return type LegCharge

to_qflat()
    Return charges in qflat form.

to_qdict()
    Return charges in qdict form.
    Raises ValueError, if not blocked.

is_blocked()
    Returns whether self is blocked, i.e. qindex map 1:1 to charge values.

is_sorted()
    Returns whether self.charges is sorted lexicographically.

is_bunched()
    Checks whether bunch() would change something.

test_contractible(other)
    Raises a ValueError if charges are incompatible for contraction with other.

    Parameters other (LegCharge) – The LegCharge of the other leg considdered for contrac-
    tion.

    Raises ValueError – If the charges are incompatible for direct contraction.
Notes

This function checks that two legs are ready for contraction. This is the case, if all of the following conditions are met:

• the ChargeInfo is equal
• the slices are equal
• the charges are the same up to opposite signs $q_{\text{conj}}$:

$$\text{self.charges} \times \text{self}.q_{\text{conj}} = - \text{other.charges} \times \text{other}.q_{\text{conj}}$$

In general, there could also be a change of the total charge, see Charge conservation with np_conserved
This special case is not considered here - instead use gauge_total_charge(), if a change of the charge is desired.

If you are sure that the legs should be contractable, check whether the charges are actually valid or whether self and other are blocked or should be sorted.

See also:

\textbf{test\_equal} self.test\_contractible(other) just performs self.
\textbf{test\_equal}(other).  

\textbf{test\_equal}(other)  
Test if charges are equal including $q_{\text{conj}}$.

Check that all of the following conditions are met:

• the ChargeInfo is equal
• the slices are equal
• the charges are the same up to the signs $q_{\text{conj}}$:

$$\text{self.charges} \times \text{self}.q_{\text{conj}} = \text{other.charges} \times \text{other}.q_{\text{conj}}$$

See also:

\textbf{test\_contractible} self.test\_equal(other) is equivalent to self.
\textbf{test\_contractible}(other).  

\textbf{get\_block\_sizes}()  
Return the sizes of the individual blocks.

Returns sizes – The sizes of the individual blocks; sizes[i] = slices[i+1] - slices[i].

Return type ndarray, shape (block_number,)

\textbf{get\_slice}(qindex)  
Return slice selecting the block for a given qindex.

\textbf{get\_qindex}(flat\_index)  
Find qindex containing a flat index.

Given a flat index, to find the corresponding entry in an Array, we need to determine the block it is saved in. For example, if slices = [[0, 3], [3, 7], [7, 12]], the flat index 5 corresponds to the second entry, qindex = 1 (since 5 is in [3:7]), and the index within the block would be 2 = 5 - 3.

Parameters flat\_index (int) – A flat index of the leg. Negative index counts from behind.
Returns

- **qindex** *(int)* – The qindex, i.e. the index of the block containing *flat_index*.
- **index_within_block** *(int)* – The index of *flat_index* within the block given by *qindex*.

**get_qindex_of_charges** *(charges)*

Return the slice selecting the block for given charge values.

Inverse function of **get_charge()**.

**Parameters**

- **charges** *(1D array_like)* – Charge values for which the slice of the block is to be determined.

**Returns**

- **slice** *(i, j)* – Slice of the charge values for

**Return type** *slice*

:raises ValueError : if the answer is not unique (because *self* is not blocked).

**get_charge** *(qindex)*

Return charge \( \text{self.charges}[\text{qindex}] \times \text{self.qconj} \) for a given *qindex*.

**sort** *(bunch=True)*

Return a copy of *self* sorted by charges (but maybe not bunched).

If bunch=True, the returned copy is completely blocked by charge.

**Parameters**

- **bunch** *(bool)* – Whether *self.bunch* is called after sorting. If True, the leg is guaranteed to be fully blocked by charge.

**Returns**

- **perm_qind** *(array (self.block_len,))* – The permutation of the qindices (before bunching) used for the sorting. To obtain the flat permutation such that \( \text{sorted_array}[\ldots, :] = \text{unsorted_array}[\ldots, \text{perm_flat}], \) use \( \text{perm_flat} = \text{unsorted_leg.perm_flat_from_perm_qind}(\text{perm_qind}) \)
- **sorted_copy** *(LegCharge)* – A shallow copy of *self*, with new qind sorted (and thus blocked if bunch) by charges.

See also:

**bunch** enlarge blocks for contiguous qind of the same charges.

**numpy.take** can apply *perm_flat* to a given axis

**tenpy.tools.misc.inverse_permutation** returns inverse of a permutation

**bunch()**

Return a copy with bunched self.charges: form blocks for contiguous equal charges.

**Returns**

- **idx** *(1D array)* – \( \text{idx}[:-1] \) are the indices of the old qind which are kept, \( \text{idx}[-1] = \text{old_block_number} \).
- **cp** *(LegCharge)* – A new LegCharge with the same charges at given indices of the leg, but (possibly) shorter *self.charges* and *self.slices*.

See also:

**sort** sorts by charges, thus enforcing complete blocking in combination with bunch.
project \( (mask) \)
Return copy keeping only the indices specified by \( mask \).

Parameters mask (1D array (bool)) – Whether to keep of the indices.

Returns

- map_qind (1D array) – Map of qindices, such that \( qind_{\text{new}} = \text{map}_qind[qind_{\text{old}}] \), and \( \text{map}_qind[qind_{\text{old}}] = -1 \) for qindices projected out.
- block_masks (1D array) – The bool mask for each of the remaining blocks.
- projected_copy (LegCharge) – Copy of self with the qind projected by \( mask \).

extend \( (\text{extra}) \)
Return a new LegCharge, which extends self with further charges.

This is needed to formally increase the dimension of an Array.

Parameters extra (LegCharge | int) – By what to extend, i.e. the charges to be appended to self. An int stands for extending the length of the array by a single new block of that size and zero charges.

Returns extended_leg – Copy of self extended by the charge blocks of the extra leg.

Return type LegCharge

charge_sectors()
Return unique rows of self.charges.

Returns charges – Rows are the rows of self.charges lexsorted and without duplicates.

Return type array[QTYPE, ndim=2]

perm_flat_from_perm_qind (perm_qind)
Convert a permutation of qind (acting on self) into a flat permutation.

perm_qind_from_perm_flat (perm_flat)
Convert flat permutation into qind permutation.

Parameters perm_flat (1D array) – A permutation acting on self, which doesn’t mix the blocks of qind.

Returns perm_qind – The permutation of self.qind described by perm_flat.

Return type 1D array

Raises ValueError – If perm_flat mixes blocks of different qindex.

LegPipe

- full name: tenpy.linalg.charges.LegPipe
- parent module: tenpy.linalg.charges
- type: class
Inheritance Diagram

```
LegCharge
  ↓
LegPipe
```

Methods

<table>
<thead>
<tr>
<th>Function Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LegPipe.<strong>init</strong></td>
<td>Initialize self.</td>
</tr>
<tr>
<td>LegPipe.bunch(*args, **kwargs)</td>
<td>Convert to LegCharge and call LegCharge.bunch().</td>
</tr>
<tr>
<td>LegPipe.charge_sectors()</td>
<td>Return unique rows of self.charges.</td>
</tr>
<tr>
<td>LegPipe.conj()</td>
<td>Return a shallow copy with opposite self.qconj.</td>
</tr>
<tr>
<td>LegPipe.copy()</td>
<td>Return a (shallow) copy of self.</td>
</tr>
<tr>
<td>LegPipe.extend(extra)</td>
<td>Return a new LegCharge, which extends self with further charges.</td>
</tr>
<tr>
<td>LegPipe.flip_charges_qconj()</td>
<td>Return a copy with both negative qconj and charges.</td>
</tr>
<tr>
<td>LegPipe.from_add_charge(legs[, chargeinfo])</td>
<td>Add the (independent) charges of two or more legs to get larger qnumber.</td>
</tr>
<tr>
<td>LegPipe.from_change_charge(leg, charge, new_qmod)</td>
<td>Remove a charge from a LegCharge.</td>
</tr>
<tr>
<td>LegPipe.from_drop_charge(leg[, charge, ...])</td>
<td>Remove a charge from a LegCharge.</td>
</tr>
<tr>
<td>LegPipe.from_hdf5(hdf5_loader, h5gr, subpath)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>LegPipe.from_qdict(chargeinfo, qdict[, qconj])</td>
<td>Create a LegCharge from qdict form.</td>
</tr>
<tr>
<td>LegPipe.from_qflat(chargeinfo, qflat[, qconj])</td>
<td>Create a LegCharge from qflat form.</td>
</tr>
<tr>
<td>LegPipe.from_qind(chargeinfo, slices, charges)</td>
<td>Just a wrapper around self.<strong>init</strong>(), see class docstring for parameters.</td>
</tr>
<tr>
<td>LegPipe.from_trivial(ind_len[, chargeinfo, ...])</td>
<td>Create trivial (qnumber=0) LegCharge for given len of indices ind_len.</td>
</tr>
<tr>
<td>LegPipe.get_block_sizes()</td>
<td>Return the sizes of the individual blocks.</td>
</tr>
<tr>
<td>LegPipe.get_charge(qindex)</td>
<td>Return charge self.charges[qindex] * self.qconj for a given qindex.</td>
</tr>
<tr>
<td>LegPipe.get_qindex( flat_index)</td>
<td>Find qindex containing a flat index.</td>
</tr>
<tr>
<td>LegPipe.get_qindex_of_charges( charges)</td>
<td>Return the slice selecting the block for given charge values.</td>
</tr>
<tr>
<td>LegPipe.get_slice(qindex)</td>
<td>Return slice selecting the block for a given qindex.</td>
</tr>
<tr>
<td>LegPipe.is_blocked()</td>
<td>Returns whether self is blocked, i.e. qindex map 1:1 to charge values.</td>
</tr>
<tr>
<td>LegPipe.is_bunched()</td>
<td>Checks whether bunch() would change something.</td>
</tr>
<tr>
<td>LegPipe.is_sorted()</td>
<td>Returns whether self.charges is sorted lexiographically.</td>
</tr>
</tbody>
</table>
Table 58 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>LegPipe.map Incoming Flat</code> (incoming_indices)</td>
<td>Map (flat) incoming indices to an index in the outgoing pipe.</td>
</tr>
<tr>
<td><code>LegPipe.outer Conj()</code></td>
<td>Like <code>conj()</code>, but don’t change <code>qconj</code> for incoming legs.</td>
</tr>
<tr>
<td><code>LegPipe.perm Flat From Perm Qind</code> (perm_qind)</td>
<td>Convert a permutation of <code>qind</code> (acting on <code>self</code>) into a flat permutation.</td>
</tr>
<tr>
<td><code>LegPipe.perm Qind From Perm Flat</code> (perm-flat)</td>
<td>Convert flat permutation into <code>qind</code> permutation.</td>
</tr>
<tr>
<td><code>LegPipe.project</code> (*args, **kwargs)</td>
<td>Convert <code>self</code> to <code>LegCharge</code> and call <code>LegCharge.project()</code>.</td>
</tr>
<tr>
<td><code>LegPipe.save HDF5</code> (hdf5_saver, h5gr, subpath)</td>
<td>Export <code>self</code> into a HDF5 file.</td>
</tr>
<tr>
<td><code>LegPipe.sort</code> (*args, **kwargs)</td>
<td>Convert to <code>LegCharge</code> and call <code>LegCharge.sort()</code>.</td>
</tr>
<tr>
<td><code>LegPipe.test Contractible</code> (other)</td>
<td>Raises a <code>ValueError</code> if charges are incompatible for contraction with other.</td>
</tr>
<tr>
<td><code>LegPipe.test Equal</code> (other)</td>
<td>Test if charges are <code>equal</code> including <code>qconj</code>.</td>
</tr>
<tr>
<td><code>LegPipe.test Sanity</code>()</td>
<td>Sanity check, raises <code>ValueErrors</code>, if something is wrong.</td>
</tr>
<tr>
<td><code>LegPipe.to LegCharge</code>()</td>
<td>Convert <code>self</code> to a <code>LegCharge</code>, discarding the information how to split the legs.</td>
</tr>
<tr>
<td><code>LegPipe.to Qdict()</code></td>
<td>Return charges in <code>qdict</code> form.</td>
</tr>
<tr>
<td><code>LegPipe.to Qflat()</code></td>
<td>Return charges in <code>qflat</code> form.</td>
</tr>
</tbody>
</table>

**class** `tenpy.linalg.charges.LegPipe` *(legs, qconj=1, sort=True, bunch=True)*

**Bases:** `tenpy.linalg.charges.LegCharge`

A `LegPipe` combines multiple legs of a tensor to one.

Often, it is necessary to “combine” multiple legs into one: for example to perform a SVD, the tensor needs to be viewed as a matrix.

This class does exactly this job: it combines multiple `LegCharges` (`incoming legs`) into one ‘pipe’ (the ‘outgoing leg’). The pipe itself is a `LegCharge`, with indices running from 0 to the product of the individual legs’ `ind_len`, corresponding to all possible combinations of input leg indices.

(This class is implemented in `tenpy.linalg.charges` but also imported in `tenpy.linalg.np_conserved` for convenience.)

**Parameters**

- `legs` (list of `LegCharge`) – The legs which are to be combined.
- `qconj` ([+1, -1]) – A flag telling whether the charge of the `resulting` pipe points inwards (+1, default) or outwards (-1).
- `sort` (bool) – Whether the outgoing pipe should be sorted. Default `True`; recommended. Note: calling `sort()` after initialization converts to a `LegCharge`.
- `bunch` (bool) – Whether the outgoing pipe should be bunched. Default `True`; recommended. Note: calling `bunch()` after initialization converts to a `LegCharge`.

**nlegs**

The number of legs.

Type `int`

**legs**

The original legs, which were combined in the pipe.

Type `tuple of LegCharge`
subshape

ind_len for each of the incoming legs.

Type tuple of int

subqshape

block_number for each of the incoming legs.

Type tuple of int

q_map

Shape (block_number, 3 + nlegs). Rows: [ b_j, b_{j+1}, I_s, i_1, ..., i_(nlegs)],
See Notes below for details.

Type array[np.intp, ndim=2]

q_map_slices

Defined such that the row indices of in range(q_map_slices[I_s], q_map_slices[I_s+1])
have q_map[:, 2] == I_s.

Type array[np.intp, ndim=1]

_perm

A permutation such that q_map[_perm, 3:] is sorted by i_l.

Type 1D array

_strides

Strides for mapping incoming qindices i_l to the index of q_map[_perm, :].

Type 1D array

Notes

For np.reshape, taking, for example, i, j, ... → k amounted to k = s_1 * i + s_2 * j + ... for appropriate strides s_1, s_2.

In the charged case, however, we want to block k by charge, so we must implicitly permute as well. This reordering is encoded in q_map.

Each qindex combination of the nlegs input legs (i_1, ..., i_{nlegs}), will end up getting placed in some slice a_j : a_{j+1} of the outgoing pipe. Within this slice, the data is simply reshaped in usual row-major fashion ('C'-order), i.e., with strides s_1 > s_2 > ....

It will be a subslice of a new total block labeled by qindex I_s. Because many charge combinations fuse to the same total charge, in general there will be many tuples (i_1, ..., i_{nlegs}) belonging to the same I_s. The rows of q_map are precisely the collections of [b_j, b_{j+1}, I_s, i_1, ..., i_(nlegs)]. Here, b_j : b_{j+1} denotes the slice of this qindex combination within the total block I_s, i.e., b_j = a_j - self.slices[I_s].

The rows of q_map are lex-sorted first by I_s, then the i. Each I_s will have multiple rows, and the order in which they are stored in q_map is the order the data is stored in the actual tensor, i.e., it might look like

```
[ ... ,
  [ b_j, b_{j+1}, I_s, i_1, ..., i_(nlegs) ],
  [ b_{j+1}, b_{j+2}, I_s, i'_1, ..., i'_(nlegs) ],
  [ 0, b_{j+2}, I_s + 1, i''_1, ..., i''_(nlegs) ],
  [ b_{j+2}, b_{j+3}, I_s + 1, i'''_1, ..., i'''_(nlegs)],
  ...
]
```

The charge fusion rule is:
Here the qindex $Q_i$ of the pipe corresponds to qindices $q_i_1$ on the individual legs.

**copy()**
Return a (shallow) copy of self.

**save_hdf5(hdf5_saver, h5gr, subpath)**
Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5().

In addition to the data saved for the LegCharge, it just saves the legs as subgroup.

**Parameters**
- **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.
- **h5gr** (:class:`Group`) – HDF5 group which is supposed to represent self.
- **subpath** (*str*) – The name of h5gr with a '/' in the end.

**classmethod from_hdf5(hdf5_loader, h5gr, subpath)**
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

**Parameters**
- **hdf5_loader** (*Hdf5Loader*) – Instance of the loading engine.
- **h5gr** (*Group*) – HDF5 group which is represent the object to be constructed.
- **subpath** (*str*) – The name of h5gr with a '/' in the end.

**Returns** obj – Newly generated class instance containing the required data.

**Return type** cls

**test_sanity()**
Sanity check, raises ValueErrors, if something is wrong.

**to_LegCharge()**
Convert self to a LegCharge, discarding the information how to split the legs.

Usually not needed, but called by functions, which are not implemented for a LegPipe.

**conj()**
Return a shallow copy with opposite self.qconj.

**Returns** conjugated – Shallow copy of self with flipped qconj. Whenever we contract two legs, they need to be conjugated to each other. The incoming legs of the pipe are also conjugated.

**Return type** LegCharge

**outer_conj()**
Like conj(), but don’t change qconj for incoming legs.

**sort(*args, **kwargs)**
Convert to LegCharge and call LegCharge.sort().

**bunch(*args, **kwargs)**
Convert to LegCharge and call LegCharge.bunch().
project(*args, **kwargs)
Convert self to LegCharge and call LegCharge.project().

In general, this could be implemented for a LegPipe, but would make split_legs() more complicated, thus we keep it simple. If you really want to project and split afterwards, use the following work-around, which is for example used in exact_diagonalization:

1) Create the full pipe and save it separately.
2) Convert the Pipe to a Leg & project the array with it.
3) [...] do calculations [...] 
4) To split the ‘projected pipe’ of A, create and empty array B with the legs of A, but replace the projected leg by the full pipe. Set A as a slice of B. Finally split the pipe.

map_incoming_flat(incoming_indices)
Map (flat) incoming indices to an index in the outgoing pipe.

Parameters incoming_indices(iterable of int) – One (flat) index on each of the incoming legs.

Returns outgoing_index – The index in the outgoing leg.

Return type int

charge_sectors()
Return unique rows of self.charges.

Returns charges – Rows are the rows of self.charges lexsorted and without duplicates.

Return type array[QTYPE, ndim=2]

extend(extra)
Return a new LegCharge, which extends self with further charges.

This is needed to formally increase the dimension of an Array.

Parameters extra(LegCharge | int) – By what to extend, i.e. the charges to be appended to self. An int stands for extending the length of the array by a single new block of that size and zero charges.

Returns extended_leg – Copy of self extended by the charge blocks of the extra leg.

Return type LegCharge

flip_charges_qconj()
Return a copy with both negative qconj and charges.

Returns conj_charges – (Shallow) copy of self with negative qconj and charges, thus representing the very same charges. test_equal() of self with conj_charges will not raise an error.

Return type LegCharge

classmethod from_add_charge(legs, chargeinfo=None)
Add the (independent) charges of two or more legs to get larger qnumber.

Parameters

• legs(iterable of LegCharge) – The legs for which the charges are to be combined/added.

• chargeinfo(ChargeInfo) – The ChargeInfo for all charges; create new if None.

Returns combined – A LegCharge with the charges of both legs. Is neither sorted nor bunched!
Return type `LegCharge`

classmethod `from_change_charge` *(leg, charge, new_qmod, new_name='', chargeinfo=None)*

Remove a charge from a LegCharge.

Parameters

- `leg` *(LegCharge)* – The leg from which to drop/remove a charge.
- `charge` *(int | str)* – Number or name of the charge (within `chinfo`) for which `mod` is to be changed.
- `new_qmod` *(int)* – The new `mod` to be set for `charge` in the `ChargeInfo`.
- `new_name` *(str)* – The new name for `charge`.
- `chargeinfo` *(ChargeInfo)* – The ChargeInfo with `charge` changed; create new if `None`.

Returns `leg` – A LegCharge with the specified charge changed. Is neither sorted nor bunched!

Return type `LegCharge`

classmethod `from_drop_charge` *(leg, charge=None, chargeinfo=None)*

Remove a charge from a LegCharge.

Parameters

- `leg` *(LegCharge)* – The leg from which to drop/remove a charge.
- `charge` *(int | str)* – Number or name of the charge (within `chinfo`) which is to be dropped. `None` means dropping all charges.
- `chargeinfo` *(ChargeInfo)* – The ChargeInfo with `charge` dropped; create new if `None`.

Returns `dropped` – A LegCharge with the specified charge dropped. Is neither sorted nor bunched!

Return type `LegCharge`

classmethod `from_qdict` *(chargeinfo, qdict, qconj=1)*

Create a LegCharge from qdict form.

Parameters

- `chargeinfo` *(ChargeInfo)* – The nature of the charge.
- `qdict` *(dict)* – A dictionary mapping a tuple of charges to slices.

classmethod `from_qflat` *(chargeinfo, qflat, qconj=1)*

Create a LegCharge from qflat form.

Does neither bunch nor sort. We recommend to sort (and bunch) afterwards, if you expect that tensors using the LegCharge have entries at all positions compatible with the charges.

Parameters

- `chargeinfo` *(ChargeInfo)* – The nature of the charge.
- `qflat` *(array_like (ind_len, qnumber))* – `qnumber` charges for each index of the leg on entry.
- `qconj` *({-1, 1})* – A flag telling whether the charge points inwards (+1) or outwards (-1).

See also:
sort sorts by charges

bunch bunches contiguous blocks of the same charge.

classmethod from_qind(chargeinfo, slices, charges, qconj=1)
Just a wrapper around self.__init__(), see class doc-string for parameters.

See also:

sort sorts by charges

bunch bunches contiguous blocks of the same charge.

classmethod from_trivial(ind_len, chargeinfo=None, qconj=1)
Create trivial (qnumber=0) LegCharge for given len of indices ind_len.

get_block_sizes()
Return the sizes of the individual blocks.

Returns sizes – The sizes of the individual blocks; sizes[i] = slices[i+1] - slices[i].

Return type ndarray, shape (block_number,)

get_charge(qindex)
Return charge self.charges[qindex] * self.qconj for a given qindex.

get_qindex(flat_index)
Find qindex containing a flat index.

Given a flat index, to find the corresponding entry in an Array, we need to determine the block it is saved in. For example, if slices = [[0, 3], [3, 7], [7, 12]], the flat index 5 corresponds to the second entry, qindex = 1 (since 5 is in [3:7]), and the index within the block would be 2 = 5 - 3.

Parameters flat_index (int) – A flat index of the leg. Negative index counts from behind.

Returns

• qindex (int) – The qindex, i.e. the index of the block containing flat_index.

• index_within_block (int) – The index of flat_index within the block given by qindex.

get_qindex_of_charges(charges)
Return the slice selecting the block for given charge values.

Inverse function of get_charge().

Parameters charges (1D array_like) – Charge values for which the slice of the block is to be determined.

Returns slice(i, j) – Slice of the charge values for

Return type slice

:raises ValueError : if the answer is not unique (because self is not blocked):

get_slice(qindex)
Return slice selecting the block for a given qindex.

is_blocked()
Returns whether self is blocked, i.e. qindex map 1:1 to charge values.

is_bunched()
Checks whether bunch() would change something.
is_sorted()
Returns whether self.charges is sorted lexiographically.

perm_flat_from_perm_qind(perm_qind)
Convert a permutation of qind (acting on self) into a flat permutation.

perm_qind_from_perm_flat(perm_flat)
Convert flat permutation into qind permutation.

Parameters perm_flat (1D array) – A permutation acting on self, which doesn’t mix the blocks of qind.

Returns perm_qind – The permutation of self.qind described by perm_flat.

Return type 1D array

Raises ValueError – If perm_flat mixes blocks of different qindex.

test_contractible(other)
Raises a ValueError if charges are incompatible for contraction with other.

Parameters other (LegCharge) – The LegCharge of the other leg considered for contraction.

Raises ValueError – If the charges are incompatible for direct contraction.

Notes
This function checks that two legs are ready for contraction. This is the case, if all of the following conditions are met:
• the ChargeInfo is equal
• the slices are equal
• the charges are the same up to opposite signs qconj:

\[ \text{self.charges} \times \text{self.qconj} = - \text{other.charges} \times \text{other.qconj} \]

In general, there could also be a change of the total charge, see Charge conservation with np_conserved This special case is not considered here - instead use gauge_total_charge(), if a change of the charge is desired.

If you are sure that the legs should be contractable, check whether the charges are actually valid or whether self and other are blocked or should be sorted.

See also:

test_equal self.test_contractible(other) just performs self.

    test_equal(other.conj()).

test_equal(other)
Test if charges are equal including qconj.

Check that all of the following conditions are met:
• the ChargeInfo is equal
• the slices are equal
• the charges are the same up to the signs qconj:
```
self.charges * self.qconj = other.charges * other.qconj
```

See also:

```
test_contractible self.test_equal(other) is equivalent to self.
test_contractible(other.conj()).
```

```
to_qdict ()
    Return charges in qdict form.
    Raises ValueError, if not blocked.

to_qflat ()
    Return charges in qflat form.
```

**Module description**

Basic definitions of a charge.

This module contains implementations for handling the quantum numbers (“charges”) of the `Array`.

In particular, the classes `ChargeInfo`, `LegCharge` and `LegPipe` are implemented here.

**Note:** The contents of this module are imported in `np_conserved`, so you usually don’t need to import this module in your application.

A detailed introduction to `np_conserved` can be found in *Charge conservation with np_conserved*.

In this module, some functions have the python decorator `@use_cython`. Functions with this decorator are replaced by the ones written in Cython, implemented in the file `tenpy/linalg/_npc_helper.pyx`. For further details, see the definition of `use_cython()`.

```
tenpy.linalg.charges.QTYPE = <class 'numpy.int64'>
    Numpy data type for the charges.
```

### 7.10.3 svd_robust

- full name: `tenpy.linalg.svd_robust`
- parent module: `tenpy.linalg`
- type: module

**Functions**

<table>
<thead>
<tr>
<th><code>svd</code>([full_matrices, compute_uv, ...])</th>
<th>Wrapper around <code>scipy.linalg.svd()</code> with gesvd backup plan.</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>svd_gesvd</code>([full_matrices, compute_uv, ...])</td>
<td>svd with LAPACK’s ‘#gesvd’ (with # = d/z for float/complex).</td>
</tr>
</tbody>
</table>

7.10. linalg 273
svd

- full name: tenpy.linalg.svd_robust.svd
- parent module: tenpy.linalg.svd_robust
- type: function

tenpy.linalg.svd_robust.svd(a, full_matrices=True, compute_uv=True, overwrite_a=False, check_finite=True, lapack_driver='gesdd', warn=True)

Wrapper around scipy.linalg.svd() with gesvd backup plan.

Tries to avoid raising an LinAlgError by using using the lapack_driver gesvd, if gesdd failed.

Parameters not described below are as in scipy.linalg.svd()

Parameters

- overwrite_a (bool) – Ignored (i.e. set to False) if lapack_driver='gesdd'. Otherwise described in scipy.linalg.svd().

- lapack_driver ({'gesdd', 'gesvd'}, optional) – Whether to use the more efficient divide-and-conquer approach ('gesdd') or general rectangular approach ('gesvd') to compute the SVD. MATLAB and Octave use the 'gesvd' approach. Default is 'gesdd'. If 'gesdd' fails, 'gesvd' is used as backup.

- warn (bool) – Whether to create a warning when the SVD failed.

Returns U, S, Vh – As described in doc-string of scipy.linalg.svd().

Return type ndarray

darray

svd_gesvd

- full name: tenpy.linalg.svd_robust.svd_gesvd
- parent module: tenpy.linalg.svd_robust
- type: function

tenpy.linalg.svd_robust.svd_gesvd(a, full_matrices=True, compute_uv=True, check_finite=True)

svd with LAPACK’s ‘#gesvd’ (with # = d/z for float/complex).

Similar as numpy.linalg.svd(), but use LAPACK ‘gesvd’ driver. Works only with 2D arrays. Outer part is based on the code of numpy.linalg.svd.

Parameters

- a – See numpy.linalg.svd() for details.

- full_matrices – See numpy.linalg.svd() for details.

- compute_uv – See numpy.linalg.svd() for details.

- check_finite – check whether input arrays contain ‘NaN’ or ‘inf’.

Returns U, S, Vh – See numpy.linalg.svd() for details.

Return type ndarray
Module description

(More) robust version of singular value decomposition.

We often need to perform an SVD. In general, an SVD is a matrix factorization that is always well defined and should also work for ill-conditioned matrices. But sadly, both numpy.linalg.svd() and scipy.linalg.svd() fail from time to time, raising LinAlgError("SVD did not converge"). The reason is that both of them call the LAPACK function #gesdd (where # depends on the data type), which takes an iterative approach that can fail. However, it is usually much faster than the alternative (and robust) #gesvd.

Our workaround is as follows: we provide a function svd() with call signature as scipy’s svd. This function is basically just a wrapper around scipy’s svd, i.e., we keep calling the faster dgesdd. But if that fails, we can still use dgesvd as a backup.

Sadly, dgesvd and zgesvd were not included into scipy until version ‘0.18.0’ (nor in numpy), which is as the time of this writing the latest stable scipy version. For scipy version newer than ‘0.18.0’, we make use of the new keyword ‘lapack_driver’ for svd, otherwise we (try to) load dgesvd and zgesvd from shared LAPACK libraries.

The tribute for the dgesvd wrapper code goes to ‘jgarcke’, originally posted at http://projects.scipy.org/numpy/ticket/990, which is now hosted at https://github.com/numpy/numpy/issues/1588 He explains a bit more in detail what fails.

The include of dgesvd to scipy was done in https://github.com/scipy/scipy/pull/5994.

Examples

The idea is that you just import the svd from this module and use it as replacement for np.linalg.svd or scipy.linalg.svd:

```python
>>> from tenpy.linalg.svd_robust import svd
>>> U, S, VT = svd([[1., 1.], [0., 1.]])
```

7.10.4 random_matrix

- full name: tenpy.linalg.random_matrix
- parent module: tenpy.linalg
- type: module

Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>COE(size)</td>
<td>Circular orthogonal ensemble (COE).</td>
</tr>
<tr>
<td>CRE(size)</td>
<td>Circular real ensemble (CRE).</td>
</tr>
<tr>
<td>CUE(size)</td>
<td>Circular unitary ensemble (CUE).</td>
</tr>
<tr>
<td>GOE(size)</td>
<td>Gaussian orthogonal ensemble (GOE).</td>
</tr>
<tr>
<td>GUE(size)</td>
<td>Gaussian unitary ensemble (GUE).</td>
</tr>
<tr>
<td>O_close_1(size[, a])</td>
<td>return an random orthogonal matrix 'close' to the Identity.</td>
</tr>
<tr>
<td>U_close_1(size[, a])</td>
<td>return an random orthogonal matrix 'close' to the identity.</td>
</tr>
<tr>
<td>box(size[, W])</td>
<td>return random number uniform in (-W, W].</td>
</tr>
<tr>
<td>standard_normal_complex(size)</td>
<td>return (R + 1.j*I) for independent R and I from np.random.standard_normal.</td>
</tr>
</tbody>
</table>
COE

- full name: tenpy.linalg.random_matrix.COE
- parent module: tenpy.linalg.random_matrix
- type: function
tenpy.linalg.random_matrix.COE(size)
  Circular orthogonal ensemble (COE).
  
  Parameters size (tuple) – (n, n), where \( n \) is the dimension of the output matrix.
  
  Returns U – Unitary, symmetric (complex) matrix drawn from the COE (=Haar measure on this space).

  Return type ndarray

CRE

- full name: tenpy.linalg.random_matrix.CRE
- parent module: tenpy.linalg.random_matrix
- type: function
tenpy.linalg.random_matrix.CRE(size)
  Circular real ensemble (CRE).
  
  Parameters size (tuple) – (n, n), where \( n \) is the dimension of the output matrix.
  
  Returns U – Orthogonal matrix drawn from the CRE (=Haar measure on O(n)).

  Return type ndarray

CUE

- full name: tenpy.linalg.random_matrix.CUE
- parent module: tenpy.linalg.random_matrix
- type: function
tenpy.linalg.random_matrix.CUE(size)
  Circular unitary ensemble (CUE).
  
  Parameters size (tuple) – (n, n), where \( n \) is the dimension of the output matrix.
  
  Returns U – Unitary matrix drawn from the CUE (=Haar measure on U(n)).

  Return type ndarray
GOE

- full name: tenpy.linalg.random_matrix.GOE
- parent module: tenpy.linalg.random_matrix
- type: function

```python
tenpy.linalg.random_matrix.GOE(size)
```

Gaussian orthogonal ensemble (GOE).

**Parameters**

- `size` (tuple) – (n, n), where n is the dimension of the output matrix.

**Returns**

H – Real, symmetric numpy matrix drawn from the GOE, i.e. 
\[ p(H) = \frac{1}{Z} \exp\left(-\frac{n}{4} \text{tr}(H^2)\right) \]

**Return type**

ndarray

GUE

- full name: tenpy.linalg.random_matrix.GUE
- parent module: tenpy.linalg.random_matrix
- type: function

```python
tenpy.linalg.random_matrix.GUE(size)
```

Gaussian unitary ensemble (GUE).

**Parameters**

- `size` (tuple) – (n, n), where n is the dimension of the output matrix.

**Returns**

H – Hermitian (complex) numpy matrix drawn from the GUE, i.e. 
\[ p(H) = \frac{1}{Z} \exp\left(-\frac{n}{4} \text{tr}(H^2)\right) \]

**Return type**

ndarray

O_close_1

- full name: tenpy.linalg.random_matrix.O_close_1
- parent module: tenpy.linalg.random_matrix
- type: function

```python
tenpy.linalg.random_matrix.O_close_1(size, a=0.01)
```

return an random orthogonal matrix 'close' to the Identity.

**Parameters**

- `size` (tuple) – (n, n), where n is the dimension of the output matrix.
- `a` (float) – Parameter determining how close the result is on O; \( \lim_{a \to 0} <|O - E| >_a = 0 \) (where E is the identity).

**Returns**

O – Orthogonal matrix close to the identity (for small a).

**Return type**

ndarray
**U_close_1**

- full name: tenpy.linalg.random_matrix.U_close_1
- parent module: tenpy.linalg.random_matrix
- type: function

```python
tenpy.linalg.random_matrix.U_close_1(size, a=0.01)
```

return an random orthogonal matrix 'close' to the identity.

**Parameters**

- **size (tuple)** – \((n, n)\), where \(n\) is the dimension of the output matrix.
- **a (float)** – Parameter determining how close the result is to the identity. \(\lim_{a \to 0} < |O - E| >_a = 0\) (where \(E\) is the identity).

**Returns**

- **U** – Unitary matrix close to the identity (for small \(a\)). Eigenvalues are chosen i.i.d. as \(\exp(1.j*a*x)\) with \(x\) uniform in [-1, 1].

**Return type**

- ndarray

---

**box**

- full name: tenpy.linalg.random_matrix.box
- parent module: tenpy.linalg.random_matrix
- type: function

```python
tenpy.linalg.random_matrix.box(size, W=1.0)
```

return random number uniform in \((-W, W]\).

---

**standard_normal_complex**

- full name: tenpy.linalg.random_matrix.standard_normal_complex
- parent module: tenpy.linalg.random_matrix
- type: function

```python
tenpy.linalg.random_matrix.standard_normal_complex(size)
```

return \((R + 1.j*I)\) for independent \(R\) and \(I\) from np.random.standard_normal.

---

**Module description**

Provide some random matrix ensembles for numpy.
The implemented ensembles are:

<table>
<thead>
<tr>
<th>ensemble</th>
<th>matrix class drawn from</th>
<th>measure</th>
<th>invariant under</th>
<th>beta</th>
</tr>
</thead>
<tbody>
<tr>
<td>GOE</td>
<td>real, symmetric</td>
<td>~ (\exp(-n/4 \text{ tr}(H^2)))</td>
<td>orthogonal O</td>
<td>1</td>
</tr>
<tr>
<td>GUE</td>
<td>hermitian</td>
<td>~ (\exp(-n/2 \text{ tr}(H^2)))</td>
<td>unitary U</td>
<td>2</td>
</tr>
<tr>
<td>CRE</td>
<td>O(n)</td>
<td>Haar</td>
<td>orthogonal O</td>
<td>/</td>
</tr>
<tr>
<td>COE</td>
<td>U in U(n) with U = U^T</td>
<td>Haar</td>
<td>orthogonal O</td>
<td>1</td>
</tr>
<tr>
<td>CUE</td>
<td>U(n)</td>
<td>Haar</td>
<td>unitary U</td>
<td>2</td>
</tr>
<tr>
<td>O_close_1</td>
<td>O(n)</td>
<td>?</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>U_close_1</td>
<td>U(n)</td>
<td>?</td>
<td>/</td>
<td>/</td>
</tr>
</tbody>
</table>
All functions in this module take a tuple \((n, n)\) as first argument, such that we can use the function `from_func()` to generate a block diagonal \(Array\) with the block from the corresponding ensemble, for example:

```python
npc.Array.from_func_square(GOE, [leg, leg.conj()])
```

## 7.10.5 sparse

- full name: `tenpy.linalg.sparse`
- parent module: `tenpy.linalg`
- type: module

### Classes

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>FlatHermitianOperator</code></td>
<td>Hermitian variant of <code>FlatLinearOperator</code>.</td>
</tr>
<tr>
<td><code>FlatLinearOperator</code></td>
<td>Square linear operator acting on numpy arrays based on (\text{matvec}) acting on (\text{npc}) Arrays.</td>
</tr>
<tr>
<td><code>NpcLinearOperator</code></td>
<td>Prototype for a linear operator acting on (\text{Array}).</td>
</tr>
<tr>
<td><code>NpcLinearOperatorWrapper</code></td>
<td>Base class for wrapping around another <code>NpcLinearOperator</code>.</td>
</tr>
<tr>
<td><code>OrthogonalNpcLinearOperator</code></td>
<td>Replace (H \rightarrow PHP) with the projector (P = 1 - \sum_o</td>
</tr>
<tr>
<td><code>ShiftNpcLinearOperator</code></td>
<td>Represents (\text{original_operator} + \text{shift} \ast \text{identity}).</td>
</tr>
<tr>
<td><code>SumNpcLinearOperator</code></td>
<td>Sum of two linear operators.</td>
</tr>
</tbody>
</table>

**FlatHermitianOperator**

- full name: `tenpy.linalg.sparse.FlatHermitianOperator`
- parent module: `tenpy.linalg.sparse`
- type: class
### Methods

<table>
<thead>
<tr>
<th>Method Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FlatHermitianOperator.</strong> <code>__init__(npc_matvec,...)</code></td>
<td>Initialize this LinearOperator.</td>
</tr>
<tr>
<td><code>adjoint()</code></td>
<td>Hermitian adjoint.</td>
</tr>
<tr>
<td><code>dot(x)</code></td>
<td>Matrix-matrix or matrix-vector multiplication.</td>
</tr>
<tr>
<td><code>eigenvectors(*args,...)</code></td>
<td>Same as <code>FlatLinearOperator(..., hermitian=True)</code>.</td>
</tr>
<tr>
<td><code>flat_to_npc(vec)</code></td>
<td>Convert flat numpy vector of selected charge sector into npc Array.</td>
</tr>
<tr>
<td><code>flat_to_npc_None_sector(vec)</code></td>
<td>Convert flat vector of undetermined charge sectors into npc Array.</td>
</tr>
<tr>
<td><code>flat_to_npc_all_sectors(vec)</code></td>
<td>Convert flat vector of all charge sectors into npc Array with extra “charge” leg.</td>
</tr>
<tr>
<td><code>from_NpcArray(mat[....])</code></td>
<td>Create a <code>FlatLinearOperator</code> from a square <code>Array</code>.</td>
</tr>
<tr>
<td><code>from_guess_with_pipe(...)</code></td>
<td>Create a <code>FlatLinearOperator</code> from a <code>matvec</code> function acting on multiple legs.</td>
</tr>
<tr>
<td><code>matmat(X)</code></td>
<td>Matrix-matrix multiplication.</td>
</tr>
<tr>
<td><code>matvec(x)</code></td>
<td>Matrix-vector multiplication.</td>
</tr>
<tr>
<td><code>npc_to_flat(npc_vec)</code></td>
<td>Convert npc Array into a 1D ndarray, inverse of <code>flat_to_npc()</code>.</td>
</tr>
<tr>
<td><code>npc_to_flat_all_sectors(npc_vec)</code></td>
<td>Convert npc Array with qtotal = self.charge_sector into ndarray.</td>
</tr>
<tr>
<td><code>rmatmat(X)</code></td>
<td>Adjoint matrix-matrix multiplication.</td>
</tr>
<tr>
<td><code>rmatvec(x)</code></td>
<td>Adjoint matrix-vector multiplication.</td>
</tr>
<tr>
<td><code>transpose()</code></td>
<td>Transpose this linear operator.</td>
</tr>
</tbody>
</table>
### Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FlatHermitianOperator.H</td>
<td>Hermitian adjoint.</td>
</tr>
<tr>
<td>FlatHermitianOperator.T</td>
<td>Transpose this linear operator.</td>
</tr>
<tr>
<td>FlatHermitianOperator.charge_sector</td>
<td>Charge sector of the vector which is acted on.</td>
</tr>
<tr>
<td>FlatHermitianOperator.ndim</td>
<td></td>
</tr>
</tbody>
</table>

```python
class tenpy.linalg.sparse.FlatHermitianOperator(*args, **kwargs)
    Bases: tenpy.linalg.sparse.FlatLinearOperator
```

Hermitian variant of FlatLinearOperator.

Note that we don’t check `matvec()` to return a hermitian result, we only define an adjoint to be `self`.

**property** H

- Hermitian adjoint.

  Returns the Hermitian adjoint of self, aka the Hermitian conjugate or Hermitian transpose. For a complex matrix, the Hermitian adjoint is equal to the conjugate transpose.

  Can be abbreviated `self.H` instead of `self.adjoint()`.

  **Returns** A_H – Hermitian adjoint of self.

  **Return type** LinearOperator

**property** T

- Transpose this linear operator.

  Returns a LinearOperator that represents the transpose of this one. Can be abbreviated `self.T` instead of `self.transpose()`.

**adjoint()**

- Hermitian adjoint.

  Returns the Hermitian adjoint of self, aka the Hermitian conjugate or Hermitian transpose. For a complex matrix, the Hermitian adjoint is equal to the conjugate transpose.

  Can be abbreviated `self.H` instead of `self.adjoint()`.

  **Returns** A_H – Hermitian adjoint of self.

  **Return type** LinearOperator

**property** charge_sector

- Charge sector of the vector which is acted on.

**dot**(x)

- Matrix-matrix or matrix-vector multiplication.

  **Parameters** x (array_like) – 1-d or 2-d array, representing a vector or matrix.

  **Returns** Ax – 1-d or 2-d array (depending on the shape of x) that represents the result of applying this linear operator on x.

  **Return type** array

**flat_to_npc**(vec)

- Convert flat numpy vector of selected charge sector into npc Array.

  If `charge_sector` is not None, convert to a 1D npc vector with leg `self.leg`. Otherwise convert vec, which can be non-zero in all charge sectors, to a npc matrix with an additional 'charge' leg to allow representing the full vector at once.
Parameters vec (1D ndarray) – Numpy vector to be converted. Should have the entries according to self.charge_sector.

Returns npc_vec – Same as vec, but converted into a npc array.

Return type Array

flat_to_npc_None_sector (vec, cutoff=1e-10)
Convert flat vector of undetermined charge sectors into npc Array.

The charge sector to be used is chosen as the block with the maximal norm, not by self.charge_sector (which might be None).

Parameters vec (1D ndarray) – Numpy vector to be converted.

Returns npc_vec – Same as vec, but converted into a npc array.

Return type Array

flat_to_npc_all_sectors (vec)
Convert flat vector of all charge sectors into npc Array with extra “charge” leg.

Deprecated since version 0.7.3: This is merged into flat_to_npc() with self.charge_sector = None.

Parameters vec (1D ndarray) – Numpy vector to be converted.

Returns npc_vec – Same as vec, but converted into a npc array.

Return type Array

classmethod from_NpcArray (mat, charge_sector=0)
Create a FlatLinearOperator from a square Array.

Parameters

• mat (Array) – A square matrix, with contractable legs.

• charge_sector (None | charges | 0) – Selects the charge sector of the vector onto which the Linear operator acts. None stands for all sectors, 0 stands for the zero-charge sector. Defaults to 0, i.e., assumes the dominant eigenvector is in charge sector 0.

classmethod from_guess_with_pipe (npc_matvec, v0_guess, labels_split=None, dtype=None)
Create a FlatLinearOperator from a matvec function acting on multiple legs.

This function creates a wrapper matvec function to allow acting on a “vector” with multiple legs. The wrapper combines the legs into a LegPipe before calling the actual matvec function, and splits them again in the end.

Parameters

• npc_matvec (function) – Function to calculate the action of the linear operator on an npc vector with the given split labels labels_split. Has to return an npc vector with the same legs.

• v0_guess (Array) – Initial guess/starting vector which can be applied to npc_matvec.

• labels_split (None | list of str) – Labels of v0_guess in the order in which they are to be combined into a LegPipe. None defaults to v0_guess, get_leg_labels().

• dtype (np.dtype | None) – The data type of the arrays. None defaults to dtype of v0_guess (!).

Returns
- **lin_op** (*cls*) – Instance of the class to be used as linear operator
- **guess_flat** (*np.ndarray*) – Numpy vector representing the guess $v_0 \_guess$.

**matmat** (*X*)
Matrix-matrix multiplication.
Performs the operation $y=A \times X$ where $A$ is an $M \times N$ linear operator and $X$ dense $N \times K$ matrix or ndarray.

**Parameters**


**Returns**

$Y$ – A matrix or ndarray with shape (M,K) depending on the type of the X argument.

**Return type**

{matrix, ndarray}

**Notes**

This matmat wraps any user-specified matmat routine or overridden _matmat method to ensure that $y$ has the correct type.

**matvec** (*x*)
Matrix-vector multiplication.
Performs the operation $y=A \times x$ where $A$ is an $M \times N$ linear operator and $x$ is a column vector or 1-d array.

**Parameters**

$x$ (*matrix*, *ndarray*) – An array with shape (N,) or (N,1).

**Returns**

$y$ – A matrix or ndarray with shape (M,) or (M,1) depending on the type and shape of the $x$ argument.

**Return type**

{matrix, ndarray}

**Notes**

This matvec wraps the user-specified matvec routine or overridden _matvec method to ensure that $y$ has the correct shape and type.

**npc_to_flat** (*npc_vec*)
Convert npc Array into a 1D ndarray, inverse of flat_to_npc().

**Parameters**

npc_vec (*Array*) – Npc Array to be converted. If self.charge_sector is not None, this should be a 1D array with that qtotal. If self.charge_sector is not None, it should have an additional "charge" leg, (as returned by flat_to_npc()).

**Returns**

vec – Same entries as npc_vec, but converted into a flat Numpy array.

**Return type**

1D ndarray

**npc_to_flat_all_sectors** (*npc_vec*)
Convert npc Array with qtotal = self.charge_sector into ndarray.

Deprecated since version 0.7.3: This is merged into npc_to_flat() with self.charge_sector = None.

**Parameters**

npc_vec (*Array*) – Npc Array to be converted. Should only have entries in self.charge_sector.

**Returns**

vec – Same as npc_vec, but converted into a flat Numpy array.

**Return type**

1D ndarray
**rmatmat** \((X)\)

Adjoint matrix-matrix multiplication.

Performs the operation \(y = A^H \cdot x\) where \(A\) is an \(M \times N\) linear operator and \(x\) is a column vector or 1-d array, or 2-d array. The default implementation defers to the adjoint.

- **Parameters** \(X\)({matrix,ndarray}) – A matrix or 2D array.
- **Returns** \(Y\) – A matrix or 2D array depending on the type of the input.
- **Return type** {matrix,ndarray}

**Notes**

This rmatmat wraps the user-specified rmatmat routine.

**rmatvec** \((x)\)

Adjoint matrix-vector multiplication.

Performs the operation \(y = A^H \cdot x\) where \(A\) is an \(M \times N\) linear operator and \(x\) is a column vector or 1-d array.

- **Parameters** \(x\)({matrix,ndarray}) – An array with shape (M,) or (M,1).
- **Returns** \(y\) – A matrix or ndarray with shape (N,) or (N,1) depending on the type and shape of the x argument.
- **Return type** {matrix,ndarray}

**Notes**

This rmatvec wraps the user-specified rmatvec routine or overridden _rmatvec method to ensure that \(y\) has the correct shape and type.

**transpose** ()

Transpose this linear operator.

Returns a LinearOperator that represents the transpose of this one. Can be abbreviated self.T instead of self.transpose().

**eigenvectors** (*args, **kwargs)

Same as FlatLinearOperator(..., hermitian=True).

---

**FlatLinearOperator**

- full name: tenpy.linalg.sparse.FlatLinearOperator
- parent module: tenpy.linalg.sparse
- type: class
**Inheritance Diagram**

```
  LinearOperator
     ↓
 FlatLinearOperator
```

**Methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>FlatLinearOperator.__init__(npc_matvec, leg, ...)</code></td>
<td>Initialize this LinearOperator.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.adjoint()</code></td>
<td>Hermitian adjoint.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.dot(x)</code></td>
<td>Matrix-matrix or matrix-vector multiplication.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.eigenvectors([num_ev, ...])</code></td>
<td>Find (dominant) eigenvector(s) of self using <code>scipy.sparse.linalg.eigs()</code>.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.flat_to_npc(vec)</code></td>
<td>Convert flat numpy vector of selected charge sector into npc Array.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.from_NpcArray(mat[, ...])</code></td>
<td>Create a <code>FlatLinearOperator</code> from a square <code>Array</code>.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.from_guess_with_pipe(...)</code></td>
<td>Create a <code>FlatLinearOperator</code> from a <code>matvec</code> function acting on multiple legs.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.matmat(X)</code></td>
<td>Matrix-matrix multiplication.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.matvec(x)</code></td>
<td>Matrix-vector multiplication.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.npc_to_flat(npc_vec)</code></td>
<td>Convert npc Array into a 1D ndarray, inverse of <code>flat_to_npc()</code>.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.npc_to_flat_all_sectors(npc_vec)</code></td>
<td>Convert npc Array with <code>qtotal = self.charge_sector</code> into ndarray.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.rmatmat(X)</code></td>
<td>Adjoint matrix-matrix multiplication.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.rmatvec(x)</code></td>
<td>Adjoint matrix-vector multiplication.</td>
</tr>
<tr>
<td><code>FlatLinearOperator.transpose()</code></td>
<td>Transpose this linear operator.</td>
</tr>
</tbody>
</table>
Class Attributes and Properties

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FlatLinearOperator.H</td>
<td>Hermitian adjoint.</td>
</tr>
<tr>
<td>FlatLinearOperator.T</td>
<td>Transpose this linear operator.</td>
</tr>
<tr>
<td>FlatLinearOperator.charge_sector</td>
<td>Charge sector of the vector which is acted on.</td>
</tr>
<tr>
<td>FlatLinearOperator.ndim</td>
<td></td>
</tr>
</tbody>
</table>

```python
class tenpy.linalg.sparse.FlatLinearOperator(*args, **kwargs)
    Bases: scipy.sparse.linalg.interface.LinearOperator

Square Linear operator acting on numpy arrays based on a `matvec` acting on npc Arrays.

Note that this class represents a square linear operator. In terms of charges, this means it has legs `[self.leg, self.leg.conj()]` and trivial (zero) qtotal.

Parameters

- `npc_matvec (function)` – Function to calculate the action of the linear operator on an npc vector (with the specified leg). Has to return an npc vector with the same leg.
- `leg (LegCharge)` – Leg of the vector on which `npc_matvec` can act on.
- `dtype (np.dtype)` – The data type of the arrays.
- `charge_sector (None | charges | 0)` – Selects the charge sector of the vector onto which the Linear operator acts. None stands for all sectors, 0 stands for the zero-charge sector. Defaults to 0, i.e., assumes the dominant eigenvector is in charge sector 0.
- `vec_label (None | str)` – Label to be set to the npc vector before acting on it with `npc_matvec`. Ignored if None.

possible_charge_sectors
Each row corresponds to one possible choice for charge_sector.

Type ndarray[QTYPE, ndim=2]

shape
The dimensions for the selected charge sector.

Type (int, int)

dtype
The data type of the arrays.

Type np.dtype

leg
Leg of the vector on which `npc_matvec` can act on.

Type LegCharge

vec_label
Label to be set to the npc vector before acting on it with `npc_matvec`. Ignored if None.

Type None | str

npc_matvec
Function to calculate the action of the linear operator on an npc vector (with one leg).

Type function

matvec_count
The number of times `npc_matvec` was called.
Type \texttt{int}

\_\texttt{mask}

The indices of \textit{leg} corresponding to the \textit{charge\_sector} to be diagonalized.

Type \texttt{ndarray[ndim=1, bool]}

\_\texttt{npc\_matvec\_multileg}

Only set if initialized with \texttt{from\_guess\_with\_pipe()}. The \textit{npc\_matvec} function to be wrapped around. Takes the npc Array in multidimensional form and returns it that way.

Type \texttt{function | None}

\_\texttt{labels\_split}

Only set if initialized with \texttt{from\_guess\_with\_pipe()}. Labels of the guess before combining them into a pipe (stored as \textit{leg}).

Type \texttt{list of str}

classmethod \texttt{from\_NpcArray(mat, charge\_sector=0)}

Create a \texttt{FlatLinearOperator} from a square \texttt{Array}.

Parameters

- \texttt{mat (Array)} – A square matrix, with contractable legs.
- \texttt{charge\_sector (None \textbar} \texttt{charges \textbar} 0) – Selects the charge sector of the vector onto which the Linear operator acts. \texttt{None} stands for \textit{all} sectors, 0 stands for the zero-charge sector. Defaults to 0, i.e., \texttt{assumes} the dominant eigenvector is in charge sector 0.

classmethod \texttt{from\_guess\_with\_pipe(npc\_matvec, v0\_guess, labels\_split=\texttt{None}, dtype=\texttt{None})}

Create a \texttt{FlatLinearOperator} from a \texttt{matvec} function acting on multiple legs.

This function creates a wrapper \texttt{matvec} function to allow acting on a “vector” with multiple legs. The wrapper combines the legs into a \texttt{LegPipe} before calling the actual \texttt{matvec} function, and splits them again in the end.

Parameters

- \texttt{npc\_matvec (function)} – Function to calculate the action of the linear operator on an npc vector with the given split labels \texttt{labels\_split}. Has to return an npc vector with the same legs.
- \texttt{v0\_guess (Array)} – Initial guess/starting vector which can be applied to \texttt{npc\_matvec}.
- \texttt{labels\_split (None \textbar} \texttt{list of str}) – Labels of \texttt{v0\_guess} in the order in which they are to be combined into a \texttt{LegPipe}. \texttt{None} defaults to \texttt{v0\_guess}. \texttt{get\_leg\_labels()}
- \texttt{dtype (np.dtype \textbar} \texttt{None)} – The data type of the arrays. \texttt{None} defaults to \texttt{dtype} of \texttt{v0\_guess} (!).

Returns

- \texttt{lin\_op (cls)} – Instance of the class to be used as linear operator
- \texttt{guess\_flat (np.ndarray)} – Numpy vector representing the guess \texttt{v0\_guess}.

property \texttt{charge\_sector}

Charge sector of the vector which is acted on.

\texttt{flat\_to\_npc(\texttt{vec})}

Convert flat numpy vector of selected charge sector into npc Array.
If `charge_sector` is not None, convert to a 1D npc vector with leg `self.leg`. Otherwise convert `vec`, which can be non-zero in all charge sectors, to a npc matrix with an additional 'charge' leg to allow representing the full vector at once.

**Parameters**

- `vec` *(1D ndarray)* – Numpy vector to be converted. Should have the entries according to `self.charge_sector`.

**Returns**

- `npc_vec` – Same as `vec`, but converted into a npc array.

**Return type**

- *Array*

### `npc_to_flat(npc_vec)`

Convert npc Array into a 1D ndarray, inverse of `flat_to_npc()`.

**Parameters**

- `npc_vec` *(Array)* – Npc Array to be converted. If `self.charge_sector` is not None, this should be a 1D Array with that `qtotal`. If `self.charge_sector` is not None, it should have an additional "charge" leg, (as returned by `flat_to_npc()`).

**Returns**

- `vec` – Same entries as `npc_vec`, but converted into a flat Numpy array.

**Return type**

- *1D ndarray*

### `flat_to_npc_all_sectors(vec)`

Convert flat vector of all charge sectors into npc Array with extra "charge" leg.

Deprecated since version 0.7.3: This is merged into `flat_to_npc()` with `self.charge_sector = None`.

**Parameters**

- `vec` *(1D ndarray)* – Numpy vector to be converted.

**Returns**

- `npc_vec` – Same as `vec`, but converted into a npc array.

**Return type**

- *Array*

### `flat_to_npc_None_sector(vec, cutoff=1e-10)`

Convert flat vector of undetermined charge sectors into npc Array.

The charge sector to be used is chosen as the block with the maximal norm, not by `self.charge_sector` (which might be `None`).

**Parameters**

- `vec` *(1D ndarray)* – Numpy vector to be converted.

**Returns**

- `npc_vec` – Same as `vec`, but converted into a npc array.

**Return type**

- *Array*

### `npc_to_flat_all_sectors(npc_vec)`

Convert npc Array with `qtotal = self.charge_sector` into ndarray.

Deprecated since version 0.7.3: This is merged into `npc_to_flat()` with `self.charge_sector = None`.

**Parameters**

- `npc_vec` *(Array)* – Npc Array to be converted. Should only have entries in `self.charge_sector`.

**Returns**

- `vec` – Same as `npc_vec`, but converted into a flat Numpy array.

**Return type**

- *1D ndarray*

### `eigenvectors(num_ev=1, max_num_ev=None, max_tol=1e-12, which='LM', v0=None, v0_npc=None, cutoff=1e-12, hermitian=False, **kwargs)`

Find (dominant) eigenvector(s) of `self` using `scipy.sparse.linalg.eigs()`.

If no `charge_sector` was selected, we look in all charge sectors.

**Parameters**
• `num_ev (int)` – Number of eigenvalues/vectors to look for.

• `max_num_ev (int)` – `scipy.sparse.linalg.speigs()` sometimes raises a `NoConvergenceError` for small `num_ev`, which might be avoided by increasing `num_ev`. As a work-around, we try it again in the case of an error, just with larger `num_ev` up to `max_num_ev`. None defaults to `num_ev + 2`.

• `max_tol (float)` – After the first `NoConvergenceError` we increase the `tol` argument to that value.

• `which (str)` – Which eigenvalues to look for, see `scipy.sparse.linalg.eigs()`. More details also in `argsort()`.

• `v0 (Array)` – Initial guess as a “flat” numpy array.

• `v0_npc (Array)` – Initial guess, to be converted by `npc_to_flat()`.

• `cutoff (float)` – Only used if `self.charge_sector` is `None`; in that case it determines when entries in a given charge-block are considered nonzero, and what counts as degenerate.

• `hermitian (bool)` – If False (default), use `scipy.sparse.linalg.eigs()` If True, assume that `self` is hermitian and use `scipy.sparse.linalg.eigsh()`.

• `**kwargs` – Further keyword arguments given to `scipy.sparse.linalg.eigsh()` or `scipy.sparse.linalg.eigs()`, respectively.

Returns

• `eta (1D ndarray)` – The eigenvalues, sorted according to `which`.

• `w` (list of `Array`) – The eigenvectors corresponding to `eta`, as `npc.Array` with LegPipe.

property `H`

Hermitian adjoint.

Returns the Hermitian adjoint of self, aka the Hermitian conjugate or Hermitian transpose. For a complex matrix, the Hermitian adjoint is equal to the conjugate transpose.

Can be abbreviated self.H instead of self.adjoint().

Returns `A_H` – Hermitian adjoint of self.

Return type `LinearOperator`

property `T`

Transpose this linear operator.

Returns a LinearOperator that represents the transpose of this one. Can be abbreviated self.T instead of self.transpose().

adjoint()

Hermitian adjoint.

Returns the Hermitian adjoint of self, aka the Hermitian conjugate or Hermitian transpose. For a complex matrix, the Hermitian adjoint is equal to the conjugate transpose.

Can be abbreviated self.H instead of self.adjoint().

Returns `A_H` – Hermitian adjoint of self.

Return type `LinearOperator`

dot `(x)`

Matrix-matrix or matrix-vector multiplication.
Parameters $x$ (array_like) – 1-d or 2-d array, representing a vector or matrix.

Returns $Ax$ – 1-d or 2-d array (depending on the shape of $x$) that represents the result of applying this linear operator on $x$.

Return type array

matmat ($X$)
Matrix-matrix multiplication.

Performs the operation $y = A*X$ where $A$ is an $M$x$N$ linear operator and $X$ dense $N$x$K$ matrix or ndarray.

Parameters $X$ ($\{matrix, \ ndarray\}$) – An array with shape (N,K).

Returns $Y$ – A matrix or ndarray with shape (M,K) depending on the type of the $X$ argument.

Return type $\{matrix, \ ndarray\}$

Notes
This matmat wraps any user-specified matmat routine or overridden _matmat method to ensure that $y$ has the correct type.

matvec ($x$)
Matrix-vector multiplication.

Performs the operation $y = A*x$ where $A$ is an $M$x$N$ linear operator and $x$ is a column vector or 1-d array.

Parameters $x$ ($\{matrix, \ ndarray\}$) – An array with shape (N,) or (N,1).

Returns $y$ – A matrix or ndarray with shape (M,) or (M,1) depending on the type and shape of the $x$ argument.

Return type $\{matrix, \ ndarray\}$

Notes
This matvec wraps the user-specified matvec routine or overridden _matvec method to ensure that $y$ has the correct shape and type.

rmatmat ($X$)
Adjoint matrix-matrix multiplication.

Performs the operation $y = A^H * x$ where $A$ is an $M$x$N$ linear operator and $x$ is a column vector or 1-d array, or 2-d array. The default implementation defers to the adjoint.

Parameters $X$ ($\{matrix, \ ndarray\}$) – A matrix or 2D array.

Returns $Y$ – A matrix or 2D array depending on the type of the input.

Return type $\{matrix, \ ndarray\}$
Notes

This rmatmat wraps the user-specified rmatmat routine.

\texttt{rmatvec}(x)
Adjoint matrix-vector multiplication.
Performs the operation \( y = A^H \times x \) where \( A \) is an \( M \times N \) linear operator and \( x \) is a column vector or 1-d array.

\textbf{Parameters} \( x \) ((\texttt{matrix, ndarray}) -- An array with shape \( (M,) \) or \( (M,1) \).

\textbf{Returns} \( y \) -- A matrix or ndarray with shape \( (N,) \) or \( (N,1) \) depending on the type and shape of the \( x \) argument.

\textbf{Return type} \{matrix, ndarray\}

Notes

This rmatvec wraps the user-specified rmatvec routine or overridden \_rmatvec method to ensure that \( y \) has the correct shape and type.

\texttt{transpose}()
Transpose this linear operator.

Returns a LinearOperator that represents the transpose of this one. Can be abbreviated \texttt{self.T} instead of \texttt{self.transpose()}.

\textbf{NpcLinearOperator}

- full name: tenpy.linalg.sparse.NpcLinearOperator
- parent module: \texttt{tenpy.linalg.sparse}
- type: class

\textbf{Inheritance Diagram}

$\hspace{1cm}$

```
NpcLinearOperator
```

7.10. linalg
Methods

NpcLinearOperator.__init__()  Initialize self.
NpcLinearOperator.adjoint()  Return the hermitian conjugate of self
NpcLinearOperator.matvec(vec)  Calculate the action of the operator on a vector vec.
NpcLinearOperator.to_matrix()  Contract self to a matrix.

Class Attributes and Properties

NpcLinearOperator.acts_on

class tenpy.linalg.sparse.NpcLinearOperator
Bases: object

Prototype for a Linear Operator acting on Array.

Note that an Array implements a matvec function. Thus you can use any (square) npc Array as an NpcLinearOperator.

dtype
The data type of its action.

    Type np.type

acts_on
Labels of the state on which the operator can act. NB: Class attribute.

    Type list of str

matvec(vec)
Calculate the action of the operator on a vector vec.

    Note that we don’t require vec to be one-dimensional. However, for square operators we require that the result of matvec has the same legs (in the same order) as vec such that they can be added. Note that this excludes a non-trivial qtotal for square operators.

to_matrix()
Contract self to a matrix.

    If self represents an operator with very small shape, e.g. because the MPS bond dimension is very small, an algorithm might choose to contract self to a single tensor.

    Returns matrix – Contraction of the represented operator.

    Return type Array

adjoint()
Return the hermitian conjugate of self

    If self is hermitian, subclasses can choose to implement this to define the adjoint operator of self.
### NpcLinearOperatorWrapper

- full name: `tenpy.linalg.sparse.NpcLinearOperatorWrapper`
- parent module: `tenpy.linalg.sparse`
- type: class

#### Inheritance Diagram

![Inheritance Diagram](image)

#### Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>__init__(orig_operator)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>adjoint()</code></td>
<td>Return the hermitian conjugate of <code>self</code>.</td>
</tr>
<tr>
<td><code>to_matrix()</code></td>
<td>Contract <code>self</code> to a matrix.</td>
</tr>
<tr>
<td><code>unwrapped()</code></td>
<td>Return to the original NpcLinearOperator.</td>
</tr>
</tbody>
</table>

#### class `tenpy.linalg.sparse.NpcLinearOperatorWrapper` (orig_operator)

Bases: `object`

Base class for wrapping around another `NpcLinearOperator`.

Attributes not explicitly set with `self.attribute = value` (or by defining methods) default to the attributes of the wrapped `orig_operator`.

**Warning:** If there are multiple levels of wrapping operators, the order might be critical to get correct results; e.g. `OrthogonalNpcLinearOperator` needs to be the outer-most wrapper to produce correct results and/or be efficient.

**Parameters**

- `orig_operator (NpcLinearOperator)` – The original operator implementing the `matvec`.

- `orig_operator`
  The original operator implementing the `matvec`.

- `unwrapped()`
  Return to the original NpcLinearOperator.

  If multiple levels of wrapping were used, this returns the most unwrapped one.
to_matrix()
Contract self to a matrix.

adjoint()
Return the hermitian conjugate of self.

If self is hermitian, subclasses can choose to implement this to define the adjoint operator of self.

OrthogonalNpcLinearOperator

- full name: tenpy.linalg.sparse.OrthogonalNpcLinearOperator
- parent module: tenpy.linalg.sparse
- type: class

Inheritance Diagram

```
NpcLinearOperatorWrapper
          ↓
OrthogonalNpcLinearOperator
```

Methods

```
OrthogonalNpcLinearOperator.__init__(...)
Initialize self.

OrthogonalNpcLinearOperator.adjoint()
Return the hermitian conjugate of self.

OrthogonalNpcLinearOperator.matvec(vec)

OrthogonalNpcLinearOperator.to_matrix()
Contract self to a matrix.

OrthogonalNpcLinearOperator.unwrapped()
Return to the original NpcLinearOperator.
```

class tenpy.linalg.sparse.OrthogonalNpcLinearOperator(orig_operator, ortho_vecs)
Bases: tenpy.linalg.sparse.NpcLinearOperatorWrapper

Replace \( H \rightarrow P H P \) with the projector \( P = 1 - \sum_o |o> <o| \).
Here, \( |o> \) are the vectors from \( \text{ortho_vecs} \).

Parameters

- \( \text{orig_operator} \) (EffectiveH) – The original EffectiveH instance to wrap around.
• **ortho_vecs** (list of *Array*) – The vectors to orthogonalize against.

```python
to_matrix()
Contract *self* to a matrix.
```

```python
adjoint()
Return the hermitian conjugate of *self*.
If *self* is hermitian, subclasses *can* choose to implement this to define the adjoint operator of *self*.
```

```python
unwrapped()
Return to the original NpcLinearOperator.
If multiple levels of wrapping were used, this returns the most unwrapped one.
```

**ShiftNpcLinearOperator**

- full name: tenpy.linalg.sparse.ShiftNpcLinearOperator
- parent module: tenpy.linalg.sparse
- type: class

**Inheritance Diagram**

```
NpcLinearOperatorWrapper
  ▼
  ShiftNpcLinearOperator
```

**Methods**

```python
ShiftNpcLinearOperator.__init__(...)
Initialize *self*.
```

```python
ShiftNpcLinearOperator.adjoint()
Return the hermitian conjugate of *self*.
```

```python
ShiftNpcLinearOperator.matvec(vec)
```

```python
ShiftNpcLinearOperator.to_matrix()
Contract *self* to a matrix.
```

```python
ShiftNpcLinearOperator.unwrapped()
Return to the original NpcLinearOperator.
```

**class** tenpy.linalg.sparse.ShiftNpcLinearOperator(*orig_operator*, *shift*)

Bases: tenpy.linalg.sparse.NpcLinearOperatorWrapper

Representes *original_operator + shift* + identity.
This can be useful e.g. for better Lanczos convergence.

to_matrix()
Contract self to a matrix.

**adjoint()**
Return the hermitian conjugate of self.

If self is hermitian, subclasses can choose to implement this to define the adjoint operator of self.

**unwrapped()**
Return to the original NpcLinearOperator.

If multiple levels of wrapping were used, this returns the most unwrapped one.

---

**SumNpcLinearOperator**

- full name: tenpy.linalg.sparse.SumNpcLinearOperator
- parent module: tenpy.linalg.sparse
- type: class

**Inheritance Diagram**

```
NpcLinearOperatorWrapper
    ↓
SumNpcLinearOperator
```

**Methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>__init__(orig_operator, ...)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>SumNpcLinearOperator.adjoint()</code></td>
<td>Return the hermitian conjugate of self.</td>
</tr>
<tr>
<td><code>SumNpcLinearOperator.matvec(vec)</code></td>
<td>Contract self to a matrix.</td>
</tr>
<tr>
<td><code>SumNpcLinearOperator.to_matrix()</code></td>
<td>Contract self to a matrix.</td>
</tr>
<tr>
<td><code>SumNpcLinearOperator.unwrapped()</code></td>
<td>Return to the original NpcLinearOperator.</td>
</tr>
</tbody>
</table>

**class tenpy.linalg.sparse.SumNpcLinearOperator** *(orig_operator, other_operator)*

Bases: tenpy.linalg.sparse.NpcLinearOperatorWrapper

Sum of two linear operators.

**to_matrix()**
Contract self to a matrix.

**adjoint()**
Return the hermitian conjugate of self.
If `self` is hermitian, subclasses can choose to implement this to define the adjoint operator of `self`.

```python
unwrapped()
```

Return to the original NpcLinearOperator.

If multiple levels of wrapping were used, this returns the most unwrapped one.

### Module description

Providing support for sparse algorithms (using matrix-vector products only).

Some linear algebra algorithms, e.g. Lanczos, do not require the full representations of a linear operator, but only the action on a vector, i.e., a matrix-vector product `matvec`. Here we define the structure of such a general operator, `NpcLinearOperator`, as it is used in our own implementations of these algorithms (e.g., `lanczos`). Moreover, the `FlatLinearOperator` allows to use all the scipy sparse methods by providing functionality to convert flat numpy arrays to and from `np_conserved` arrays.

### 7.10.6 lanczos

- full name: `tenpy.linalg.lanczos`
- parent module: `tenpy.linalg`
- type: module

#### Classes

![Diagram of classes: LanczosGroundState and LanczosEvolution](image)

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>LanczosEvolution(H, psi0, options)</code></td>
<td>Calculate `exp(deltaH)</td>
</tr>
<tr>
<td><code>LanczosGroundState(H, psi0, options[, ...])</code></td>
<td>Lanczos algorithm working on npc arrays.</td>
</tr>
</tbody>
</table>
Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>gram_schmidt(vecs[, rcond, verbose])</code></td>
<td>In place Gram-Schmidt Orthogonalization and normalization for npc Arrays.</td>
</tr>
<tr>
<td><code>lanczos(H, psi[, options, orthogonal_to])</code></td>
<td>Simple wrapper calling LanczosGroundState(H, psi, options, orthogonal_to).run()</td>
</tr>
<tr>
<td><code>lanczos_arpack(H, psi[, options, orthogonal_to])</code></td>
<td>Use scipy.sparse.linalg.eigsh() to find the ground state of H.</td>
</tr>
<tr>
<td><code>plot_stats(ax, Es)</code></td>
<td>Plot the convergence of the energies.</td>
</tr>
</tbody>
</table>

**gram_schmidt**

- full name: tenpy.linalg.lanczos.gram_schmidt
- parent module: tenpy.linalg.lanczos
- type: function

    ```python
    tenpy.linalg.lanczos.gram_schmidt(vecs, rcond=1e-14, verbose=0)
    
    In place Gram-Schmidt Orthogonalization and normalization for npc Arrays.
    
    Parameters
    
    - `vecs` (list of Array) – The vectors which should be orthogonalized. All with the same order of the legs. Entries are modified in place. If a norm < rcond, the entry is set to None.
    - `rcond` (float) – Vectors of norm < rcond (after projecting out previous vectors) are discarded.
    - `verbose` (int) – Print additional output if verbose >= 1.
    
    Returns
    
    - `vecs` (list of Array) – The ortho-normalized vectors (without any None).
    - `ov` (2D Array) – For j >= i, ov[j, i] = npc.inner(vecs[j], vecs[i], 'range', do_conj=True) (where vecs[j] was orthogonalized to all vecs[k], k < i).
    ```

**lanczos**

- full name: tenpy.linalg.lanczos.lanczos
- parent module: tenpy.linalg.lanczos
- type: function

    ```python
    tenpy.linalg.lanczos.lanczos(H, psi, options={}, orthogonal_to=[])
    
    Simple wrapper calling LanczosGroundState(H, psi, options, orthogonal_to).run()
    
    Deprecated since version 0.6.0: Going to remove the orthogonal_to argument. Instead, replace H with OrthogonalNpcLinearOperator(H, orthogonal_to) using the OrthogonalNpcLinearOperator.
    
    Parameters
    
    - `H` – See LanczosGroundState.
    - `psi` – See LanczosGroundState.
    - `options` – See LanczosGroundState.
    ```
• **orthogonal_to** – See LanczosGroundState.

**Returns** See LanczosGroundState.run().

**Return type** E0, psi0, N

---

**lanczos_arpack**

- full name: tenpy.linalg.lanczos.lanczos_arpack
- parent module: tenpy.linalg.lanczos
- type: function

```
tenpy.linalg.lanczos.lanczos_arpack(H, psi, options={}, orthogonal_to=[])```

Use `scipy.sparse.linalg.eigsh()` to find the ground state of \( H \).

This function has the same call/return structure as `lanczos()`, but uses the ARPACK package through the functions `speigsh()` instead of the custom `lanczos` implementation in `LanczosGroundState`. This function is mostly intended for debugging, since it requires to convert the vector from `np_conserved Array` into a flat `numpy array` and back during each **matvec**-operation!

Deprecated since version 0.6.0: Going to remove the `orthogonal_to` argument. Instead, replace \( H \) with `OrthogonalNpcLinearOperator(H, orthogonal_to)` using the `OrthogonalNpcLinearOperator`.

**Parameters**

- \( H \) – See LanczosGroundState. \( H \) and \( psi \) should have/use labels.
- \( psi \) – See LanczosGroundState. \( H \) and \( psi \) should have/use labels.
- `options` – See LanczosGroundState. \( H \) and \( psi \) should have/use labels.
- `orthogonal_to` – See LanczosGroundState. \( H \) and \( psi \) should have/use labels.

**Returns**

- \( E0 \) (**float**) – Ground state energy.
- \( psi0 \) (**Array**) – Ground state vector.

---

**plot_stats**

- full name: tenpy.linalg.lanczos.plot_stats
- parent module: tenpy.linalg.lanczos
- type: function

```
tenpy.linalg.lanczos.plot_stats(ax, Es)```

Plot the convergence of the energies.

**Parameters**

- `ax` (**matplotlib.axes.Axes**) – The axes on which we should plot.
- `Es` (**list of ndarray.**) – The energies `Lanczos.Es`.
Module description

Lanczos algorithm for np_conserved arrays.

7.11 models

- full name: tenpy.models
- parent module: tenpy
- type: module

Module description

Definition of the various models.
For an introduction to models see Models.
The module tenpy.models.model contains base classes for models. The module tenpy.models.lattice contains base classes and implementations of lattices. All other modules in this folder contain model classes derived from these base classes.

Submodules

<table>
<thead>
<tr>
<th>lattice</th>
<th>Classes to define the lattice structure of a model.</th>
</tr>
</thead>
<tbody>
<tr>
<td>model</td>
<td>This module contains some base classes for models.</td>
</tr>
</tbody>
</table>

7.11.1 lattice

- full name: tenpy.models.lattice
- parent module: tenpy.models
- type: module

Classes
<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chain(L, site, **kwargs)</td>
<td>A chain of L equal sites.</td>
</tr>
<tr>
<td>Honeycomb(Lx, Ly, sites, **kwargs)</td>
<td>A honeycomb lattice.</td>
</tr>
<tr>
<td>IrregularLattice(regular_lattice[, remove, ...])</td>
<td>A variant of a regular lattice, where we might have extra sites or sites missing.</td>
</tr>
<tr>
<td>Kagome(Lx, Ly, sites, **kwargs)</td>
<td>A Kagome lattice.</td>
</tr>
<tr>
<td>Ladder(L, sites, **kwargs)</td>
<td>A ladder coupling two chains.</td>
</tr>
<tr>
<td>Lattice(Ls, unit_cell[, order, bc, bc_MPS, ...])</td>
<td>A general, regular lattice.</td>
</tr>
<tr>
<td>SimpleLattice(Ls, site, **kwargs)</td>
<td>A lattice with a unit cell consisting of just a single site.</td>
</tr>
<tr>
<td>Square(Lx, Ly, site, **kwargs)</td>
<td>A square lattice.</td>
</tr>
<tr>
<td>Triangular(Lx, Ly, site, **kwargs)</td>
<td>A triangular lattice.</td>
</tr>
<tr>
<td>TrivialLattice(mps_sites, **kwargs)</td>
<td>Trivial lattice consisting of a single (possibly large) unit cell in 1D.</td>
</tr>
</tbody>
</table>

**Chain**

- full name: tenpy.models.lattice.Chain
- parent module: tenpy.models.lattice
- type: class

**Inheritance Diagram**
Methods

- **Chain.__init__(L, site, **kwargs)**: Initialize self.
- **Chain.count_neighbors([u, key])**: Count e.g.
- **Chain.coupling_shape(dx)**: Calculate correct shape of the strengths for a coupling.
- **Chain.enlarge_mps_unit_cell([factor])**: Repeat the unit cell for infinite MPS boundary conditions; in place.
- **Chain.from_hdf5(hdf5_loader, h5gr, subpath)**: Load instance from a HDF5 file.
- **Chain.lat2mps_idx(lat_idx)**: Translate lattice indices \((x_0, \ldots, x_{(D-1)}, u)\) to MPS index \(i\).
- **Chain.mps2lat_idx(i)**: Translate MPS index \(i\) to lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\).
- **Chain.mps2lat_values(A[, axes, u])**: same as Lattice.mps2lat_values(), but ignore \(u\), setting it to 0.
- **Chain.mps2lat_values_masked(A[, axes, ...])**: Reshape/reorder an array \(A\) to replace an MPS index by lattice indices.
- **Chain.mps_idx_fix_u([u])**: return an index array of MPS indices for which the site within the unit cell is \(u\).
- **Chain.mps_lat_idx_fix_u([u])**: Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.
- **Chain.mps_sites()**: Return a list of sites for all MPS indices.
- **Chain.multi_coupling_shape(dx)**: Calculate correct shape of the strengths for a multi_coupling.
- **Chain.number_nearest_neighbors([u])**: Deprecated.
- **Chain.number_next_nearest_neighbors([u])**: Deprecated.
- **Chain.ordering(order)**: Provide possible orderings of the \(N\) lattice sites.
- **Chain.plot_basis(ax[, origin, shade])**: Plot arrows indicating the basis vectors of the lattice.
- **Chain.plot_bc_identified(ax[, direction, ...])**: Mark two sites identified by periodic boundary conditions.
- **Chain.plot_coupling(ax[, coupling, wrap])**: Plot lines connecting nearest neighbors of the lattice.
- **Chain.plot_order(ax[, order, textkwargs])**: Plot a line connecting sites in the specified “order” and text labels enumerating them.
- **Chain.plot_sites(ax[, markers])**: Plot the sites of the lattice with markers.
- **Chain.position(lat_idx)**: return ‘space’ position of one or multiple sites.
- **Chain.possible_couplings(u1, u2, dx)**: Find possible MPS indices for two-site couplings.
- **Chain.possible_multi_couplings(ops)**: Generalization of possible_couplings() to couplings with more than 2 sites.
- **Chain.save_hdf5(hdf5_saver, h5gr, subpath)**: Export self into a HDF5 file.
- **Chain.site(i)**: return Site instance corresponding to an MPS index \(i\).
- **Chain.test_sanity()**: Sanity check.

Class Attributes and Properties

- **Chain.Lu**
- **Chain.boundary_conditions**
- **Chain.dim**
- **Chain.nearest_neighbors**
- **Chain.next_nearest_neighbors**

... continues on next page
Table 77 – continued from previous page

<table>
<thead>
<tr>
<th>Chain.next_next_nearest_neighbors</th>
<th>Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.</th>
</tr>
</thead>
</table>

```python
class tenpy.models.lattice.Chain(L, site, **kwargs)
```

Bases: `tenpy.models.lattice.SimpleLattice`  
A chain of L equal sites.

**Parameters**

- `L (int)` – The length of the chain.
- `site (Site)` – The local lattice site. The `unit_cell` of the `Lattice` is just `[site]`.
- `**kwargs` – Additional keyword arguments given to the `Lattice`. `pairs` are initialized with `[next_]next_[next_]nearest_neighbors`. `positions` can be specified as a single vector.

```python
dim = 1
```
the dimension of the lattice

**ordering (order)**

Provide possible orderings of the `N` lattice sites.

The following orders are defined in this method compared to `Lattice.ordering()`:

<table>
<thead>
<tr>
<th>Order</th>
<th>Resulting order</th>
</tr>
</thead>
<tbody>
<tr>
<td>'default'</td>
<td>0, 1, 2, 3, 4, ... , L-1</td>
</tr>
<tr>
<td>'folded'</td>
<td>L-1, 1, L-2, ... , L//2</td>
</tr>
</tbody>
</table>

This order might be useful if you want to consider a ring with periodic boundary conditions with a finite MPS: It avoids the ultra-long range of the coupling from site 0 to L present in the default order.

**property boundary_conditions**

Human-readable list of boundary conditions from `bc` and `bc_shift`.

**Returns** `boundary_conditions` – List of "open" or "periodic", one entry for each direction of the lattice.

**Return type** list of str

**count_neighbors (u=0, key='nearest_neighbors')**

Count e.g. the number of nearest neighbors for a site in the bulk.

**Parameters**
• **u** (*int*) – Specifies the site in the unit cell, for which we should count the number of
neighbors (or whatever *key* specifies).

• **key** (*str*) – Key of pairs to select what to count.

**Returns**  
*number* – Number of nearest neighbors (or whatever *key* specified) for the *u*-th site in
the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value
at the edges of a lattice with open boundary conditions.

**Return type**  
*int*

coupling_shape(*dx*)

Calculate correct shape of the *strengths* for a coupling.

**Parameters**  
*dx* (*tuple of int*) – Translation vector in the lattice for a coupling of two
operators. Corresponds to *dx* argument of *tenpy.models.model.CouplingModel.add_multi_coupling()*.

**Returns**

• **coupling_shape** (*tuple of int*) – Len *dim*. The correct shape for an array specifying the
coupling strength. *lat_indices* has only rows within this shape.

• **shift_lat_indices** (*array*) – Translation vector from origin to the lower left corner of box
spanned by *dx*.

enlarge_mps_unit_cell(*factor=2*)

Repeat the unit cell for infinite MPS boundary conditions; in place.

**Parameters**  
*factor* (*int*) – The new number of sites in the MPS unit cell will be increased
from *N_sites* to *factor*\**N_sites_per_ring*. Since MPS unit cells are repeated in
the *x*-direction in our convention, the lattice shape goes from (*Lx*, *Ly*, ..., *Lu*) to
(*Lx*\**factor*, *Ly*, ..., *Lu*).

classmethod from_hdf5(*hdf5_loader, h5gr, subpath*)

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with *save_hdf5()*.

**Parameters**

• **hdf5_loader** (*Hdf5Loader*) – Instance of the loading engine.

• **h5gr** (*Group*) – HDF5 group which is represent the object to be constructed.

• **subpath** (*str*) – The *name* of *h5gr* with a ‘/’ in the end.

**Returns**  
*obj* – Newly generated class instance containing the required data.

**Return type**  
*cls*

lat2mps_idx(*lat_idx*)

Translate lattice indices (*x_0*, ..., *x_(D-1)*, *u*) to MPS index *i*.

**Parameters**

• **lat_idx** (*array_like [*., dim+1]*) – The last dimension corresponds to
lattice indices (*x_0*, ..., *x_(D-1)*, *u*). All lattice indices should be positive and
smaller than the corresponding entry in *self.shape*. Exception: for “infinite” *bc_MPS*,
an *x_0* outside indicates shifts across the boundary.

**Returns**  
*i* – MPS index/indices corresponding to *lat_idx*. Has the same shape as *lat_idx* without
the last dimension.

**Return type**  
*array_like*
mps2lat_idx(i)
Translate MPS index i to lattice indices \((x_0, \ldots, x_{\text{dim}-1}, u)\).

Parameters
- **i** *(int | array_like of int) – MPS index/indices.*

Returns
- **lat_idx** – First dimensions like \(i\), last dimension has len \(\text{dim}+1\) and contains the lattice indices \((x_0, \ldots, x_{\text{dim}-1}, u)\) corresponding to \(i\). For \(i\) across the MPS unit cell and “infinite” bc_MPS, we shift \(x_0\) accordingly.

Return type
array

mps2lat_values(A, axes=0, u=None)
same as Lattice.mps2lat_values(), but ignore \(u\), setting it to 0.

mps2lat_values_masked(A, axes=-1, mps_inds=None, include_u=None)
Reshape/reorder an array \(A\) to replace an MPS index by lattice indices.

This is a generalization of mps2lat_values() allowing for the case of an arbitrary set of MPS indices present in each axis of \(A\).

Parameters
- **A** *(ndarray) – Some values.*
- **axes** *(iterable of int) – Chooses the axis of \(A\) which should be replaced. If multiple axes are given, you also need to give multiple index arrays as mps_inds.*
- **mps_inds** *(list of 1D ndarray) – Specifies for each axis in axes, for which MPS indices we have values in the corresponding axis of \(A\). Defaults to [np.arange(A.shape[ax]) for ax in axes]. For indices across the MPS unit cell and “infinite” bc_MPS, we shift \(x_0\) accordingly.*
- **include_u** *(list of bool) – Specifies for each axis in axes, whether the \(u\) index of the lattice should be included into the output array res_A. Defaults to len(self.unit_cell) > 1.*

Returns
- **res_A** – Reshaped and reordered copy of \(A\). Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index \(j\) maps to lattice site \((x0, x1, x2)\), then res_A[... , x0, x1, x2, ...] = A[... , mps_inds[j], ...].

Return type
np.ma.MaskedArray

mps_idx_fix_u(u=None)
return an index array of MPS indices for which the site within the unit cell is \(u\).

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This functions returns an index array of the mps indices which belong to sites given by self.unit_cell[u].

Parameters
- **u** *(None | int) – Selects a site of the unit cell. None (default) means all sites.*

Returns
- **mps_idx** – MPS indices for which self.site(i) is self.unit_cell[u]. Ordered ascending.

Return type
array

mps_lat_idx_fix_u(u=None)
Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.

Parameters
- **u** *(None | int) – Selects a site of the unit cell. None (default) means all sites.*

Returns
- **mps_idx** *(array) – MPS indices \(i\) for which self.site(i) is self.unit_cell[u].*
• **lat_idx** (2D array) – The row \(j\) contains the lattice index (without \(u\)) corresponding to \(\text{mps}\_\text{idx}[j]\).

**mps_sites()**

Return a list of sites for all MPS indices.

Equivalent to \([self.\text{site}(i) \text{ for } i \in \text{range}(self.N_{\text{sites}})]\).

This should be used for sites of 1D tensor networks (MPS, MPO,...).

**multi_coupling_shape** \((dx)\)

Calculate correct shape of the strengths for a multi_coupling.

**Parameters**

- **dx** (2D array, shape \((N_{\text{ops}}, \text{dim})\)) – \(dx[i, :]\) is the translation vector in the lattice for the \(i\)-th operator. Corresponds to the \(dx\) of each operator given in the argument \(\text{ops}\) of \text{tenpy.models.model.CouplingModel}.add_multi_coupling()**.

**Returns**

- **coupling_shape** (tuple of int) – Len \(\text{dim}\). The correct shape for an array specifying the coupling strength. \(\text{lat}\_\text{indices}\) has only rows within this shape.

- **shift_lat_indices** (array) – Translation vector from origin to the lower left corner of box spanned by \(dx\). (Unlike for \(\text{coupling}_\text{shape()\ it can also contain entries > 0)}**

**number_nearest_neighbors** \((u=0)\)

Deprecated.

Deprecated since version 0.5.0: Use \(\text{count_neighbors()}\) instead.

**number_next_nearest_neighbors** \((u=0)\)

Deprecated.

Deprecated since version 0.5.0: Use \(\text{count_neighbors()}\) instead.

**property order**

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with \(\text{plot_order()}\).

**plot_basis** \((ax, \text{origin}=(0.0, 0.0), \text{shade=None, **kwargs})\)

Plot arrows indicating the basis vectors of the lattice.

**Parameters**

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.

- ****kwargs – Keyword arguments for \(ax.\text{arrow}\).

**plot_bc_identified** \((ax, \text{direction=- 1, origin=None, cylinder_axis=False, **kwargs})\)

Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

**Parameters**

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.

- **direction** (int) – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.

- **cylinder_axis** (bool) – Whether to plot the cylinder axis as well.
- **origin** *(None | np.ndarray)* – The origin starting from where we mark the identified sites. Defaults to the first entry of `unit_cell_positions`.

- **kwargs** – Keyword arguments for the used `ax.plot`.

`plot_coupling(ax, coupling=None, wrap=False, **kwargs)`

Plot lines connecting nearest neighbors of the lattice.

**Parameters**

- `ax` *(matplotlib.axes.Axes)* – The axes on which we should plot.

- `coupling` *(list of (u1, u2, dx))* – By default (None), use `self.pairs['nearest_neighbors']`. Specifies the connections to be plotted; iterating over lattice indices \((i0, i1, \ldots, u1)\), we plot a connection from the site \((i0, i1, \ldots, u1)\) to the site \((i0+dx[0], i1+dx[1], \ldots, u2)\), taking into account the boundary conditions.

- `wrap` *(bool)* – If True, wrap

- **kwargs** – Further keyword arguments given to `ax.plot()`.

`plot_order(ax, order=None, textkwargs={'color': 'r'}, **kwargs)`

Plot a line connecting sites in the specified “order” and text labels enumerating them.

**Parameters**

- `ax` *(matplotlib.axes.Axes)* – The axes on which we should plot.

- `order` *(None | 2D array (self.N_sites, self.dim+1))* – The order as returned by `ordering()`; by default (None) use `order`.

- `textkwargs` *(None | dict)* – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for `ax.text()`.

- **kwargs** – Further keyword arguments given to `ax.plot()`.

`plot_sites(ax, markers=['o', '^', 's', 'p', 'h', 'D'], **kwargs)`

Plot the sites of the lattice with markers.

**Parameters**

- `ax` *(matplotlib.axes.Axes)* – The axes on which we should plot.

- `markers` *(list)* – List of values for the keyword `marker` of `ax.plot()` to distinguish the different sites in the unit cell, a site \(u\) in the unit cell is plotted with a marker `markers[u % len(markers)]`.

- **kwargs** – Further keyword arguments given to `ax.plot()`.

`position(lat_idx)`

return ‘space’ position of one or multiple sites.

**Parameters** `lat_idx` *(ndarray, (..., dim+1))* – Lattice indices.

**Returns** `pos` – The position of the lattice sites specified by `lat_idx` in real-space.

**Return type** ndarray, (..., dim)

`possible_couplings(u1, u2, dx)`

Find possible MPS indices for two-site couplings.

For periodic boundary conditions (`bc[a] == False`) the index \(x_a\) is taken modulo \(L_s[a]\) and runs through \(range(L_s[a])\). For open boundary conditions, \(x_a\) is limited to \(0 <= x_a < L_s[a]\) and \(0 <= x_a+dx[a] < lat.Ls[a]\).
Parameters

- **u1** *(int)* – Indices within the unit cell; the *u1* and *u2* of `add_coupling()`
- **u2** *(int)* – Indices within the unit cell; the *u1* and *u2* of `add_coupling()`
- **dx** *(array)* – Length *dim*. The translation in terms of basis vectors for the coupling.

Returns

- **mps1, mps2** *(array)* – For each possible two-site coupling the MPS indices for the *u1* and *u2*.
- **lat_indices** *(2D int array)* – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** *(tuple of int)* – Len *dim*. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

`possible_multi_couplings(ops)`

Generalization of `possible_couplings()` to couplings with more than 2 sites.

Parameters **ops** *(list of (opname, dx, u))* – Same as the argument **ops** of `add_multi_coupling()`.

Returns

- **mps_ijkl** *(2D int array)* – Each row contains MPS indices *i,j,k,.* for each of the operators positions. The positions are defined by *dx* (*j,k,.* relative to *i*) and boundary conditions of `self` (how much the box for given *dx* can be shifted around without hitting a boundary - these are the different rows).
- **lat_indices** *(2D int array)* – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** *(tuple of int)* – Len *dim*. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

`save_hdf5(hdf5_saver, h5gr, subpath)`

Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

Specifically, it saves `unit_cell`, `Ls`, `unit_cell_positions`, `basis`, `boundary_conditions`, `pairs` under their name, `bc_MPS` as "boundary_conditions_MPS", and `order` as "order_for_MPS". Moreover, it saves `dim` and `N_sites` as HDF5 attributes.

Parameters

- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.
- **h5gr** *(class 'Group')* – HDF5 group which is supposed to represent `self`.
- **subpath** *(str)* – The name of `h5gr` with a `'/`' in the end.

`site(i)`

Return `Site` instance corresponding to an MPS index *i*

`test_sanity()`

Sanity check.

Raises ValueErrors, if something is wrong.
Honeycomb

- full name: tenpy.models.lattice.Honeycomb
- parent module: tenpy.models.lattice
- type: class

Inheritance Diagram

```
  Lattice
   ^
   |  Honeycomb
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Honeycomb.<strong>init</strong>(Lx, Ly, sites, **kwargs)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>Honeycomb.count_neighbors([u, key])</td>
<td>Count e.g.</td>
</tr>
<tr>
<td>Honeycomb.coupling_shape(dx)</td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td>Honeycomb.enlarge_mps_unit_cell([factor])</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>Honeycomb.from_hdf5(hdf5_loader, h5gr, sub-path)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>Honeycomb.lat2mps_idx(lat_idx)</td>
<td>Translate lattice indices ((x_0, \ldots, x_{\text{dim}-1}, u)) to MPS index (i).</td>
</tr>
<tr>
<td>Honeycomb.mps2lat_idx(i)</td>
<td>Translate MPS index (i) to lattice indices ((x_0, \ldots, x_{\text{dim}-1}, u)).</td>
</tr>
<tr>
<td>Honeycomb.mps2lat_values(A[, axes, u])</td>
<td>Reshape/reorder (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>Honeycomb.mps2lat_values_masked(A[, axes, ...])</td>
<td>Reshape/reorder an array (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>Honeycomb.mps_idx_fix_u([u])</td>
<td>Return an index array of MPS indices for which the site within the unit cell is (u).</td>
</tr>
<tr>
<td>Honeycomb.mps_lat_idx_fix_u([u])</td>
<td>Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td>Honeycomb.mps_sites()</td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td>Honeycomb.multi_coupling_shape(dx)</td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td>Honeycomb.number_nearest_neighbors([u])</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>Honeycomb.number_next_nearest_neighbors()</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>Honeycomb.ordering(order)</td>
<td>Provide possible orderings of the (N) lattice sites.</td>
</tr>
</tbody>
</table>

continues on next page
Table 78 – continued from previous page

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</tr>
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<tbody>
<tr>
<td>Honeycomb.plot_basis(ax[, origin, shade])</td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td>Honeycomb.plot_bc_identified(ax[,...])</td>
<td>Mark two sites identified by periodic boundary conditions.</td>
</tr>
<tr>
<td>Honeycomb.plot_coupling(ax[, coupling, wrap])</td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
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<td>Honeycomb.plot_order(ax[, order, textkwargs])</td>
<td>Plot a line connecting sites in the specified “order” and text labels enumerating them.</td>
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<td>Honeycomb.plot_sites(ax[, markers])</td>
<td>Plot the sites of the lattice with markers.</td>
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<td>Honeycomb.position(lat_idx)</td>
<td>return 'space' position of one or multiple sites.</td>
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<td>Honeycomb.possible_couplings(u1, u2, dx)</td>
<td>Find possible MPS indices for two-site couplings.</td>
</tr>
<tr>
<td>Honeycomb.possible_multi_couplings(ops)</td>
<td>Generalization of possible_couplings() to couplings with more than 2 sites.</td>
</tr>
<tr>
<td>Honeycomb.save_hdf5(hdf5_saver, h5gr, subpath)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>Honeycomb.site(i)</td>
<td>return Site instance corresponding to an MPS index i</td>
</tr>
<tr>
<td>Honeycomb.test_sanity()</td>
<td>Sanity check.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Honeycomb.Lu</td>
<td>the (expected) number of sites in the unit cell, len(unit_cell).</td>
</tr>
<tr>
<td>Honeycomb.boundary_conditions</td>
<td>Human-readable list of boundary conditions from bc and bc_shift.</td>
</tr>
<tr>
<td>Honeycomb.dim</td>
<td>the dimension of the lattice</td>
</tr>
<tr>
<td>Honeycomb.fifth_nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Honeycomb.fourth_nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Honeycomb.next_nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Honeycomb.next_next_nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Honeycomb.order</td>
<td>Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.</td>
</tr>
</tbody>
</table>

```python
class tenpy.models.lattice.Honeycomb(Lx, Ly, sites, **kwargs)

Bases: tenpy.models.lattice.Lattice

A honeycomb lattice.

Parameters

- **Lx** *(int)* – The length in each direction.
- **Ly** *(int)* – The length in each direction.
- **sites** *(list of Site)* – The two local lattice sites making the unit cell of the Lattice. If only a single Site is given, it is used for both sites.
- ****kwargs** – Additional keyword arguments given to the Lattice. basis, pos and pairs are set accordingly. For the Honeycomb lattice 'fourth_nearest_neighbors', 'fifth_nearest_neighbors' are set in pairs.

dim = 2
the dimension of the lattice
```
7.11. models
\( \text{Lu} = 2 \)
the (expected) number of sites in the unit cell, \( \text{len}(\text{unit\_cell}) \).

**ordering** *(order)*
Provide possible orderings of the \( N \) lattice sites.

The following orders are defined in this method compared to \( \text{Lattice.ordering()} \):

<table>
<thead>
<tr>
<th>order</th>
<th>equivalent priority</th>
<th>equivalent snake winding</th>
</tr>
</thead>
<tbody>
<tr>
<td>'default'</td>
<td>(0, 2, 1)</td>
<td>(False, False, False)</td>
</tr>
<tr>
<td>'snake'</td>
<td>(0, 2, 1)</td>
<td>(False, True, False)</td>
</tr>
</tbody>
</table>

**property boundary_conditions**
Human-readable list of boundary conditions from \( \text{bc} \) and \( \text{bc\_shift} \).

**Returns boundary_conditions** – List of "open" or "periodic", one entry for each direction of the lattice.
Return type  list of str

count_neighbors(u=0, key='nearest_neighbors')
Count e.g. the number of nearest neighbors for a site in the bulk.

Parameters

• u (int) – Specifies the site in the unit cell, for which we should count the number of
neighbors (or whatever key specifies).

• key (str) – Key of pairs to select what to count.

Returns  number – Number of nearest neighbors (or whatever key specified) for the u-th site in
the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value
at the edges of a lattice with open boundary conditions.

Return type  int
coupling_shape(dx)
Calculate correct shape of the strengths for a coupling.

Parameters dx (tuple of int) – Translation vector in the lattice for a coupling of two
operators. Corresponds to dx argument of tenpy.models.model.CouplingModel.
add_multi_coupling().

Returns

• coupling_shape (tuple of int) – Len dim. The correct shape for an array specifying the
coupling strength. lat_indices has only rows within this shape.

• shift_lat_indices (array) – Translation vector from origin to the lower left corner of box
spanned by dx.
enlarge_mps_unit_cell(factor=2)
Repeat the unit cell for infinite MPS boundary conditions; in place.

Parameters factor (int) – The new number of sites in the MPS unit cell will be increased
from N_sites to factor*N_sites_per_ring. Since MPS unit cells are repeated in
the x-direction in our convention, the lattice shape goes from (Lx, Ly, ..., Lu) to
(Lx*factor, Ly, ..., Lu).
classmethod from_hdf5(hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

Parameters

• hdf5_loader (Hdf5Loader) – Instance of the loading engine.

• h5gr (Group) – HDF5 group which is represent the object to be constructed.

• subpath (str) – The name of h5gr with a '/' in the end.

Returns  obj – Newly generated class instance containing the required data.

Return type  cls
lat2mps_idx(lat_idx)
Translate lattice indices (x_0, ..., x_{D-1}, u) to MPS index i.

Parameters lat_idx (array_like [:, dim+1])– The last dimension corresponds to
lattice indices (x_0, ..., x_{D-1}, u). All lattice indices should be positive and
smaller than the corresponding entry in self.shape. Exception: for “infinite” bc_MPS,
an x_0 outside indicates shifts across the boundary.
**Returns**  
i – MPS index/indices corresponding to `lat_idx`. Has the same shape as `lat_idx` without the last dimension.

**Return type**  
`array_like`

`mps2lat_idx(i)`  
Translate MPS index `i` to lattice indices `(x_0, ..., x_{dim-1}, u)`.

**Parameters**  
`i (int | array_like of int)` – MPS index/indices.

**Returns**  
`lat_idx` – First dimensions like `i`, last dimension has len `dim`+1 and contains the lattice indices `(x_0, ..., x_{dim-1}, u)` corresponding to `i`. For `i` across the MPS unit cell and “infinite” `bc_MPS`, we shift `x_0` accordingly.

**Return type**  
`array`

`mps2lat_values(A, axes=0, u=None)`  
Reshape/reorder `A` to replace an MPS index by lattice indices.

**Parameters**

- `A (ndarray)` – Some values. Must have `A.shape[axes] = self.N_sites` if `u` is `None`, or `A.shape[axes] = self.N_cells` if `u` is an int.
- `axes ((iterable of) int)` – chooses the axis which should be replaced.
- `u (None | int)` – Optionally choose a subset of MPS indices present in the axes of `A`, namely the indices corresponding to `self.unit_cell[u]`, as returned by `mps_idx_fix_u()`. The resulting array will not have the additional dimension(s) of `u`.

**Returns**  
`res_A` – Reshaped and reordered versions of `A`. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index `j` maps to lattice site `(x0, x1, x2)`, then `res_A[..., x0, x1, x2, ...] = A[..., j, ...]`.

**Return type**  
`ndarray`

**Examples**

Say you measure expectation values of an onsite term for an MPS, which gives you an 1D array `A`, where `A[i]` is the expectation value of the site given by `self.mps2lat_idx(i)`. Then this function gives you the expectation values ordered by the lattice:

```python
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[tuple(lat.mps2lat_idx(5))] == A[5]
True
```

If you have a correlation function `C[i, j]`, it gets just slightly more complicated:

```python
>>> print(lat.shape, C.shape)
(10, 3, 2) (60, 60)
>>> lat.mps2lat_values(C, axes=[0, 1]).shape
(10, 3, 2, 10, 3, 2)
```

If the unit cell consists of different physical sites, an onsite operator might be defined only on one of the sites in the unit cell. Then you can use `mps_idx_fix_u()` to get the indices of sites it is defined on, measure the operator on these sites, and use the argument `u` of this function.
```python
>>> u = 0
>>> idx_subset = lat.mps_idx_fix_u(u)
>>> A_u = A[idx_subset]
>>> A_u_res = lat.mps2lat_values(A_u, u=u)
>>> A_u_res.shape
(10, 3)
>>> np.all(A_res[:, :, u] == A_u_res[:, :])
True
```

**mps2lat_values_masked** *(A, axes=-1, mps_inds=None, include_u=None)*

Reshape/reorder an array `A` to replace an MPS index by lattice indices.

This is a generalization of `mps2lat_values()` allowing for the case of an arbitrary set of MPS indices present in each axis of `A`.

**Parameters**

- `A` *(ndarray)* – Some values.
- `axes` *(iterable of int)* – Chooses the axis of `A` which should be replaced. If multiple axes are given, you also need to give multiple index arrays as `mps_inds`.
- `mps_inds` *(list of 1D ndarray)* – Specifies for each axis in `axes`, for which MPS indices we have values in the corresponding axis of `A`. Defaults to `[np.arange(A.shape[ax]) for ax in axes]`. For indices across the MPS unit cell and “infinite” `bc_MPS`, we shift `x_0` accordingly.
- `include_u` *(list of bool)* – Specifies for each axis in `axes`, whether the `u` index of the lattice should be included into the output array `res_A`. Defaults to `len(self.unit_cell) > 1`.

**Returns**

- `res_A` – Reshaped and reordered copy of `A`. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index `j` maps to lattice site `(x0, x1, x2)`, then `res_A[..., x0, x1, x2, ...] = A[..., mps_inds[j], ...]`.

**Return type** `np.ma.MaskedArray`

**mps_idx_fix_u** *(u=None)*

return an index array of MPS indices for which the site within the unit cell is `u`.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This function returns an index array of the mps indices which belong to sites given by `self.unit_cell[u]`.

**Parameters**

- `u` *(None | int)* – Selects a site of the unit cell. `None` (default) means all sites.

**Returns**

- `mps_idx` – MPS indices for which `self.site(i)` is `self.unit_cell[u]`. Ordered ascending.

**Return type** `array`

**mps_lat_idx_fix_u** *(u=None)*

Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.

**Parameters**

- `u` *(None | int)* – Selects a site of the unit cell. `None` (default) means all sites.

**Returns**

- `mps_idx` *(array)* – MPS indices `i` for which `self.site(i)` is `self.unit_cell[u]`. 

• **lat_idx** *(2D array)* – The row \( j \) contains the lattice index (without \( u \)) corresponding to \( \text{mps_idx}[j] \).

```python
mps_sites()
```

Return a list of sites for all MPS indices.

Equivalent to \([\text{self}.\text{site}(i) \text{ for } i \text{ in } \text{range(self.N_sites)}]\).

This should be used for sites of 1D tensor networks (MPS, MPO, ...).

```python
multi_coupling_shape(dx)
```

Calculate correct shape of the strengths for a multi_coupling.

**Parameters**
- **dx** *(2D array, shape (N_ops, dim))* – \( dx[i, :] \) is the translation vector in the lattice for the \( i \)-th operator. Corresponds to the \( dx \) of each operator given in the argument \( \text{ops} \) of \( \text{tenpy.models.model.CouplingModel.add_multi_coupling()} \).

**Returns**
- **coupling_shape** *(tuple of int)* – \( \text{Len dim} \). The correct shape for an array specifying the coupling strength. \( \text{lat_indices} \) has only rows within this shape.
- **shift_lat_indices** *(array)* – Translation vector from origin to the lower left corner of box spanned by \( dx \). (Unlike for \( \text{coupling_shape()} \) it can also contain entries > 0)

```python
number_nearest_neighbors(u=0)
```

Deprecated.

Deprecated since version 0.5.0: Use \( \text{count_neighbors()} \) instead.

```python
number_next_nearest_neighbors(u=0)
```

Deprecated.

Deprecated since version 0.5.0: Use \( \text{count_neighbors()} \) instead.

**property order**

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with \( \text{plot_order()} \).

```python
plot_basis(ax, origin=(0.0, 0.0), shade=None, **kwargs)
```

Plot arrows indicating the basis vectors of the lattice.

**Parameters**
- **ax** *(matplotlib.axes.Axes)* – The axes on which we should plot.
- ****kwargs – Keyword arguments for \( \text{ax}.\text{arrow} \).

```python
plot_bc_identified(ax, direction=-1, origin=None, cylinder_axis=False, **kwargs)
```

Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

**Parameters**
- **ax** *(matplotlib.axes.Axes)* – The axes on which we should plot.
- **direction** *(int)* – The direction of the lattice along which we should mark the identified sites. If \( \text{None} \), mark it along all directions with periodic boundary conditions.
- **cylinder_axis** *(bool)* – Whether to plot the cylinder axis as well.
• `origin`: The origin starting from where we mark the identified sites. Defaults to the first entry of `unit_cell_positions`.

• `**kwargs` – Keyword arguments for the used `ax.plot`.

`plot_coupling(ax, coupling=None, wrap=False, **kwargs)`
Plot lines connecting nearest neighbors of the lattice.

Parameters

• `ax` (`matplotlib.axes.Axes`) – The axes on which we should plot.

• `coupling` (`list of (u1, u2, dx)`) – By default (None), use `self.pairs['nearest_neighbors']`. Specifies the connections to be plotted; iterating over lattice indices (i0, i1, ...), we plot a connection from the site (i0, i1, ..., u1) to the site (i0+dx[0], i1+dx[1], ..., u2), taking into account the boundary conditions.

• `wrap` (`bool`) – If True, wrap

• `**kwargs` – Further keyword arguments given to `ax.plot()`.

`plot_order(ax, order=None, textkwargs={'color': 'r'}, **kwargs)`
Plot a line connecting sites in the specified “order” and text labels enumerating them.

Parameters

• `ax` (`matplotlib.axes.Axes`) – The axes on which we should plot.

• `order` (`None | 2D array (self.N_sites, self.dim+1)`) – The order as returned by `ordering()`; by default (None) use `order`.

• `textkwargs` (`None | dict`) – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for `ax.text()`.

• `**kwargs` – Further keyword arguments given to `ax.plot()`.

`plot Sites(ax, markers=['o', '^', 's', 'p', 'h', 'D'], **kwargs)`
Plot the sites of the lattice with markers.

Parameters

• `ax` (`matplotlib.axes.Axes`) – The axes on which we should plot.

• `markers` (`list`) – List of values for the keyword `marker` of `ax.plot()` to distinguish the different sites in the unit cell, a site `u` in the unit cell is plotted with a marker `markers[u % len(markers)]`.

• `**kwargs` – Further keyword arguments given to `ax.plot()`.

`position(lat_idx)`
return 'space' position of one or multiple sites.

Parameters

• `lat_idx` (`ndarray, (..., dim+1)`) – Lattice indices.

Returns `pos` – The position of the lattice sites specified by `lat_idx` in real-space.

Return type `ndarray, (..., dim)`

`possible_couplings(u1, u2, dx)`
Find possible MPS indices for two-site couplings.

For periodic boundary conditions (`bc[a] == False`) the index `x_a` is taken modulo `Ls[a]` and runs through `range(Ls[a])`. For open boundary conditions, `x_a` is limited to `0 <= x_a < Ls[a]` and `0 <= x_a+dx[a] < lat.Ls[a]`. 

7.11. models
Parameters

- **u1** (*int*) – Indices within the unit cell; the $u1$ and $u2$ of `add_coupling()`
- **u2** (*int*) – Indices within the unit cell; the $u1$ and $u2$ of `add_coupling()`
- **dx** (*array*) – Length $\text{dim}$. The translation in terms of basis vectors for the coupling.

Returns

- **mps1, mps2** (*array*) – For each possible two-site coupling the MPS indices for the $u1$ and $u2$.
- **lat_indices** (*2D int array*) – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** (*tuple of int*) – $\text{Len } \text{dim}$. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

`possible_multi_couplings(ops)`

Generalization of `possible_couplings()` to couplings with more than 2 sites.

Parameters **ops** (list of (opname, dx, u)) – Same as the argument `ops` of `add_multi_coupling()`.

Returns

- **mps_ijkl** (*2D int array*) – Each row contains MPS indices $i,j,k,\ldots$ for each of the operators positions. The positions are defined by `dx` ($j,k,\ldots$ relative to $i$) and boundary coundary conditions of `self` (how much the box for given `dx` can be shifted around without hitting a boundary - these are the different rows).
- **lat_indices** (*2D int array*) – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** (*tuple of int*) – $\text{Len } \text{dim}$. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

`sav`; `_hdf5(hdf5_saver, h5gr, subpath)`

Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

Specifically, it saves `unit_cell`, `Ls`, `unit_cell_positions`, `basis`, `boundary_conditions`, `pairs` under their name, `bc_MPS` as "`boundary_conditions_MPS"", and `order` as "`order_for_MPS". Moreover, it saves `dim` and `N_sites` as HDF5 attributes.

Parameters

- **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.
- **h5gr**:class:’Group’ – HDF5 group which is supposed to represent `self`.
- **subpath** (*str*) – The name of `h5gr` with a "/" in the end.

`site(i)`

return `Site` instance corresponding to an MPS index $i$

`test_sanity()`

Sanity check.

Raises ValueErrors, if something is wrong.
IrregularLattice

- full name: tenpy.models.lattice.IrregularLattice
- parent module: tenpy.models.lattice
- type: class

Inheritance Diagram

```
Lattice
   ↓
IrregularLattice
```

Methods

```
IrregularLattice.__init__(regular_lattice[, ...]) Initialize self.

IrregularLattice.count_neighbors([u, key]) Count e.g.

IrregularLattice.coupling_shape(dx) Calculate correct shape of the strengths for a coupling.

IrregularLattice.enlarge_mps_unit_cell([factor]) Repeat the unit cell for infinite MPS boundary conditions; in place.

IrregularLattice.from_hdf5(hdf5_loader, ...) Load instance from a HDF5 file.

IrregularLattice.lat2mps_idx(lat_idx) Translate lattice indices (x_0, ..., x_{D-1}, u) to MPS index i.

IrregularLattice.mps2lat_idx(i) Translate MPS index i to lattice indices (x_0, ..., x_{dim-1}, u).

IrregularLattice.mps2lat_values(A[, axes, u]) Reshape/reorder A to replace an MPS index by lattice indices.

IrregularLattice.mps2lat_values_masked(A[, ...]) Reshape/reorder an array A to replace an MPS index by lattice indices.

IrregularLattice.mps_idx_fix_u([u]) return an index array of MPS indices for which the site within the unit cell is u.

IrregularLattice.mps_lat_idx_fix_u([u]) Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.

IrregularLattice.mps_sites() Return a list of sites for all MPS indices.

IrregularLattice.multi_coupling_shape(dx) Calculate correct shape of the strengths for a multi_coupling.
```

continues on next page
IrregularLattice.
n_number_nearest_neighbors((u))  Deprecated.

IrregularLattice.
n_number_next_nearest_neighbors((u))  Deprecated.

IrregularLattice.ordering(order)  Provide possible orderings of the lattice sites.

IrregularLattice.plot_basis(ax[, origin, shade])  Plot arrows indicating the basis vectors of the lattice.

IrregularLattice.plot_bc_identified(ax[, ...])  Mark two sites identified by periodic boundary conditions.

IrregularLattice.plot_coupling(ax[, ...])  Plot lines connecting nearest neighbors of the lattice.

IrregularLattice.plot_order(ax[, order, ...])  Plot a line connecting sites in the specified “order” and text labels enumerating them.

IrregularLattice.plot_sites(ax[, markers])  Plot the sites of the lattice with markers.

IrregularLattice.position(lat_idx)  return ‘space’ position of one or multiple sites.

IrregularLattice.possible_couplings(u1, u2, dx)  Find possible MPS indices for two-site couplings.

IrregularLattice.possible_multi_couplings(ops)  Generalization of possible_couplings() to couplings with more than 2 sites.

IrregularLattice.save_hdf5(hdf5_saver, h5gr,...)  Export self into a HDF5 file.

IrregularLattice.site(i)  return Site instance corresponding to an MPS index i

IrregularLattice.test_sanity()  Sanity check.

Class Attributes and Properties

IrregularLattice.Lu
IrregularLattice.boundary_conditions  Human-readable list of boundary conditions from bc and bc_shift.
IrregularLattice.dim  The dimension of the lattice.
IrregularLattice.nearest_neighbors
IrregularLattice.next_nearest_neighbors
IrregularLattice.next_next_nearest_neighbors
IrregularLattice.order  Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

class tenpy.models.lattice.IrregularLattice(regular_lattice, remove=None, add=None, add_unit_cell=[], add_positions=None)
Bases: tenpy.models.lattice.Lattice
A variant of a regular lattice, where we might have extra sites or sites missing.

Note: The lattice defines only the geometry of the sites, not the couplings; you can have position-dependent couplings/onsite terms despite having a regular lattice.

By adjusting the order and a few private attributes and methods, we can make functions like possible_couplings() work with a more “irregular” lattice structure, where some of the sites are missing and other sites added instead.

Parameters
• **regular_lattice** (*Lattice*) – The lattice this is based on.

• **remove** (*2D array | None*) – Each row is a lattice index \((x_0, \ldots, x_{(dim-1)}, u)\) of a site to be removed. If **None**, don’t remove something.

• **add** (*Tuple*[2D array, list] | **None***) – Each row of the 2D array is a lattice index \((x_0, \ldots, x_{(dim-1)}, u)\) specifying where a site is to be added; \(u\) is the index of the site within the final unit cell of the irregular lattice. For each row of the 2D array, there is one entry in the list specifying where the site is inserted in the MPS; the values are compared to the MPS indices of the **regular** lattice and sorted into it, so “2.5” goes between what was site 2 and 3 in the regular lattice. An entry **None** indicates that the site should be inserted after the lattice site \((x_0, \ldots, x_{(dim-1)}, -1)\) of the **regular_lattice**.

• **add_unit_cell** (*list of Site*) – Extra sites to be added to the unit cell.

• **add_positions** (*iterable of 1D arrays*) – For each extra site in **add_unit_cell** the position within the unit cell. Defaults to `np.zeros((len(add_unit_cell), dim))`.

**regular_lattice**

The lattice this is based on.

**Type** *Lattice*

**remove**, **add**

See above. Used in **ordering()** only.

**Type** *2D array | None*

---

**Examples**

Let’s imagine that we have two different sites; for concreteness we can thing of a fermion site, which we represent with `'F'`, and a spin site `'S'`. If you want to preserve charges, take a look at `set_common_charges()` for the proper way to initialize the sites.

You could now imagine that to have fermion chain with spins on the “bonds”. In the periodic/infinite case, you would simply define

```python
>>> lat = Lattice([2], unit_cell=['F', 'S'], bc='periodic', bc_MPS='infinite')
>>> lat.mps_sites()
['F', 'S', 'F', 'S']
```

For a finite system, you don’t want to terminate with a spin on the right, so you need to remove the very last site by specifying the lattice index \([L-1, 1]\) of that site:

```python
>>> L = 4
>>> reg_lat = Lattice([L], unit_cell=['F', 'S'], bc='open', bc_MPS='finite')
>>> irr_lat = IrregularLattice(reg_lat, remove=[[L - 1, 1]])
>>> irr_lat.mps_sites()
['F', 'S', 'F', 'S', 'F', 'S', 'F']
```

Another simple example would be to add a spin in the center of a fermion chain. In that case, we add another site to the unit cell and specify the lattice index as \([\lfloor(L-1)/2, 1\rfloor]\) (where the 1 is the index of `'S'` in the unit cell \(['F', 'S']\) of the irregular lattice). The **None** for the MPS index is equivalent to \(\lfloor(L-1)/2\) in this case.
```python
>>> reg_lat = Lattice([L], unit_cell=['F'])
>>> irr_lat = IrregularLattice(reg_lat, add=[[[L - 1]//2, 1]], [None]),
... add_unit_cell=['S'])
>>> irr_lat.mps_sites()
['F', 'F', 'S', 'F', 'F']
```

**save_hdf5 (hdf5_saver, h5gr, subpath)**

Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5(). Specifically, it saves unit_cell, Ls, unit_cell_positions, basis, boundary_conditions, pairs under their name, bc_MPS as "boundary_conditions_MPS", and order as "order_for_MPS". Moreover, it saves dim and N_sites as HDF5 attributes.

**Parameters**

- **hdf5_saver (Hdf5Saver)** – Instance of the saving engine.
- **h5gr (:class:`Group`)** – HDF5 group which is supposed to represent self.
- **subpath (str)** – The name of h5gr with a '/' in the end.

**classmethod from_hdf5 (hdf5_loader, h5gr, subpath)**

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

**Parameters**

- **hdf5_loader (Hdf5Loader)** – Instance of the loading engine.
- **h5gr (Group)** – HDF5 group which is represent the object to be constructed.
- **subpath (str)** – The name of h5gr with a '/' in the end.

**Returns** obj – Newly generated class instance containing the required data.

**Return type** cls

**ordering (order)**

Provide possible orderings of the lattice sites.

**Parameters** order – Argument for the Lattice.ordering() of the regular_lattice, or 2D ndarray providing the order of the regular lattice.

**Returns** order – The order to be used for order, i.e. order with added/removed sites as specified by remove and add.

**Return type** array, shape (N, D+1)

**property order**

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with plot_order().

**property mps_idx_fix_u (u=None)**

return an index array of MPS indices for which the site within the unit cell is u.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This functions returns an index array of the mps indices which belong to sites given by self. unit_cell[u].
Parameters `u` *(None | int)* – Selects a site of the unit cell. *None* (default) means all sites.

Returns `mps_idx` – MPS indices for which `self.site(i)` is `self.unit_cell[u]`. Ordered ascending.

Return type `array`

**property boundary_conditions**

Human-readable list of boundary conditions from `bc` and `bc_shift`.

Returns `boundary_conditions` – List of "open" or "periodic", one entry for each direction of the lattice.

Return type `list of str`

**count_neighbors** *(u=0, key='nearest_neighbors')*

Count e.g. the number of nearest neighbors for a site in the bulk.

Parameters

- `u` *(int)* – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever `key` specifies).
- `key` *(str)* – Key of `pairs` to select what to count.

Returns `number` – Number of nearest neighbors (or whatever `key` specified) for the `u`-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

Return type `int`

**coupling_shape** *(dx)*

Calculate correct shape of the strengths for a coupling.

Parameters `dx` *(tuple of int)* – Translation vector in the lattice for a coupling of two operators. Corresponds to `dx` argument of `tenpy.models.model.CouplingModel.add_multi_coupling()`.

Returns

- `coupling_shape` *(tuple of int)* – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.
- `shift_lat_indices` *(array)* – Translation vector from origin to the lower left corner of box spanned by `dx`.

**property dim**

The dimension of the lattice.

**enlarge_mps_unit_cell** *(factor=2)*

Repeat the unit cell for infinite MPS boundary conditions; in place.

Parameters `factor` *(int)* – The new number of sites in the MPS unit cell will be increased from `N_sites` to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

**lat2mps_idx** *(lat_idx)*

Translate lattice indices `(x_0, ..., x_(D-1), u)` to MPS index `i`.

Parameters `lat_idx` *(array_like [.., dim+1])* – The last dimension corresponds to lattice indices `(x_0, ..., x_(D-1), u)`. All lattice indices should be positive and smaller than the corresponding entry in `self.shape`. Exception: for “infinite” `bc_MPS, an x_0 outside indicates shifts across the boundary.
Returns $i$ – MPS index/indices corresponding to $lat_idx$. Has the same shape as $lat_idx$ without the last dimension.

Return type array_like

$\text{mps2lat_idx}(i)$

Translate MPS index $i$ to lattice indices $(x_0, \ldots, x_{(\text{dim}-1)}, u)$.

Parameters $i$ (int | array_like of int) – MPS index/indices.

Returns $lat_idx$ – First dimensions like $i$, last dimension has len $\text{dim}+1$ and contains the lattice indices $(x_0, \ldots, x_{\text{dim}-1}, u)$ corresponding to $i$. For $i$ across the MPS unit cell and “infinite” bc_MPS, we shift $x_0$ accordingly.

Return type array

$\text{mps2lat_values}(A, \text{axes}=0, u=None)$

Reshape/reorder $A$ to replace an MPS index by lattice indices.

Parameters

- $A$ (ndarray) – Some values. Must have $A.shape[\text{axes}] = \text{self.N_sites}$ if $u$ is None, or $A.shape[\text{axes}] = \text{self.N_cells}$ if $u$ is an int.
- $\text{axes}$ ((iterable of) int) – chooses the axis which should be replaced.
- $u$ (None | int) – Optionally choose a subset of MPS indices present in the axes of $A$, namely the indices corresponding to $\text{self.unit_cell}[u]$, as returned by $\text{mps_idx_fix_u}()$. The resulting array will not have the additional dimension(s) of $u$.

Returns $\text{res_A}$ – Reshaped and reordered versions of $A$. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index $j$ maps to lattice site $(x0, x1, x2)$, then $\text{res_A}[\ldots, x0, x1, x2, \ldots] = A[\ldots, j, \ldots]$.

Return type ndarray

Examples

Say you measure expectation values of an onsite term for an MPS, which gives you an 1D array $A$, where $A[i]$ is the expectation value of the site given by $\text{self.mps2lat_idx}(i)$. Then this function gives you the expectation values ordered by the lattice:

```python
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[tuple(lat.mps2lat_idx(5))] == A[5]
True
```

If you have a correlation function $C[i, j]$, it gets just slightly more complicated:

```python
>>> print(lat.shape, C.shape)
(10, 3, 2) (60, 60)
>>> lat.mps2lat_values(C, axes=[0, 1]).shape
(10, 3, 2, 10, 3, 2)
```

If the unit cell consists of different physical sites, an onsite operator might be defined only on one of the sites in the unit cell. Then you can use $\text{mps_idx_fix_u}()$ to get the indices of sites it is defined on, measure the operator on these sites, and use the argument $u$ of this function.
```python
>>> u = 0
>>> idx_subset = lat.mps_idx_fix_u(u)
>>> A_u = A[idx_subset]
>>> A_u_res = lat.mps2lat_values(A_u, u=u)
>>> A_u_res.shape
(10, 3)
>>> np.all(A_res[:, :, u] == A_u_res[:, :])
True
```

**mps2lat_values_masked** *(A, axes=-1, mps_ind=None, include_u=None)*

Reshape/reorder an array A to replace an MPS index by lattice indices.

This is a generalization of `mps2lat_values()` allowing for the case of an arbitrary set of MPS indices present in each axis of A.

**Parameters**

- **A** *(ndarray)* – Some values.
- **axes** *(iterable of int)* – Chooses the axis of A which should be replaced. If multiple axes are given, you also need to give multiple index arrays as `mps_ind`
- **mps_ind** *(list of 1D ndarray)* – Specifies for each axis in `axes`, for which MPS indices we have values in the corresponding axis of A. Defaults to `[np.arange(A.shape[ax]) for ax in axes]`. For indices across the MPS unit cell and “infinite” `bc_MPS`, we shift `x_0` accordingly.
- **include_u** *(list of bool)* – Specifies for each axis in `axes`, whether the u index of the lattice should be included into the output array `res_A`. Defaults to `len(self.unit_cell) > 1`.

**Returns**

- **res_A** – Reshaped and reordered copy of A. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index `j` maps to lattice site `(x0, x1, x2)`, then `res_A[... , x0, x1, x2, ...] = A[... , mps_ind[j], ...]`.

**Return type** `np.ma.MaskedArray`

**mps_lat_idx_fix_u** *(u=None)*

Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.

**Parameters**

- **u** *(None | int)* – Selects a site of the unit cell. None (default) means all sites.

**Returns**

- **mps_idx** *(array)* – MPS indices `i` for which `self.site(i)` is `self.unit_cell[u]`.
- **lat_idx** *(2D array)* – The row `j` contains the lattice index (without `u`) corresponding to `mps_idx[j]`.

**mps_sites** ()

Return a list of sites for all MPS indices.

Equivalent to `[self.site(i) for i in range(self.N_sites)]`.

This should be used for `sites` of 1D tensor networks (MPS, MPO,...).

**multi_coupling_shape** *(dx)*

Calculate correct shape of the strengths for a multi_coupling.
Parameters  

**dx** (2D array, shape (N_ops, dim)) – dx[i, :) is the translation vector in the lattice for the i-th operator. Corresponds to the dx of each operator given in the argument ops of `tenpy.models.model.CouplingModel.add_multi_coupling()`.

Returns

- **coupling_shape** (tuple of int) – Len dim. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.
- **shift_lat_indices** (array) – Translation vector from origin to the lower left corner of box spanned by dx. (Unlike for `coupling_shape()` it can also contain entries > 0)

**number_nearest_neighbors** (u=0)

Deprecated.

Deprecated since version 0.5.0: Use `count_neighbors()` instead.

**number_next_nearest_neighbors** (u=0)

Deprecated.

Deprecated since version 0.5.0: Use `count_neighbors()` instead.

**plot_basis** (ax, origin=(0.0, 0.0), shade=None, **kwargs)

Plot arrows indicating the basis vectors of the lattice.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **kwargs** – Keyword arguments for `ax.arrow`.

**plot_bc_identified** (ax, direction=-1, origin=None, cylinder_axis=False, **kwargs)

Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **direction** (int) – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.
- **cylinder_axis** (bool) – Whether to plot the cylinder axis as well.
- **origin** (None | np.ndarray) – The origin starting from where we mark the identified sites. Defaults to the first entry of `unit_cell_positions`.
- **kwargs** – Keyword arguments for the used `ax.plot`.

**plot_coupling** (ax, coupling=None, wrap=False, **kwargs)

Plot lines connecting nearest neighbors of the lattice.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **coupling** (list of (u1, u2, dx)) – By default (None), use `self.pairs['nearest_neighbors']`. Specifies the connections to be plotted; iterating over lattice indices (i0, i1, ...), we plot a connection from the site (i0, i1, ..., u1) to the site (i0+dx[0], i1+dx[1], ..., u2), taking into account the boundary conditions.
- **wrap** (bool) – If True, wrap
- **kwargs** – Further keyword arguments given to `ax.plot()`.
plot_order(ax, order=None, textkwargs={"color": 'r'}, **kwargs)
Plot a line connecting sites in the specified “order” and text labels enumerating them.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **order** (None | 2D array (self.N_sites, self.dim+1)) – The order as returned by ordering(); by default (None) use order.
- **textkwargs** (None | dict) – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for ax.text().
- **kwargs** – Further keyword arguments given to ax.plot().

plot_sites(ax, markers=['o', '^', 's', 'p', 'h', 'D'], **kwargs)
Plot the sites of the lattice with markers.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **markers** (list) – List of values for the keyword marker of ax.plot() to distinguish the different sites in the unit cell, a site \( u \) in the unit cell is plotted with a marker \( \text{markers}[u \% \text{len(markers)}] \).
- **kwargs** – Further keyword arguments given to ax.plot().

position(lat_idx)
return 'space' position of one or multiple sites.

Parameters **lat_idx** (ndarray, (..., dim+1)) – Lattice indices.

Returns pos – The position of the lattice sites specified by lat_idx in real-space.

Possible return types ndarray, (..., dim)

possible_couplings(u1, u2, dx)
Find possible MPS indices for two-site couplings.

For periodic boundary conditions (bc[a] == False) the index x_a is taken modulo Ls[a] and runs through range(Ls[a]). For open boundary conditions, x_a is limited to 0 <= x_a < Ls[a] and 0 <= x_a+dx[a] < lat.Ls[a].

Parameters

- **u1** (int) – Indices within the unit cell; the u1 and u2 of add_coupling()
- **u2** (int) – Indices within the unit cell; the u1 and u2 of add_coupling()
- **dx** (array) – Length dim. The translation in terms of basis vectors for the coupling.

Returns

- **mps1, mps2** (array) – For each possible two-site coupling the MPS indices for the u1 and u2.
- **lat_indices** (2D int array) – Rows of lat_indices correspond to rows of mps_ijkl and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** (tuple of int) – Len dim. The correct shape for an array specifying the coupling strength. lat_indices has only rows within this shape.

possible_multi_couplings(ops)
Generalization of possible_couplings() to couplings with more than 2 sites.
Parameters **ops** (list of (opname, dx, u)) – Same as the argument *ops* of `add_multi_coupling()`.

Returns

- **mps_ijkl** *(2D int array)* – Each row contains MPS indices *i,j,k, l,...* for each of the operators positions. The positions are defined by *dx* (*j,k,l,...* relative to *i*) and boundary conditions *self* (how much the box for given *dx* can be shifted around without hitting a boundary - these are the different rows).
- **lat_indices** *(2D int array)* – Rows of *lat_indices* correspond to rows of *mps_ijkl* and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** *(tuple of int)* – Len *dim*. The correct shape for an array specifying the coupling strength. *lat_indices* has only rows within this shape.

```
site(i)
    return Site instance corresponding to an MPS index *i*

test_sanity()
    Sanity check.
    Raises ValueErrorS, if something is wrong.
```

**Kagome**

- full name: `tenpy.models.lattice.Kagome`
- parent module: `tenpy.models.lattice`
- type: class

**Inheritance Diagram**
Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kagome.<strong>init</strong>(Lx, Ly, sites, **kwargs)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>Kagome.count_neighbors([u, key])</td>
<td>Count e.g.</td>
</tr>
<tr>
<td>Kagome.coupling_shape(dx)</td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td>Kagome.enlarge_mps_unit_cell([factor])</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>Kagome.from_hdf5(hdf5_loader, h5gr, subpath)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>Kagome.lat2mps_idx(lat_idx)</td>
<td>Translate lattice indices (x_0, ..., x_{D-1}, u) to MPS index i.</td>
</tr>
<tr>
<td>Kagome.mps2lat_idx(i)</td>
<td>Translate MPS index i to lattice indices (x_0, ..., x_{dim-1}, u).</td>
</tr>
<tr>
<td>Kagome.mps2lat_values(A[, axes, u])</td>
<td>Reshape/reorder A to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>Kagome.mps2lat_values_masked(A[, axes, ...])</td>
<td>Reshape/reorder an array A to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>Kagome.mps_idx_fix_u([u])</td>
<td>return an index array of MPS indices for which the site within the unit cell is u.</td>
</tr>
<tr>
<td>Kagome.mps_lat_idx_fix_u([u])</td>
<td>Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td>Kagome.mps_sites()</td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td>Kagome.multi_coupling_shape(dx)</td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td>Kagome.number_nearest_neighbors([u])</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>Kagome.number_next_nearest_neighbors([u])</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>Kagome.ordering(order)</td>
<td>Provide possible orderings of the N lattice sites.</td>
</tr>
<tr>
<td>Kagome.plot_basis(ax[, origin, shade])</td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td>Kagome.plot_bc_identified(ax[, direction, ...])</td>
<td>Mark two sites indified by periodic boundary conditions.</td>
</tr>
<tr>
<td>Kagome.plot_coupling(ax[, coupling, wrap])</td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
</tr>
<tr>
<td>Kagome.plot_order(ax[, order, textkwargs])</td>
<td>Plot a line connecting sites in the specified “order” and text labels enumerating them.</td>
</tr>
<tr>
<td>Kagome.plot_sites(ax[, markers])</td>
<td>Plot the sites of the lattice with markers.</td>
</tr>
<tr>
<td>Kagome.position(lat_idx)</td>
<td>return ‘space’ position of one or multiple sites.</td>
</tr>
<tr>
<td>Kagome.possible_couplings(u1, u2, dx)</td>
<td>Find possible MPS indices for two-site couplings.</td>
</tr>
<tr>
<td>Kagome.possible_multi_couplings(ops)</td>
<td>Generalization of possible_couplings() to couplings with more than 2 sites.</td>
</tr>
<tr>
<td>Kagome.save_hdf5(hdf5_saver, h5gr, subpath)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>Kagome.site(i)</td>
<td>return Site instance corresponding to an MPS index i</td>
</tr>
<tr>
<td>Kagome.test_sanity()</td>
<td>Sanity check.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kagome.Lu</td>
<td>the (expected) number of sites in the unit cell, len(unit_cell).</td>
</tr>
<tr>
<td>Kagome.boundary_conditions</td>
<td>Human-readable list of boundary conditions from bc and bc_shift.</td>
</tr>
<tr>
<td>Kagome.dim</td>
<td>the dimension of the lattice</td>
</tr>
</tbody>
</table>

continues on next page
### Table 83 – continued from previous page

<table>
<thead>
<tr>
<th>Kagome.next_nearest_neighbors</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Kagome.order</td>
<td>Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.</td>
</tr>
</tbody>
</table>

**class** `tenpy.models.lattice.Kagome(Lx, Ly, sites, **kwargs)`

**Bases:** `tenpy.models.lattice.Lattice`

A Kagome lattice.

Parameters

- **Lx** (*int*) – The length in each direction.
- **Ly** (*int*) – The length in each direction.
- **sites** ((list of) *Site*) – The two local lattice sites making the *unit_cell* of the *Lattice*. If only a single *Site* is given, it is used for both sites.
- ****kwargs – Additional keyword arguments given to the *Lattice*. *basis*, *pos* and *pairs* are set accordingly.

**property** `boundary_conditions`

Human-readable list of boundary conditions from `bc` and `bc_shift`.

**Returns** `boundary_conditions` – List of "open" or "periodic", one entry for each direction of the lattice.

**Return type** list of str
count_neighbors \( (u=0, \text{key='nearest_neighbors'}) \)
Count e.g. the number of nearest neighbors for a site in the bulk.

Parameters

- \( u \) (int) – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever \( \text{key} \) specifies).
- \( \text{key} \) (str) – Key of pairs to select what to count.

Returns number – Number of nearest neighbors (or whatever \( \text{key} \) specified) for the \( u \)-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

Return type int
coupling_shape \( (dx) \)
Calculate correct shape of the strengths for a coupling.

Parameters \( dx \) (tuple of int) – Translation vector in the lattice for a coupling of two operators. Corresponds to \( dx \) argument of \text{tenpy.models.model.CouplingModel.add_multi_coupling}().

Returns

- coupling_shape (tuple of int) – Len \( \text{dim} \). The correct shape for an array specifying the coupling strength. \( \text{lat_indices} \) has only rows within this shape.
- shift_lat_indices (array) – Translation vector from origin to the lower left corner of box spanned by \( dx \).

dim = 2
the dimension of the lattice
enlarge_mps_unit_cell \( (\text{factor}=2) \)
Repeat the unit cell for infinite MPS boundary conditions; in place.

Parameters \( \text{factor} \) (int) – The new number of sites in the MPS unit cell will be increased from \( N_{\text{sites}} \) to \( \text{factor} \cdot N_{\text{sites\_per\_ring}} \). Since MPS unit cells are repeated in the \( x \)-direction in our convention, the lattice shape goes from \( (L_x, L_y, \ldots, L_u) \) to \( (L_x \cdot \text{factor}, L_y, \ldots, L_u) \).

classmethod from_hdf5 \( (\text{hdf5\_loader, h5gr, subpath}) \)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with \text{save_hdf5}().

Parameters

- \( \text{hdf5\_loader} \) (\text{Hdf5Loader}) – Instance of the loading engine.
- \( \text{h5gr} \) (Group) – HDF5 group which is represent the object to be constructed.
- \( \text{subpath} \) (str) – The name of \( \text{h5gr} \) with a '/' in the end.

Returns \( \text{obj} \) – Newly generated class instance containing the required data.

Return type cls
lat2mps_idx \( (\text{lat\_idx}) \)
Translate lattice indices \( (x_0, \ldots, x_{(D-1)}, u) \) to MPS index \( i \).

Parameters \( \text{lat\_idx} \) (array_like \[., dim+1]) – The last dimension corresponds to lattice indices \( (x_0, \ldots, x_{(D-1)}, u) \). All lattice indices should be positive and
smaller than the corresponding entry in \texttt{self.shape}. Exception: for “infinite” \texttt{bc\_MPS}, an \texttt{x\_0} outside indicates shifts across the boundary.

\textbf{Returns} \texttt{i} – MPS index/indices corresponding to \texttt{lat\_idx}. Has the same shape as \texttt{lat\_idx} without the last dimension.

\textbf{Return type} \texttt{array\_like}

\texttt{mps2lat\_idx(i)}

Translate MPS index \texttt{i} to lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\).

\textbf{Parameters} \texttt{i} (int | array\_like of int) -- MPS index/indices.

\textbf{Returns} \texttt{lat\_idx} -- First dimensions like \texttt{i}, last dimension has \texttt{len dim+1 and contains the lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\)} corresponding to \texttt{i}. For \texttt{i} across the MPS unit cell and “infinite” \texttt{bc\_MPS}, we shift \texttt{x\_0} accordingly.

\textbf{Return type} \texttt{array}

\texttt{mps2lat\_values}(A, axes=0, u=None)

Reshape/reorder \texttt{A} to replace an MPS index by lattice indices.

\textbf{Parameters}

- \texttt{A} (ndarray) -- Some values. Must have \texttt{A.shape[axes]} = self.N\_sites if \texttt{u} is None, or \texttt{A.shape[axes]} = self.N\_cells if \texttt{u} is an int.

- \texttt{axes} (iterable of int) -- chooses the axis which should be replaced.

- \texttt{u} (None | int) -- Optionally choose a subset of MPS indices present in the axes of \texttt{A}, namely the indices corresponding to \texttt{self.unit\_cell[u]}, as returned by \texttt{mps\_idx\_fix\_u()}.

\textbf{Returns} \texttt{res\_A} -- Reshaped and reordered versions of \texttt{A}. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index \texttt{j} maps to lattice site \((x0, x1, x2)\), then \texttt{res\_A[\ldots, x0, x1, x2, \ldots] = A[\ldots, j, \ldots]}.

\textbf{Return type} \texttt{ndarray}

\textbf{Examples}

Say you measure expection values of an onsite term for an MPS, which gives you an 1D array \texttt{A}, where \texttt{A[i]} is the expectation value of the site given by \texttt{self.mps2lat\_idx(i)}. Then this function gives you the expectation values ordered by the lattice:

```
>>> print(lat.shape, A.shape)
(10, 3, 2)  (60,)
>>> A_res = lat.mps2lat\_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[tuple(lat.mps2lat\_idx(5))] == A[5]
True
```

If you have a correlation function \texttt{C[i, j]}, it gets just slightly more complicated:

```
>>> print(lat.shape, C.shape)
(10, 3, 2)  (60, 60)
>>> lat.mps2lat\_values(C, axes=[0, 1]).shape
(10, 3, 2, 10, 3, 2)
```
If the unit cell consists of different physical sites, an onsite operator might be defined only on one of the sites in the unit cell. Then you can use \texttt{mps\_idx\_fix\_u()} to get the indices of sites it is defined on, measure the operator on these sites, and use the argument \texttt{u} of this function.

```python
>>> u = 0
>>> idx Subset = lat.mps_idx_fix_u(u)
>>> A_u = A[idx Subset]
>>> A_u_res = lat.mps2lat_values(A_u, u=u)
>>> A_u_res.shape
(10, 3)
>>> np.all(A_res[:,:,:,u] == A_u_res[:,:])
True
```

\texttt{mps2lat\_values\_masked}(\texttt{A, axes=None, mps\_inds=None, include\_u=None})

Reshape/reorder an array \texttt{A} to replace an MPS index by lattice indices.

This is a generalization of \texttt{mps2lat\_values()} allowing for the case of an arbitrary set of MPS indices present in each axis of \texttt{A}.

**Parameters**

- \texttt{A} (ndarray) – Some values.
- \texttt{axes} ((iterable of) int) – Chooses the axis of \texttt{A} which should be replaced. If multiple axes are given, you also need to give multiple index arrays as \texttt{mps\_inds}.
- \texttt{mps\_inds} (list of 1D ndarray) – Specifies for each axis in \texttt{axes}, for which MPS indices we have values in the corresponding axis of \texttt{A}. Defaults to \texttt{[np.arange(A.shape[ax]) for ax in axes]}. For indices across the MPS unit cell and “infinite” bc\_MPS, we shift \texttt{x\_0} accordingly.
- \texttt{include\_u} (list of bool) – Specifies for each axis in \texttt{axes}, whether the \texttt{u} index of the lattice should be included into the output array \texttt{res\_A}. Defaults to \texttt{len(self.unit\_cell) > 1}.

**Returns** \texttt{res\_A} – Reshaped and reordered copy of \texttt{A}. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index \texttt{j} maps to lattice site \((x0, x1, x2)\), then \texttt{res\_A[\ldots, x0, x1, x2, \ldots] = A[\ldots, mps\_inds[j], \ldots]}.

**Return type** np.ma.MaskedArray

\texttt{mps\_idx\_fix\_u}(\texttt{u=None})

return an index array of MPS indices for which the site within the unit cell is \texttt{u}.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This functions returns an index array of the mps indices which belong to sites given by \texttt{self.unit\_cell[u]}.

**Parameters** \texttt{u} (None | int) – Selects a site of the unit cell. \texttt{None} (default) means all sites.

**Returns** \texttt{mps\_idx} – MPS indices for which \texttt{self.site(i)} is \texttt{self.unit\_cell[u]}. Ordered ascending.

**Return type** array

\texttt{mps\_lat\_idx\_fix\_u}(\texttt{u=None})

Similar as \texttt{mps\_idx\_fix\_u()}, but return also the corresponding lattice indices.

**Parameters** \texttt{u} (None | int) – Selects a site of the unit cell. \texttt{None} (default) means all sites.

**Returns**
• **mps_idx** (*array*) – MPS indices \( i \) for which `self.site(i)` is `self.
unit_cell[u]`.

• **lat_idx** (*2D array*) – The row \( j \) contains the lattice index (without \( u \)) corresponding to `mps_idx[j]`.

`mps_sites()`

Return a list of sites for all MPS indices.

Equivalent to `[self.site(i) for i in range(self.N_sites)]`.

This should be used for sites of 1D tensor networks (MPS, MPO...).

`multi_coupling_shape(dx)`

Calculate correct shape of the strengths for a multi_coupling.

Parameters:

- **dx** (*2D array, shape (N_ops, dim*)) – \( dx[i,:]\) is the translation vector in the lattice for the \( i \)-th operator. Corresponds to the \( dx \) of each operator given in the argument `ops` of `tenpy.models.model.CouplingModel.add_multi_coupling()`.

Returns

- **coupling_shape** (*tuple of int*) – Len \( dim \). The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

- **shift_lat_indices** (*array*) – Translation vector from origin to the lower left corner of box spanned by \( dx \). (Unlike for `coupling_shape()` it can also contain entries > 0)

`number_nearest_neighbors(u=0)`

Deprecated.

Deprecated since version 0.5.0: Use `count_neighbors()` instead.

`number_next_nearest_neighbors(u=0)`

Deprecated.

Deprecated since version 0.5.0: Use `count_neighbors()` instead.

`property order`  

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with `plot_order()`.

`ordering(order)`  

Provide possible orderings of the \( N \) lattice sites.

This function can be overwritten by derived lattices to define additional orderings. The following orders are defined in this method:

<table>
<thead>
<tr>
<th>order</th>
<th>equivalent priority</th>
<th>equivalent snake_winding</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Cstyle'</td>
<td>(0, 1,..., dim-1, dim)</td>
<td>(False,..., False, False)</td>
</tr>
<tr>
<td>'default'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>'snake'</td>
<td>(0, 1,..., dim-1, dim)</td>
<td>(True,..., True, True)</td>
</tr>
<tr>
<td>'snakeCstyle'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>'Fstyle'</td>
<td>(dim-1,..., 1, 0, dim)</td>
<td>(False,..., False, False)</td>
</tr>
<tr>
<td>'snakeFstyle'</td>
<td>(dim-1,..., 1, 0, dim)</td>
<td>(False,..., False, False)</td>
</tr>
</tbody>
</table>
7.11. models
Note: For lattices with a non-trivial unit cell (e.g. Honeycomb, Kagome), the grouped order might be more appropriate, see `get_order_grouped()`

Parameters:

- **order** (str | ('standard', snake_winding, priority) | ('grouped', groups)) – Specifies the desired ordering using one of the strings of the above tables. Alternatively, an ordering is specified by a tuple with first entry specifying a function, 'standard' for `get_order()` and 'grouped' for `get_order_grouped()`, and other arguments in the tuple as specified in the documentation of these functions.

Returns **order** – the order to be used for `order`.

Return type array, shape (N, D+1), dtype np.intp

See also:

- **get_order** generates the order from equivalent priority and snake_winding.
- **get_order_grouped** variant of `get_order`.
- **plot_order** visualizes the resulting order.

**plot_basis**(ax, origin=(0.0, 0.0), shade=None, **kwargs)
Plot arrows indicating the basis vectors of the lattice.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- ****kwargs – Keyword arguments for ax.arrow.

**plot_bc_identified**(ax, direction=-1, origin=None, cylinder_axis=False, **kwargs)
Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **direction** (int) – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.
- **cylinder_axis** (bool) – Whether to plot the cylinder axis as well.
- **origin** (None | np.ndarray) – The origin starting from where we mark the identified sites. Defaults to the first entry of `unit_cell_positions`.
- ****kwargs – Keyword arguments for the used ax.plot.

**plot_coupling**(ax, coupling=None, wrap=False, **kwargs)
Plot lines connecting nearest neighbors of the lattice.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **coupling** (list of (u1, u2, dx)) – By default (None), use self.pairs['nearest_neighbors']. Specifies the connections to be plotted; iteating over lattice indices (i0, i1, ...), we plot a connection from the site (i0, i1, ...,
to the site \((i0+dx[0], i1+dx[1], \ldots, u2)\), taking into account the boundary conditions.

- **wrap** (bool) – If True, wrap
- **kwargs** – Further keyword arguments given to `ax.plot()`.

### plot_order

```
plot_order(ax, order=None, textkwars={'color': 'r'}, **kwargs)
```

Plot a line connecting sites in the specified “order” and text labels enumerating them.

**Parameters**

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **order** (None | 2D array (self.N_sites, self.dim+1)) – The order as returned by `ordering()`; by default (None) use `order`.
- **textkwars** (None | dict) – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for `ax.text()`.
- **kwargs** – Further keyword arguments given to `ax.plot()`.

### plot_sites

```
plot_sites(ax, markers=['o', '^', 's', 'p', 'h', 'D'], **kwargs)
```

Plot the sites of the lattice with markers.

**Parameters**

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **markers** (list) – List of values for the keyword marker of `ax.plot()` to distinguish the different sites in the unit cell, a site \(u\) in the unit cell is plotted with a marker `markers[u % len(markers)]`.
- **kwargs** – Further keyword arguments given to `ax.plot()`.

### position

```
position(lat_idx)
```

return 'space' position of one or multiple sites.

**Parameters**

- **lat_idx** (ndarray, (... , dim+1)) – Lattice indices.

**Returns**

- **pos** – The position of the lattice sites specified by `lat_idx` in real-space.

**Return type**

ndarray, (... , dim)

### possible_couplings

```
possible_couplings(u1, u2, dx)
```

Find possible MPS indices for two-site couplings.

For periodic boundary conditions (\(bc[a] == \text{False}\)) the index \(x_a\) is taken modulo \(Ls[a]\) and runs through `range(Ls[a])`. For open boundary conditions, \(x_a\) is limited to \(0 <= x_a < Ls[a]\) and \(0 <= x_a+dx[a] < lat.Ls[a]\).

**Parameters**

- **u1** (int) – Indices within the unit cell; the \(u1\) and \(u2\) of `add_coupling()`
- **u2** (int) – Indices within the unit cell; the \(u1\) and \(u2\) of `add_coupling()`
- **dx** (array) – Length \(dim\). The translation in terms of basis vectors for the coupling.

**Returns**

- **mps1, mps2** (array) – For each possible two-site coupling the MPS indices for the \(u1\) and \(u2\).
- **lat_indices** (2D int array) – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.
• **coupling_shape** *(tuple of int)* – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

**possible_multi_couplings** *(ops)*  
Generalization of `possible_couplings()` to couplings with more than 2 sites.

**Parameters ops** *(list of (opname, dx, u))* – Same as the argument `ops` of `add_multi_coupling()`.

**Returns**

• **mps_ijkl** *(2D int array)* – Each row contains MPS indices `i,j,k,\.\.\.` for each of the operators positions. The positions are defined by `dx` (j,k,\.\.\. relative to `i`) and boundary conditions of `self` (how much the box for given `dx` can be shifted around without hitting a boundary - these are the different rows).

• **lat_indices** *(2D int array)* – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.

• **coupling_shape** *(tuple of int)* – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

**save_hdf5** *(hdf5_saver, h5gr, subpath)*  
Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

Specifically, it saves `unit_cell`, `Ls`, `unit_cell_positions`, `basis`, `boundary_conditions`, `pairs` under their name, `bc_MPS` as "boundary_conditions_MPS", and `order` as "order_for_MPS". Moreover, it saves `dim` and `N_sites` as HDF5 attributes.

**Parameters**

• **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.

• **h5gr** *(class `Group`)* – HDF5 group which is supposed to represent `self`.

• **subpath** *(str)* – The name of `h5gr` with a `'/'` in the end.

**site** *(i)*  
Return `Site` instance corresponding to an MPS index `i`

**test_sanity** *( )*  
Sanity check.

Raises `ValueErrors`, if something is wrong.

`Lu = 3`

the (expected) number of sites in the unit cell, `len(unit_cell)`.

**Ladder**

• full name: `tenpy.models.lattice.Ladder`

• parent module: `tenpy.models.lattice`

• type: class
Inheritance Diagram

Ladder
down
Lattice

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ladder.<strong>init</strong>(L, sites, **kwargs)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>Ladder.count_neighbors([u, key])</td>
<td>Count e.g.</td>
</tr>
<tr>
<td>Ladder.coupling_shape(dx)</td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td>Ladder.enlarge_mps_unit_cell([factor])</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>Ladder.from_hdf5(hdf5_loader, h5gr, subpath)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>Ladder.lat2mps_idx(lat_idx)</td>
<td>Translate lattice indices ( (x_0, ..., x_{D-1}, u) ) to MPS index ( i ).</td>
</tr>
<tr>
<td>Ladder.mps2lat_idx(i)</td>
<td>Translate MPS index ( i ) to lattice indices ( (x_0, ..., x_{(\text{dim}-1)}, u) ).</td>
</tr>
<tr>
<td>Ladder.mps2lat_values(A[, axes, u])</td>
<td>Reshape/reorder ( A ) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>Ladder.mps2lat_values_masked(A[, axes, ...,])</td>
<td>Reshape/reorder an array ( A ) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>Ladder.mps_idx_fix_u([u])</td>
<td>Return an index array of MPS indices for which the site within the unit cell is ( u ).</td>
</tr>
<tr>
<td>Ladder.mps_lat_idx_fix_u([u])</td>
<td>Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td>Ladder.mps_sites()</td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td>Ladder.multi_coupling_shape(dx)</td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td>Ladder.number_nearest_neighbors([u])</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>Ladder.number_next_nearest_neighbors([u])</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>Ladder.ordering(order)</td>
<td>Provide possible orderings of the ( N ) lattice sites.</td>
</tr>
<tr>
<td>Ladder.plot_basis(ax[, origin, shade])</td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td>Ladder.plot_bc_identified(ax[, direction, ...])</td>
<td>Mark two sites indiffed by periodic boundary conditions.</td>
</tr>
<tr>
<td>Ladder.plot_coupling(ax[, coupling, wrap])</td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
</tr>
<tr>
<td>Ladder.plot_order(ax[, order, textkwargs])</td>
<td>Plot a line connecting sites in the specified &quot;order&quot; and text labels enumerating them.</td>
</tr>
<tr>
<td>Ladder.plot_sites(ax[, markers])</td>
<td>Plot the sites of the lattice with markers.</td>
</tr>
<tr>
<td>Ladder.position(lat_idx)</td>
<td>Return 'space' position of one or multiple sites.</td>
</tr>
</tbody>
</table>
Table 84 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ladder.possible_couplings</td>
<td>Find possible MPS indices for two-site couplings.</td>
</tr>
<tr>
<td>Ladder.possible_multi_couplings</td>
<td>Generalization of possible_couplings() to couplings with more than 2 sites.</td>
</tr>
<tr>
<td>Ladder.save_hdf5</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>Ladder.site(i)</td>
<td>Return Site instance corresponding to an MPS index i.</td>
</tr>
<tr>
<td>Ladder.test_sanity()</td>
<td>Sanity check.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

- **Ladder.Lu**
  the (expected) number of sites in the unit cell, `len(unit_cell)`.

- **Ladder.boundary_conditions**
  Human-readable list of boundary conditions from `bc` and `bc_shift`.

- **Ladder.dim**
  the dimension of the lattice

- **Ladder.nearest_neighbors**

- **Ladder.next_nearest_neighbors**

- **Ladder.next_next_nearest_neighbors**

- **Ladder.order**
  Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

```python
class tenpy.models.lattice.Ladder(L, sites, **kwargs)
    Bases: tenpy.models.lattice.Lattice

A ladder coupling two chains.
```

Parameters

- **L (int)** – The length of each chain, we have 2*L sites in total.
- **sites** (list of Site) – The two local lattice sites making the `unit_cell` of the Lattice. If only a single Site is given, it is used for both chains.
- ****kwargs** – Additional keyword arguments given to the Lattice. `basis`, `pos` and `pairs` are set accordingly.

- **Lu = 2**
  the (expected) number of sites in the unit cell, `len(unit_cell)`.

- **dim = 1**
  the dimension of the lattice

**property boundary_conditions**
Human-readable list of boundary conditions from `bc` and `bc_shift`. 
Returns `boundary_conditions` – List of "open" or "periodic", one entry for each direction of the lattice.

Return type  list of str

`count_neighbors (u=0, key='nearest_neighbors')`
Count e.g. the number of nearest neighbors for a site in the bulk.

Parameters

• `u (int)` – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever `key` specifies).

• `key (str)` – Key of pairs to select what to count.

Returns `number` – Number of nearest neighbors (or whatever `key` specified) for the `u`-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

Return type  int

`coupling_shape(dx)`
Calculate correct shape of the strengths for a coupling.

Parameters `dx (tuple of int)` – Translation vector in the lattice for a coupling of two operators. Corresponds to `dx` argument of `tenpy.models.model.CouplingModel.add_multi_coupling()`.

Returns

• `coupling_shape (tuple of int)` – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

• `shift_lat_indices (array)` – Translation vector from origin to the lower left corner of box spanned by `dx`.

`enlarge_mps_unit_cell (factor=2)`
Repeat the unit cell for infinite MPS boundary conditions; in place.

Parameters `factor (int)` – The new number of sites in the MPS unit cell will be increased from `N_sites` to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

`classmethod from_hdf5 (hdf5_loader, h5gr, subpath)`
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

Parameters

• `hdf5_loader (Hdf5Loader)` – Instance of the loading engine.

• `h5gr (Group)` – HDF5 group which is represent the object to be constructed.

• `subpath (str)` – The name of `h5gr` with a ' /' in the end.

Returns `obj` – Newly generated class instance containing the required data.

Return type  cls

`lat2mps_idx (lat_idx)`
Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index `i`.

7.11. models 341
Parameters `lat_idx` (array_like [., dim+1]) -- The last dimension corresponds to lattice indices \((x_0, \ldots, x_{D-1}, u)\). All lattice indices should be positive and smaller than the corresponding entry in `self.shape`. Exception: for "infinite" bc_MPS, an \(x_0\) outside indicates shifts across the boundary.

Returns `i` -- MPS index/indices corresponding to `lat_idx`. Has the same shape as `lat_idx` without the last dimension.

Return type array_like

`mps2lat_idx(i)`
Translate MPS index \(i\) to lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\).

Parameters \(i\) (int | array_like of int) -- MPS index/indices.

Returns `lat_idx` -- First dimensions like \(i\), last dimension has len `dim`+1 and contains the lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\) corresponding to \(i\). For \(i\) across the MPS unit cell and "infinite" bc_MPS, we shift \(x_0\) accordingly.

Return type array

`mps2lat_values(A, axes=0, u=None)`
Reshape/reorder \(A\) to replace an MPS index by lattice indices.

Parameters
- \(A\) (ndarray) -- Some values. Must have \(A.shape[axes] = self.N_sites\) if \(u\) is None, or \(A.shape[axes] = self.N_cells\) if \(u\) is an int.
- \(axes\) ((iterable of) int) -- chooses the axis which should be replaced.
- \(u\) (None | int) -- Optionally choose a subset of MPS indices present in the axes of \(A\), namely the indices corresponding to `self.unit_cell[u]`, as returned by `mps_idx_fix_u()`. The resulting array will not have the additional dimension(s) of \(u\).

Returns `res_A` -- Reshaped and reordered versions of \(A\). Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index \(j\) maps to lattice site \((x0, x1, x2)\), then `res_A[..., x0, x1, x2, ...] = A[..., j, ...]`.

Return type ndarray

Examples
Say you measure expectation values of an onsite term for an MPS, which gives you an 1D array \(A\), where \(A[i]\) is the expectation value of the site given by `self.mps2lat_idx(i)`. Then this function gives you the expectation values ordered by the lattice:

```python
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[tuple(lat.mps2lat_idx(5))] == A[5]
True
```

If you have a correlation function \(C[i, j]\), it gets just slightly more complicated:

```python
>>> print(lat.shape, C.shape)
(10, 3, 2) (60, 60)
```
If the unit cell consists of different physical sites, an onsite operator might be defined only on one of the sites in the unit cell. Then you can use `mps_idx_fix_u()` to get the indices of sites it is defined on, measure the operator on these sites, and use the argument `u` of this function.

```python
>>> u = 0
>>> idx_subset = lat.mps_idx_fix_u(u)
>>> A_u = A[idx_subset]
>>> A_u_res = lat.mps2lat_values(A_u, u=u)
>>> A_u_res.shape
(10, 3)
>>> np.all(A_res[:, :, u] == A_u_res[:, :])
True
```

**mps2lat_values_masked(A, axes=1, mps_inds=None, include_u=None)**

Reshape/reorder an array `A` to replace an MPS index by lattice indices. This is a generalization of `mps2lat_values()` allowing for the case of an arbitrary set of MPS indices present in each axis of `A`.

**Parameters**

- `A` *(ndarray)* – Some values.
- `axes` *(iterable of int)* – Chooses the axis of `A` which should be replaced. If multiple axes are given, you also need to give multiple index arrays as `mps_inds`.
- `mps_inds` *(list of 1D ndarray)* – Specifies for each axis in `axes`, for which MPS indices we have values in the corresponding axis of `A`. Defaults to `[np.arange(A.shape[ax]) for ax in axes]`. For indices across the MPS unit cell and “infinite” `bc_MPS`, we shift `x_0` accordingly.
- `include_u` *(list of bool)* – Specifies for each axis in `axes`, whether the `u` index of the lattice should be included into the output array `res_A`. Defaults to `len(self.unit_cell) > 1`.

**Returns** `res_A` – Reshaped and reordered copy of `A`. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index `j` maps to lattice site `(x0, x1, x2)`, then `res_A[..., x0, x1, x2, ...] = A[..., mps_inds[j], ...]`.

**Return type** `np.ma.MaskedArray`

**mps_idx_fix_u(u=None)**

return an index array of MPS indices for which the site within the unit cell is `u`.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This functions returns an index array of the mps indices which belong to sites given by `self.unit_cell[u]`.

**Parameters** `u` *(None | int)* – Selects a site of the unit cell. `None` (default) means all sites.

**Returns** `mps_idx` – MPS indices for which `self.site(i)` is `self.unit_cell[u]`. Ordered ascending.

**Return type** `array`

**mps_lat_idx_fix_u(u=None)**

Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
Parameters **u** *(None | int)* – Selects a site of the unit cell. None (default) means all sites.

Returns

- **mps_idx** *(array)* – MPS indices *i* for which `self.site(i)` is `self.unit_cell[u]`.
- **lat_idx** *(2D array)* – The row *j* contains the lattice index (without *u*) corresponding to `mps_idx[j]`.

**mps_sites()**

Return a list of sites for all MPS indices.

Equivalent to `[self.site(i) for i in range(self.N_sites)]`.

This should be used for sites of 1D tensor networks (MPS, MPO,...).

**multi_coupling_shape** *(dx)*

Calculate correct shape of the strengths for a multi_coupling.

Parameters **dx** *(2D array, shape (N_ops, dim))* – `dx[i, :]` is the translation vector in the lattice for the *i*-th operator. Corresponds to the `dx` of each operator given in the argument `ops` of `tenpy.models.model.CouplingModel.add_multi_coupling()`.

Returns

- **coupling_shape** *(tuple of int)* – Len *dim*. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.
- **shift_lat_indices** *(array)* – Translation vector from origin to the lower left corner of box spanned by `dx`. (Unlike for `coupling_shape()` it can also contain entries > 0)

**number_nearest_neighbors** *(u=0)*

Deprecated.

Deprecated since version 0.5.0: Use `count_neighbors()` instead.

**number_next_nearest_neighbors** *(u=0)*

Deprecated.

Deprecated since version 0.5.0: Use `count_neighbors()` instead.

**property order**

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with `plot_order()`.

**ordering** *(order)*

Provide possible orderings of the *N* lattice sites.

This function can be overwritten by derived lattices to define additional orderings. The following orders are defined in this method:

<table>
<thead>
<tr>
<th>order</th>
<th>equivalent priority</th>
<th>equivalent snake_winding</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Cstyle'</td>
<td>(0, 1, ..., dim-1, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'default'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>'snake'</td>
<td>(0, 1, ..., dim-1, dim)</td>
<td>(True, ..., True, True)</td>
</tr>
<tr>
<td>'snakeCstyle'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>'Fstyle'</td>
<td>(dim-1, ..., 1, 0, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'snakeFstyle'</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
7.11. models
Note: For lattices with a non-trivial unit cell (e.g. Honeycomb, Kagome), the grouped order might be more appropriate, see get_order_grouped()

Parameters order (str | (‘standard’, snake_winding, priority) | (‘grouped’, groups)) – Specifies the desired ordering using one of the strings of the above tables. Alternatively, an ordering is specified by a tuple with first entry specifying a function, 'standard' for get_order() and 'grouped' for get_order_grouped(), and other arguments in the tuple as specified in the documentation of these functions.

Returns order – the order to be used for order.

Return type array, shape (N, D+1), dtype np.intp

See also:

generate_order generates the order from equivalent priority and snake_winding.
generate_order_grouped variant of get_order.
plot_order visualizes the resulting order.

plot_basis(ax, origin=(0.0, 0.0), shade=None, **kwargs)
Plot arrows indicating the basis vectors of the lattice.

Parameters

• ax (matplotlib.axes.Axes) – The axes on which we should plot.
• **kwargs – Keyword arguments for ax.arrow.

plot_bc_identified(ax, direction=-1, origin=None, cylinder_axis=False, **kwargs)
Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

Parameters

• ax (matplotlib.axes.Axes) – The axes on which we should plot.
• direction (int) – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.
• cylinder_axis (bool) – Whether to plot the cylinder axis as well.
• origin (None | np.ndarray) – The origin starting from where we mark the identified sites. Defaults to the first entry of unit_cell_positions.
• **kwargs – Keyword arguments for the used ax.plot.

plot_coupling(ax, coupling=None, wrap=False, **kwargs)
Plot lines connecting nearest neighbors of the lattice.

Parameters

• ax (matplotlib.axes.Axes) – The axes on which we should plot.
• coupling (list of (u1, u2, dx)) – By default (None), use self.pairs['nearest_neighbors']. Specifies the connections to be plotted; iterating over lattice indices (i0, i1, ...), we plot a connection from the site (i0, i1, ...,
to the site \((i0+dx[0], i1+dx[1], \ldots, u2)\), taking into account the boundary conditions.

- **wrap** (bool) – If True, wrap
- **kwargs** – Further keyword arguments given to `ax.plot()`.

### plot_order

Plot a line connecting sites in the specified “order” and text labels enumerating them.

**Parameters**

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **order** (None | 2D array (self.N_sites, self.dim+1)) – The order as returned by `ordering()`; by default (None) use `order`.
- **textkwargs** (None | dict) – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for `ax.text()`.
- **kwargs** – Further keyword arguments given to `ax.plot()`.

### plot_sites

Plot the sites of the lattice with markers.

**Parameters**

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **markers** (list) – List of values for the keyword `marker` of `ax.plot()` to distinguish the different sites in the unit cell, a site \(u\) in the unit cell is plotted with a marker `markers[u % len(markers)]`.
- **kwargs** – Further keyword arguments given to `ax.plot()`.

### position

Return 'space' position of one or multiple sites.

**Parameters**

- **lat_idx** (ndarray, (..., dim+1)) – Lattice indices.

**Returns**

- **pos** – The position of the lattice sites specified by `lat_idx` in real-space.

**Return type**

ndarray, (..., dim)

### possible_couplings

Find possible MPS indices for two-site couplings.

For periodic boundary conditions (`bc[a] == False`) the index \(x_a\) is taken modulo \(Ls[a]\) and runs through `range(Ls[a])`. For open boundary conditions, \(x_a\) is limited to \(0 <= x_a < Ls[a]\) and \(0 <= x_a+dx[a] < lat.Ls[a]\).

**Parameters**

- **u1** (int) – Indices within the unit cell; the \(u1\) and \(u2\) of `add_coupling()`
- **u2** (int) – Indices within the unit cell; the \(u1\) and \(u2\) of `add_coupling()`
- **dx** (array) – Length `dim`. The translation in terms of basis vectors for the coupling.

**Returns**

- **mps1, mps2** (array) – For each possible two-site coupling the MPS indices for the \(u1\) and \(u2\).
- **lat_indices** (2D int array) – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** *(tuple of int)* – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

**possible_multi_couplings** *(ops)*  
Generalization of `possible_couplings()` to couplings with more than 2 sites.

Parameters `ops` *(list of (opname, dx, u))* – Same as the argument `ops` of `add_multi_coupling()`.

Returns

- **mps_ijkl** *(2D int array)* – Each row contains MPS indices `ijkl`... for each of the operators positions. The positions are defined by `dx` `(j,k,...` relative to `i`) and boundary conditions of `self` (how much the box for given `dx` can be shifted around without hitting a boundary - these are the different rows).

- **lat_indices** *(2D int array)* – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.

- **coupling_shape** *(tuple of int)* – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

**save_hdf5** *(hdf5_saver, h5gr, subpath)*  
Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

Specifically, it saves `unit_cell`, `Ls`, `unit_cell_positions`, `basis`, `boundary_conditions`, `pairs` under their name, `bc_MPS` as "boundary_conditions_MPS", and `order` as "order_for_MPS". Moreover, it saves `dim` and `N_sites` as HDF5 attributes.

Parameters

- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.

- **h5gr** *(:`class` `Group`)* – HDF5 group which is supposed to represent `self`.

- **subpath** *(str)* – The `name` of `h5gr` with a `'/'` in the end.

**site** *(i)*  
return `Site` instance corresponding to an MPS index `i`

**test_sanity** ()  
Sanity check.

Raises ValueErrors, if something is wrong.

**Lattice**

- full name: `tenpy.models.lattice.Lattice`

- parent module: `tenpy.models.lattice`

- type: class
Inheritance Diagram

```
Inheritance Diagram

[367x748]
Lattice

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice.<strong>init</strong>((Ls, unit_cell[, order, bc, ...]))</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>Lattice.count_neighbors([u, key])</td>
<td>Count e.g.</td>
</tr>
<tr>
<td>Lattice.coupling_shape(dx)</td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td>Lattice.enlarge_mps_unit_cell([factor])</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>Lattice.from_hdf5(hdf5_loader, h5gr, subpath)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>Lattice.lat2mps_idx(lat_idx)</td>
<td>Translate lattice indices (x_0, ..., x_{dim-1}, u) to MPS index i.</td>
</tr>
<tr>
<td>Lattice.mps2lat_idx(i)</td>
<td>Translate MPS index i to lattice indices (x_0, ..., x_{dim-1}, u).</td>
</tr>
<tr>
<td>Lattice.mps2lat_values(A[, axes, u])</td>
<td>Reshape/reorder A to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>Lattice.mps2lat_values_masked(A[, axes, ...,])</td>
<td>Reshape/reorder an array A to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>Lattice.mps_idx_fix_u([u])</td>
<td>return an index array of MPS indices for which the site within the unit cell is u.</td>
</tr>
<tr>
<td>Lattice.mps_lat_idx_fix_u([u])</td>
<td>Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td>Lattice.mps_sites()</td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td>Lattice.multi_coupling_shape(dx)</td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td>Lattice.number_nearest_neighbors([u])</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>Lattice.number_next_nearest_neighbors([u])</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>Lattice.ordering(order)</td>
<td>Provide possible orderings of the N lattice sites.</td>
</tr>
<tr>
<td>Lattice.plot_basis(ax[, origin, shade])</td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td>Lattice.plot_bc_identified(ax[, direction, ...])</td>
<td>Mark two sites identified by periodic boundary conditions.</td>
</tr>
<tr>
<td>Lattice.plot_coupling(ax[, coupling, wrap])</td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
</tr>
<tr>
<td>Lattice.plot_order(ax[, order, textkwargs])</td>
<td>Plot a line connecting sites in the specified “order” and text labels enumerating them.</td>
</tr>
<tr>
<td>Lattice.plot_sites(ax[, markers])</td>
<td>Plot the sites of the lattice with markers.</td>
</tr>
<tr>
<td>Lattice.position(lat_idx)</td>
<td>return <code>space</code> position of one or multiple sites.</td>
</tr>
<tr>
<td>Lattice.possible_couplings(u1, u2, dx)</td>
<td>Find possible MPS indices for two-site couplings.</td>
</tr>
<tr>
<td>Lattice.possible_multi_couplings(ops)</td>
<td>Generalization of possible_couplings() to couplings with more than 2 sites.</td>
</tr>
<tr>
<td>Lattice.save_hdf5(hdf5_saver, h5gr, subpath)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>Lattice.site(i)</td>
<td>return Site instance corresponding to an MPS index i</td>
</tr>
</tbody>
</table>
```
Table 86 – continued from previous page

Lattice.test_sanity()  
Sanity check.

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice.Lu</td>
<td>the (expected) number of sites in the unit cell, (\text{len(unit_cell)}).</td>
</tr>
<tr>
<td>Lattice.boundary_conditions</td>
<td>Human-readable list of boundary conditions from (bc) and (bc_shift).</td>
</tr>
<tr>
<td>Lattice.dim</td>
<td>the dimension of the lattice</td>
</tr>
<tr>
<td>Lattice.nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Lattice.next_nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Lattice.next_next_nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Lattice.order</td>
<td>Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.</td>
</tr>
</tbody>
</table>

```python
class tenpy.models.lattice.Lattice(Ls, unit_cell, order='default', bc='open', 
bc_MPS='finite', basis=None, positions=None, nearest_neighbors=None, 
next_nearest_neighbors=None, next_next_nearest_neighbors=None, pairs=None)
```

Bases: object

A general, regular lattice.

The lattice consists of a unit cell which is repeated in \(dim\) different directions. A site of the lattice is thus identified by lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\), where \(0 \leq x_l < Ls[l]\) pick the position of the unit cell in the lattice and \(0 \leq u < \text{len(unit\_cell)}\) picks the site within the unit cell. The site is located in ‘space’ at \(\sum_l x_l \times \text{basis}[l] + \text{unit\_cell\_positions}[u]\) (see \text{position()}). (Note that the position in space is only used for plotting, not for defining the couplings.)

In addition to the pure geometry, this class also defines an order of all sites. This order maps the lattice to a finite 1D chain and defines the geometry of MPSs and MPOs. The MPS index \(i\) corresponds thus to the lattice sites given by \((x_0, \ldots, x_{(dim-1)}, u) = \text{tuple(self.order}[i])\). Infinite boundary conditions of the MPS repeat in the first spatial direction of the lattice, i.e., if the site at \((x_0, x_1, \ldots, x_{(dim-1)}, u)\) has MPS index \(i\), the site at \((x_0 + Ls[0], x_1, \ldots, x_{(dim-1)}, u)\) corresponds to MPS index \(i + N\_sites\). Use \text{mps2lat\_idx()} and \text{lat2mps\_idx()} for conversion of indices. The function \text{mps2lat\_values()} performs the necessary reshaping and re-ordering from arrays indexed in MPS form to arrays indexed in lattice form.

Deprecated since version 0.5.0: The parameters and attributes nearest_neighbors, next_nearest_neighbors and next_next_nearest_neighbors are deprecated. Instead, we use a dictionary pairs with those names as keys and the corresponding values as specified before.

Parameters

- **Ls** (list of int) – the length in each direction
- **unit_cell** (list of Site) – The sites making up a unit cell of the lattice. If you want to specify it only after initialization, use None entries in the list.
- **order** (str | ('standard', snake_winding, priority) | ('grouped', groups)) – A string or tuple specifying the order, given to \text{ordering()}.
- **bc** (iterable of) ('open' | 'periodic' | int) – Boundary conditions in each direction of the lattice. A single string holds for all directions. An integer shift means that we have periodic boundary conditions along this direction, but shift/tilt by
• bc_MPS ('finite' | 'segment' | 'infinite') – Boundary conditions for an MPS/MPO living on the ordered lattice. If the system is 'infinite', the infinite direction is always along the first basis vector (justifying the definition of N_rings and N_sites_per_ring).

• basis (iterable of 1D arrays) – For each direction one translation vectors shifting the unit cell. Defaults to the standard ONB np.eye(dim).

• positions (iterable of 1D arrays) – For each site of the unit cell the position within the unit cell. Defaults to np.zeros((len(unit_cell), dim)).

• nearest_neighbors (None | list of (u1, u2, dx)) – Deprecated. Specify as pairs['nearest_neighbors'] instead.

• next_nearest_neighbors (None | list of (u1, u2, dx)) – Deprecated. Specify as pairs['next_nearest_neighbors'] instead.

• next_next_nearest_neighbors (None | list of (u1, u2, dx)) – Deprecated. Specify as pairs['next_next_nearest_neighbors'] instead.

• pairs (dict) – Of the form {'nearest_neighbors': [(u1, u2, dx), ...], ...}. Typical keys are 'nearest_neighbors', 'next_nearest_neighbors'. For each of them, it specifies a list of tuples (u1, u2, dx) which can be used as parameters for add_coupling() to generate couplings over each pair of e.g., 'nearest_neighbors'. Note that this adds couplings for each pair only in one direction!

Ls

the length in each direction.

Type  tuple of int

shape

the ‘shape’ of the lattice, same as Ls + (len(unit_cell), )

Type  tuple of int

N_cells

the number of unit cells in the lattice, np.prod(self.Ls).

Type  int

N_sites

the number of sites in the lattice, np.prod(self.shape).

Type  int

N_sites_per_ring

Defined as N_sites / Ls[0], for an infinite system the number of cites per “ring”.

Type  int

N_rings

Alias for Ls[0], for an infinite system the number of “rings” in the unit cell.

Type  int

unit_cell

the sites making up a unit cell of the lattice.

Type  list of Site
...
test_sanity()
Sanity check.

    Raises ValueErrors, if something is wrong.

save_hdf5(hdf5_saver, h5gr, subpath)
Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5().

Specifically, it saves unit_cell, Ls, unit_cell_positions, basis, boundary_conditions, pairs under their name, bc_MPS as "boundary_conditions_MPS ", and order as "order_for_MPS". Moreover, it saves dim and N_sites as HDF5 attributes.

Parameters

- hdf5_saver (Hdf5Saver) – Instance of the saving engine.
- h5gr (:class:`Group`) – HDF5 group which is supposed to represent self.
- subpath (str) – The name of h5gr with a '/' in the end.

classmethod from_hdf5(hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

Parameters

- hdf5_loader (Hdf5Loader) – Instance of the loading engine.
- h5gr (Group) – HDF5 group which is represent the object to be constructed.
- subpath (str) – The name of h5gr with a '/' in the end.

Returns obj – Newly generated class instance containing the required data.

Return type cls

property dim
the dimension of the lattice

property order
Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

    Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

    You can visualize the order with plot_order().

ordering(order)
Provide possible orderings of the N lattice sites.

This function can be overwritten by derived lattices to define additional orderings. The following orders are defined in this method:

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<td></td>
<td></td>
</tr>
<tr>
<td>'Fstyle'</td>
<td>(dim-1, ..., 1, 0, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'snakeFstyle'</td>
<td>(dim-1, ..., 1, 0, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
</tbody>
</table>
Chapter 7. License
Note: For lattices with a non-trivial unit cell (e.g. Honeycomb, Kagome), the grouped order might be more appropriate, see `get_order_grouped()`.

**Parameters**

- **order**: (str | ('standard', snake_winding, priority) | ('grouped', groups)) – Specifies the desired ordering using one of the strings of the above tables. Alternatively, an ordering is specified by a tuple with first entry specifying a function, 'standard' for `get_order()` and 'grouped' for `get_order_grouped()`, and other arguments in the tuple as specified in the documentation of these functions.

  **Returns** order – the order to be used for `order`.

  **Return type** array, shape (N, D+1), dtype np.intp

See also:

- `get_order` generates the order from equivalent priority and snake_winding.
- `get_order_grouped` variant of `get_order`.
- `plot_order` visualizes the resulting order.

**property boundary_conditions**

Human-readable list of boundary conditions from `bc` and `bc_shift`.

  **Returns** boundary_conditions – List of "open" or "periodic", one entry for each direction of the lattice.

  **Return type** list of str

**enlarge_mps_unit_cell** (factor=2)

Repeat the unit cell for infinite MPS boundary conditions; in place.

  **Parameters**

- **factor**: (int) – The new number of sites in the MPS unit cell will be increased from `N_sites` to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

**position** (lat_idx)

return 'space' position of one or multiple sites.

  **Parameters**

- **lat_idx**: (ndarray, (... , dim+1)) – Lattice indices.

  **Returns** pos – The position of the lattice sites specified by `lat_idx` in real-space.

  **Return type** ndarray, (... , dim)

**site** (i)

return Site instance corresponding to an MPS index `i`

**mps_sites** ()

Return a list of sites for all MPS indices.

Equivalent to `[self.site(i) for i in range(self.N_sites)]`.

This should be used for `sites` of 1D tensor networks (MPS, MPO, ...).

**mps2lat_idx** (i)

Translate MPS index `i` to lattice indices `(x_0, ..., x_(dim-1), u)`.

  **Parameters** i (int / array_like of int) – MPS index/indices.
Returns **lat_idx** – First dimensions like $i$, last dimension has len \(dim + 1\) and contains the lattice indices \((x_0, ..., x_{(dim-1)}, u)\) corresponding to $i$. For $i$ across the MPS unit cell and “infinite” bc\_MPS, we shift $x_0$ accordingly.

**Return type** array

**lat2mps_idx(lat_idx)**

Translate lattice indices \((x_0, ..., x_{(D-1)}, u)\) to MPS index $i$.

**Parameters**

- **lat_idx** *(array_like \([.., dim+1]\))* – The last dimension corresponds to lattice indices \((x_0, ..., x_{(D-1)}, u)\). All lattice indices should be positive and smaller than the corresponding entry in self.shape. Exception: for “infinite” bc\_MPS, an $x_0$ outside indicates shifts across the boundary.

**Returns** $i$ – MPS index/indices corresponding to lat\_idx. Has the same shape as lat\_idx without the last dimension.

**Return type** array_like

**mps_idx_fix_u(u=None)**

return an index array of MPS indices for which the site within the unit cell is $u$.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This function returns an index array of the mps indices which belong to sites given by self.unit\_cell\[u\].

**Parameters**

- **u** *(None | int)* – Selects a site of the unit cell. None (default) means all sites.

**Returns** mps\_idx – MPS indices for which self.site(i) is self.unit\_cell\[u\]. Ordered ascending.

**Return type** array

**mps_lat_idx_fix_u(u=None)**

Similar as mps\_idx\_fix\_u(), but return also the corresponding lattice indices.

**Parameters**

- **u** *(None | int)* – Selects a site of the unit cell. None (default) means all sites.

**Returns**

- **mps_idx (array)** – MPS indices $i$ for which self.site(i) is self.unit\_cell\[u\].
- **lat_idx (2D array)** – The row $j$ contains the lattice index (without $u$) corresponding to mps\_idx\[j\].

**mps2lat_values(A, axes=0, u=None)**

Reshape/reorder $A$ to replace an MPS index by lattice indices.

**Parameters**

- **A** *(ndarray)* – Some values. Must have A.shape[axes] = self.N\_sites if $u$ is None, or A.shape[axes] = self.N\_cells if $u$ is an int.
- **axes** *(iterable of) int* – chooses the axis which should be replaced.
- **u** *(None | int)* – Optionally choose a subset of MPS indices present in the axes of $A$, namely the indices corresponding to self.unit\_cell\[u\], as returned by mps\_idx\_fix\_u(). The resulting array will not have the additional dimension(s) of $u$.

**Returns** res\_A – Reshaped and reordered versions of A. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index $j$ maps to lattice site \((x0, x1, x2)\), then res\_A[... , x0, x1, x2, ...] = A[... , j, ...].
Return type  ndarray

Examples
Say you measure expectation values of an onsite term for an MPS, which gives you an 1D array $A$, where $A[i]$ is the expectation value of the site given by `self.mps2lat_idx(i)`. Then this function gives you the expectation values ordered by the lattice:

```python
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[tuple(lat.mps2lat_idx(5))] == A[5]
True
```

If you have a correlation function $C[i, j]$, it gets just slightly more complicated:

```python
>>> print(lat.shape, C.shape)
(10, 3, 2) (60, 60)
>>> lat.mps2lat_values(C, axes=[0, 1]).shape
(10, 3, 2, 10, 3, 2)
```

If the unit cell consists of different physical sites, an onsite operator might be defined only on one of the sites in the unit cell. Then you can use `mps_idx_fix_u()` to get the indices of sites it is defined on, measure the operator on these sites, and use the argument $u$ of this function.

```python
>>> u = 0
>>> idx_subset = lat.mps_idx_fix_u(u)
>>> A_u = A[idx_subset]
>>> A_u_res = lat.mps2lat_values(A_u, u=u)
>>> A_u_res.shape
(10, 3)
>>> np.all(A_res[:, :, u] == A_u_res[:, :])
True
```

`mps2lat_values_masked(A, axes=-1, mps_inds=None, include_u=None)`
Reshape/reorder an array $A$ to replace an MPS index by lattice indices.

This is a generalization of `mps2lat_values()` allowing for the case of an arbitrary set of MPS indices present in each axis of $A$.

Parameters
- **A** (*ndarray*) – Some values.
- **axes** (*iterable of int*) – Chooses the axis of $A$ which should be replaced. If multiple axes are given, you also need to give multiple index arrays as `mps_inds`.
- **mps_inds** (*list of 1D ndarray*) – Specifies for each axis in `axes`, for which MPS indices we have values in the corresponding axis of $A$. Defaults to `[np.arange(A.shape[ax]) for ax in axes]`. For indices accross the MPS unit cell and "infinite" `bc_MPS`, we shift $x_0$ accordingly.
- **include_u** (*list of bool*) – Specifies for each axis in `axes`, whether the $u$ index of the lattice should be included into the output array `res_A`. Defaults to `len(self.unit_cell) > 1`. 7.11. models
Returns \texttt{res\_A} – Reshaped and reordered copy of \(A\). Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index \(j\) maps to lattice site \((x_0, x_1, x_2)\), then 
\[ \text{res\_A}[..., x_0, x_1, x_2, ...] = A[..., \text{mps\_inds}[j], ...]. \]

Return type \texttt{np.ma.MaskedArray}

\texttt{count\_neighbors}(u=0, key='nearest\_neighbors')
Count e.g. the number of nearest neighbors for a site in the bulk.

Parameters

- \(u\) (\texttt{int}) – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever \textit{key} specifies).
- \textit{key} (\texttt{str}) – Key of \textit{pairs} to select what to count.

Returns \texttt{number} – Number of nearest neighbors (or whatever \textit{key} specified) for the \(u\)-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

Return type \texttt{int}

\texttt{number\_nearest\_neighbors}(u=0)
Deprecated.

Deprecated since version 0.5.0: Use \texttt{count\_neighbors()} instead.

\texttt{number\_next\_nearest\_neighbors}(u=0)
Deprecated.

Deprecated since version 0.5.0: Use \texttt{count\_neighbors()} instead.

\texttt{coupling\_shape}(dx)
Calculate correct shape of the \textit{strengths} for a coupling.

Parameters \(dx\) (\texttt{tuple of int}) – Translation vector in the lattice for a coupling of two operators. Corresponds to \(dx\) argument of \texttt{tenpy.models.model.CouplingModel.add\_multi\_coupling()}.

Returns

- \texttt{coupling\_shape} (\texttt{tuple of int}) – Len \textit{dim}. The correct shape for an array specifying the coupling strength. \textit{lat\_indices} has only rows within this shape.
- \texttt{shift\_lat\_indices} (\texttt{array}) – Translation vector from origin to the lower left corner of box spanned by \(dx\).

\texttt{possible\_couplings}(u1, u2, dx)
Find possible MPS indices for two-site couplings.

For periodic boundary conditions (\texttt{bc[a] == False}) the index \(x_a\) is taken modulo \texttt{Ls[a]} and runs through \texttt{range(Ls[a])}. For open boundary conditions, \(x_a\) is limited to \(0 \leq x_a < Ls[a]\) and 
\(0 \leq x_a + dx[a] < \text{lat.Ls[a]}.\)

Parameters

- \(u1\) (\texttt{int}) – Indices within the unit cell; the \(u1\) and \(u2\) of \texttt{add\_coupling()}.
- \(u2\) (\texttt{int}) – Indices within the unit cell; the \(u1\) and \(u2\) of \texttt{add\_coupling()}.
- \(dx\) (\texttt{array}) – Length \textit{dim}. The translation in terms of basis vectors for the coupling.

Returns

- \texttt{mps1, mps2} (\texttt{array}) – For each possible two-site coupling the MPS indices for the \(u1\) and \(u2\).
• **lat_indices** (2D int array) – Rows of *lat_indices* correspond to rows of *mps_ijkl* and contain the lattice indices of the “lower left corner” of the box containing the coupling.

• **coupling_shape** (tuple of int) – Len *dim*. The correct shape for an array specifying the coupling strength. *lat_indices* has only rows within this shape.

**multi_coupling_shape** (*dx*)

Calculate correct shape of the *strengths* for a multi_coupling.

**Parameters**
- *dx* (2D array, shape (N_ops, *dim*)) – *dx*[i, :] is the translation vector in the lattice for the *i*-th operator. Corresponds to the *dx* of each operator given in the argument *ops* of `tenpy.models.model.CouplingModel.add_multi_coupling()`.

**Returns**
- **coupling_shape** (tuple of int) – Len *dim*. The correct shape for an array specifying the coupling strength. *lat_indices* has only rows within this shape.

- **shift_lat_indices** (array) – Translation vector from origin to the lower left corner of box spanned by *dx*. (Unlike for *coupling_shape()* it can also contain entries > 0)

**possible_multi_couplings** (*ops*)

Generalization of `possible_couplings()` to couplings with more than 2 sites.

**Parameters**
- *ops* (list of (opname, dx, u)) – Same as the argument *ops* of `add_multi_coupling()`.

**Returns**
- **mps_ijkl** (2D int array) – Each row contains MPS indices i,j,k,l,... for each of the operators positions. The positions are defined by *dx* (j,k,l,... relative to *i*) and boundary conditions of *self* (how much the box for given *dx* can be shifted around without hitting a boundary - these are the different rows).

- **lat_indices** (2D int array) – Rows of *lat_indices* correspond to rows of *mps_ijkl* and contain the lattice indices of the “lower left corner” of the box containing the coupling.

- **coupling_shape** (tuple of int) – Len *dim*. The correct shape for an array specifying the coupling strength. *lat_indices* has only rows within this shape.

**plot_sites** (*ax*, markers=['o', '^', 's', 'p', 'h', 'D'], **kwargs)

Plot the sites of the lattice with markers.

**Parameters**
- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.

- **markers** (list) – List of values for the keyword *marker* of *ax.plot()* to distinguish the different sites in the unit cell, a site *u* in the unit cell is plotted with a marker *markers[u % len(markers)]*.

- ****kwargs** – Further keyword arguments given to *ax.plot()*.

**plot_order** (*ax*, order=None, textkwargs={'color': 'r'}, **kwargs)

Plot a line connecting sites in the specified “order” and text labels enumerating them.

**Parameters**
- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.

- **order** (None | 2D array (self.N_sites, self.dim+1)) – The order as returned by `ordering()`; by default (None) use *order*.

- **textkwargs** (None | dict) – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for *ax.text()*.
plot_coupling \( (ax, \text{coupling}=\text{None}, \text{wrap}=\text{False}, **\text{kwargs}) \)
Plot lines connecting nearest neighbors of the lattice.

Parameters

- \( \text{ax} \) (matplotlib.axes.Axes) – The axes on which we should plot.
- \( \text{coupling} \) (list of \((u1, u2, dx)\)) – By default (None), use self.pairs['nearest_neighbors']. Specifies the connections to be plotted; iterating over lattice indices \((i0, i1, \ldots)\), we plot a connection from the site \((i0, i1, \ldots, u1)\) to the site \((i0+dx[0], i1+dx[1], \ldots, u2)\), taking into account the boundary conditions.
- \( \text{wrap} \) (bool) – If True, wrap
- \( **\text{kwargs} \) – Further keyword arguments given to \text{ax.plot}()

plot_basis \( (ax, \text{origin}=(0.0, 0.0), \text{shade}=\text{None}, **\text{kwargs}) \)
Plot arrows indicating the basis vectors of the lattice.

Parameters

- \( \text{ax} \) (matplotlib.axes.Axes) – The axes on which we should plot.
- \( **\text{kwargs} \) – Keyword arguments for \text{ax.arrow}.

plot_bc_identified \( (ax, \text{direction}=-1, \text{origin}=\text{None}, \text{cylinder_axis}=\text{False}, **\text{kwargs}) \)
Mark two sites identified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

Parameters

- \( \text{ax} \) (matplotlib.axes.Axes) – The axes on which we should plot.
- \( \text{direction} \) (int) – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.
- \( \text{cylinder_axis} \) (bool) – Whether to plot the cylinder axis as well.
- \( \text{origin} \) (None | np.ndarray) – The origin starting from where we mark the identified sites. Defaults to the first entry of \text{unit_cell_positions}.
- \( **\text{kwargs} \) – Keyword arguments for the used \text{ax.plot}.

SimpleLattice

- full name: tenpy.models.lattice.SimpleLattice
- parent module: tenpy.models.lattice
- type: class
Inheritance Diagram

```
Lattice
  ↓
SimpleLattice
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SimpleLattice.<strong>init</strong></td>
<td>Initialize self.</td>
</tr>
<tr>
<td>SimpleLattice.count_neighbors</td>
<td>Count e.g.</td>
</tr>
<tr>
<td>SimpleLattice.coupling_shape</td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td>SimpleLattice.enlarge_mps_unit_cell</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>SimpleLattice.from_hdf5</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>SimpleLattice.lat2mps_idx</td>
<td>Translate lattice indices (x_0, \ldots, x_{\text{dim}-1}, u) to MPS index (i).</td>
</tr>
<tr>
<td>SimpleLattice.mps2lat_idx</td>
<td>Translate MPS index (i) to lattice indices (x_0, \ldots, x_{\text{dim}-1}, u).</td>
</tr>
<tr>
<td>SimpleLattice.mps2lat_values</td>
<td>same as Lattice.mps2lat_values(), but ignore (u), setting it to 0.</td>
</tr>
<tr>
<td>SimpleLattice.mps2lat_values_masked</td>
<td>Reshape/reorder an array (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>SimpleLattice.mps_idx_fix_u</td>
<td>return an index array of MPS indices for which the site within the unit cell is (u).</td>
</tr>
<tr>
<td>SimpleLattice.mps_lat_idx_fix_u</td>
<td>Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td>SimpleLattice.mps_sites</td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td>SimpleLattice.multi_coupling_shape</td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td>SimpleLattice.number_nearest_neighbors</td>
<td><a href="https://docs.python.org/3/whatsnew/3.6.html">deprecated.</a></td>
</tr>
<tr>
<td>SimpleLattice.number_next_nearest_neighbor</td>
<td><a href="https://docs.python.org/3/whatsnew/3.6.html">deprecated.</a></td>
</tr>
<tr>
<td>SimpleLattice.ordering</td>
<td>Provide possible orderings of the (N) lattice sites.</td>
</tr>
<tr>
<td>SimpleLattice.plot_basis</td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td>SimpleLattice.plot_bc_identified</td>
<td>Mark two sites indifly by periodic boundary conditions.</td>
</tr>
<tr>
<td>SimpleLattice.plot_coupling</td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
</tr>
<tr>
<td>SimpleLattice.plot_order</td>
<td>Plot a line connecting sites in the specified “order” and text labels enumerating them.</td>
</tr>
</tbody>
</table>

continues on next page
Table 88 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>SimpleLattice.plot_sites(ax[, markers])</code></td>
<td>Plot the sites of the lattice with markers.</td>
</tr>
<tr>
<td><code>SimpleLattice.position(lat_idx)</code></td>
<td>return ‘space’ position of one or multiple sites.</td>
</tr>
<tr>
<td><code>SimpleLattice.possible_couplings(u1, u2, dx)</code></td>
<td>Find possible MPS indices for two-site couplings.</td>
</tr>
<tr>
<td><code>SimpleLattice.possible_multi_couplings(ops)</code></td>
<td>Generalization of <code>possible_couplings()</code> to couplings with more than 2 sites.</td>
</tr>
<tr>
<td><code>SimpleLattice.save_hdf5(hdf5_saver, h5gr, ...)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>SimpleLattice.site(i)</code></td>
<td>return Site instance corresponding to an MPS index i</td>
</tr>
<tr>
<td><code>SimpleLattice.test_sanity()</code></td>
<td>Sanity check.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>SimpleLattice.Lu</code></td>
<td>the (expected) number of sites in the unit cell, <code>len(unit_cell)</code>.</td>
</tr>
<tr>
<td><code>SimpleLattice.boundary_conditions</code></td>
<td>Human-readable list of boundary conditions from <code>bc</code> and <code>bc_shift</code>.</td>
</tr>
<tr>
<td><code>SimpleLattice.dim</code></td>
<td>The dimension of the lattice.</td>
</tr>
<tr>
<td><code>SimpleLattice.nearest_neighbors</code></td>
<td></td>
</tr>
<tr>
<td><code>SimpleLattice.next_nearest_neighbors</code></td>
<td></td>
</tr>
<tr>
<td><code>SimpleLattice.next_next_nearest_neighbors</code></td>
<td></td>
</tr>
<tr>
<td><code>SimpleLattice.order</code></td>
<td>Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.</td>
</tr>
</tbody>
</table>

class `tenpy.models.lattice.SimpleLattice(Ls, site, **kwargs)`

Bases: `tenpy.models.lattice.Lattice`

A lattice with a unit cell consisting of just a single site.

In many cases, the unit cell consists just of a single site, such that the the last entry of `u` of an ‘lattice index’ can only be 0. From the point of internal algorithms, we handle this class like a `Lattice` – in that way we don’t need to distinguish special cases in the algorithms.

Yet, from the point of a tenpy user, for example if you measure an expectation value on each site in a `SimpleLattice`, you expect to get an `ndarray` of dimensions `self.Ls`, not `self.shape`. To avoid that problem, `SimpleLattice` overwrites just the meaning of `u=None` in `mps2lat_values()` to be the same as `u=0`.

Parameters

- `Ls` (list of int) – the length in each direction
- `site` (Site) – the lattice site. The `unit_cell` of the `Lattice` is just `[site]`.
- `**kwargs` – Additional keyword arguments given to the `Lattice`. If `order` is specified in the form (`'standard'`, `snake_windingi`, `priority`), the `snake_winding` and `priority` should only be specified for the spatial directions. Similarly, `positions` can be specified as a single vector.

Lu = 1
the (expected) number of sites in the unit cell, `len(unit_cell)`.

`mps2lat_values(A, axes=0, u=None)`
same as `Lattice.mps2lat_values()`, but ignore `u`, setting it to 0.
**property boundary_conditions**

Human-readable list of boundary conditions from bc and bc_shift.

**Returns** boundary_conditions – List of "open" or "periodic", one entry for each direction of the lattice.

**Return type** list of str

**count_neighbors** (u=0, key='nearest_neighbors')

Count e.g. the number of nearest neighbors for a site in the bulk.

**Parameters**

- u (int) – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever key specifies).
- key (str) – Key of pairs to select what to count.

**Returns** number – Number of nearest neighbors (or whatever key specified) for the u-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

**Return type** int

**coupling_shape**(dx)

Calculate correct shape of the strengths for a coupling.

**Parameters** dx (tuple of int) – Translation vector in the lattice for a coupling of two operators. Corresponds to dx argument of tenpy.models.model.CouplingModel.add_multi_coupling().

**Returns**

- coupling_shape (tuple of int) – Len dim. The correct shape for an array specifying the coupling strength. lat_indices has only rows within this shape.
- shift_lat_indices (array) – Translation vector from origin to the lower left corner of box spanned by dx.

**property dim**

The dimension of the lattice.

**enlarge_mps_unit_cell**(factor=2)

Repeat the unit cell for infinite MPS boundary conditions; in place.

**Parameters**

- factor (int) – The new number of sites in the MPS unit cell will be increased from N_sites to factor*N_sites_per_ring. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from (Lx, Ly, ..., Lu) to (Lx*factor, Ly, ..., Lu).

**classmethod from_hdf5**(hdf5_loader, h5gr, subpath)

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

**Parameters**

- hdf5_loader (Hdf5Loader) – Instance of the loading engine.
- h5gr (Group) – HDF5 group which is represent the object to be constructed.
- subpath (str) – The name of h5gr with a '/' in the end.

**Returns**

- obj – Newly generated class instance containing the required data.

**Return type** cls
\textbf{\texttt{lat2mps_idx}}(\textit{lat_idx})

Translate lattice indices \((x_0, \ldots, x_{(D-1)}, u)\) to MPS index \(i\).

- **Parameters** \texttt{lat_idx} \((\text{array_like } [\ldots, \text{dim+1}])\) – The last dimension corresponds to lattice indices \((x_0, \ldots, x_{(D-1)}, u)\). All lattice indices should be positive and smaller than the corresponding entry in \texttt{self.shape}. Exception: for “infinite” bc\_MPS, an \(x_0\) outside indicates shifts across the boundary.

- **Returns** \(i\) – MPS index/indices corresponding to \texttt{lat_idx}. Has the same shape as \texttt{lat_idx} without the last dimension.

- **Return type** array_like

\textbf{\texttt{mps2lat_idx}}(\textit{i})

Translate MPS index \(i\) to lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\).

- **Parameters** \texttt{i} \((\text{int } | \text{array_like of int})\) – MPS index/indices.

- **Returns** \texttt{lat_idx} – First dimensions like \(i\), last dimension has \(\text{len dim}+1\) and contains the lattice indices `(\(x_0, \ldots, x_{(dim-1)}, u)\)` corresponding to \(i\). For \(i\) accross the MPS unit cell and “infinite” bc\_MPS, we shift \(x_0\) accordingly.

- **Return type** array

\textbf{\texttt{mps2lat_values_masked}}(\textit{A, axes=-1, mps_inds=None, include_u=None})

Reshape/reorder an array \(A\) to replace an MPS index by lattice indices.

This is a generalization of \texttt{mps2lat_values()} allowing for the case of an arbitrary set of MPS indices present in each axis of \(A\).

- **Parameters**

  - \(A\) \((\text{ndarray})\) – Some values.
  - \texttt{axes} \((\text{iterable of int})\) – Chooses the axis of \(A\) which should be replaced. If multiple axes are given, you also need to give multiple index arrays as \texttt{mps inds}.
  - \texttt{mps inds} \((\text{list of 1D ndarray})\) – Specifies for each axis in \texttt{axes}, for which MPS indices we have values in the corresponding axis of \(A\). Defaults to \([\text{np.arange}(A.\text{shape}[ax])\text{ for } ax \text{ in } \texttt{axes}]\). For indices accross the MPS unit cell and “infinite” bc\_MPS, we shift \(x_0\) accordingly.
  - \texttt{include_u} \((\text{list of bool})\) – Specifies for each axis in \texttt{axes}, whether the \(u\) index of the lattice should be included into the output array \texttt{res A}. Defaults to \(\text{len(self.\text{unit_cell})} > 1\).

- **Returns** \texttt{res_A} – Reshaped and reordered copy of \(A\). Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index \(j\) maps to lattice site \((x0, x1, x2)\), then \(\texttt{res_A}[\ldots, x0, x1, x2, \ldots] = A[\ldots, \texttt{mps inds}[j], \ldots]\).

- **Return type** np.ma.MaskedArray

\textbf{\texttt{mps_idx_fix_u}}(\textit{u=None})

return an index array of MPS indices for which the site within the unit cell is \(u\).

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This functions returns an index array of the mps indices which belong to sites given by \texttt{self.\text{unit_cell}[u]}.

- **Parameters** \texttt{u} \((\text{None } | \text{int})\) – Selects a site of the unit cell. \texttt{None} (default) means all sites.

- **Returns** \texttt{mps_idx} – MPS indices for which \texttt{self.site(i)} is \texttt{self.unit_cell[u]}. Ordered ascending.
Return type array

mps_lat_idx_fix_u(u=None)
Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.

Parameters u (None | int) – Selects a site of the unit cell. None (default) means all sites.

Returns

• mps_idx (array) – MPS indices $i$ for which self.site($i$) is self.
  unit_cell[u].

• lat_idx (2D array) – The row $j$ contains the lattice index (without $u$) corresponding to
  mps_idx[$j$].

mps_sites()
Return a list of sites for all MPS indices.

Equivalent to [self.site(i) for i in range(self.N_sites)].

This should be used for sites of 1D tensor networks (MPS, MPO,…).

multi_coupling_shape(dx)
Calculate correct shape of the strengths for a multi_coupling.

Parameters dx (2D array, shape (N_ops, dim)) – $dx[i, :]$ is the translation vector in the
lattice for the $i$-th operator. Corresponds to the $dx$ of each operator given in the argument ops
of tenpy.models.model.CouplingModel.add_multi_coupling().

Returns

• coupling_shape (tuple of int) – Len dim. The correct shape for an array specifying the
coupling strength. lat_indices has only rows within this shape.

• shift_lat_indices (array) – Translation vector from origin to the lower left corner of box
spanned by $dx$. (Unlike for coupling_shape() it can also contain entries > 0)

number_nearest_neighbors(u=0)
Deprecated.

Deprecated since version 0.5.0: Use count_neighbors() instead.

number_next_nearest_neighbors(u=0)
Deprecated.

Deprecated since version 0.5.0: Use count_neighbors() instead.

property order
Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path
through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with plot_order().

ordering(order)
Provide possible orderings of the $N$ lattice sites.

This function can be overwritten by derived lattices to define additional orderings. The following orders
are defined in this method:
<table>
<thead>
<tr>
<th>order</th>
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</tr>
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<tr>
<td>'Cstyle'</td>
<td>(0, 1, ..., dim-1, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'default'</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>(0, 1, ..., dim-1, dim)</td>
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</tr>
</tbody>
</table>

Note: For lattices with a non-trivial unit cell (e.g. Honeycomb, Kagome), the grouped order might be more appropriate, see `get_order_grouped()`

**Parameters**

| order | (str | ('standard', snake_winding, priority) | ('grouped', groups) | Specifies the desired ordering using one of the strings of the above tables. Alternatively, an ordering is specified by a tuple with first entry specifying a function, 'standard' for `get_order()` and 'grouped' for `get_order_grouped()`, and other arguments in the tuple as specified in the documentation of these functions.  

**Returns**

- order – the order to be used for `order`

**Return type**

array, shape (N, D+1), dtype np.intp
See also:

get_order generates the order from equivalent priority and snake_winding.

get_order_grouped variant of get_order.

plot_order visualizes the resulting order.

plot_basis \((ax, \text{origin}=(0.0, 0.0), \text{shade}=\text{None}, **\text{kwargs})\)
Plot arrows indicating the basis vectors of the lattice.

**Parameters**

- **ax** *(matplotlib.axes.Axes)* – The axes on which we should plot.
- **kwargs** – Keyword arguments for ax.arrow.

plot_bc_identified \((ax, \text{direction}=-1, \text{origin}=\text{None}, \text{cylinder_axis}=\text{False}, **\text{kwargs})\)
Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

**Parameters**

- **ax** *(matplotlib.axes.Axes)* – The axes on which we should plot.
- **direction** *(int)* – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.
- **cylinder_axis** *(bool)* – Whether to plot the cylinder axis as well.
- **origin** *(None | np.ndarray)* – The origin starting from where we mark the identified sites. Defaults to the first entry of unit_cell_positions.
- **kwargs** – Keyword arguments for the used ax.plot.

plot_coupling \((ax, \text{coupling}=\text{None}, \text{wrap}=\text{False}, **\text{kwargs})\)
Plot lines connecting nearest neighbors of the lattice.

**Parameters**

- **ax** *(matplotlib.axes.Axes)* – The axes on which we should plot.
- **coupling** *(list of (u1, u2, dx))* – By default (None), use self.pairs['nearest_neighbors']. Specifies the connections to be plotted; iterating over lattice indices \((i0, i1, \ldots, u1)\) to the site \((i0+dx[0], i1+dx[1], \ldots, u2)\), taking into account the boundary conditions.
- **wrap** *(bool)* – If True, wrap
- **kwargs** – Further keyword arguments given to ax.plot().

plot_order \((ax, \text{order}=\text{None}, \text{textkwargs}='color': 'r'), **\text{kwargs})\)
Plot a line connecting sites in the specified “order” and text labels enumerating them.

**Parameters**

- **ax** *(matplotlib.axes.Axes)* – The axes on which we should plot.
- **order** *(None | 2D array (self.N_sites, self.dim+1))* – The order as returned by ordering(); by default (None) use order.
- **textkwargs** *(None | dict)* – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for ax.text().
**kwargs – Further keyword arguments given to ax.plot().

**plot_sites** *(ax, markers=['o', '^', 's', 'p', 'h', 'D'], **kwargs)*

Plot the sites of the lattice with markers.

**Parameters**

- **ax** *(matplotlib.axes.Axes)* – The axes on which we should plot.
- **markers** *(list)* – List of values for the keyword *marker* of ax.plot() to distinguish the different sites in the unit cell, a site $u$ in the unit cell is plotted with a marker $\text{markers}[u \% \text{len(markers)}]$.
- **kwargs** – Further keyword arguments given to ax.plot().

**position** *(lat_idx)*

return ‘space’ position of one or multiple sites.

**Parameters**

- **lat_idx** *(ndarray, (... , dim+1))* – Lattice indices.

**Returns**

**pos** – The position of the lattice sites specified by *lat_idx* in real-space.

**Return type**

ndarray, (... , dim)

**possible_couplings** *(u1, u2, dx)*

Find possible MPS indices for two-site couplings.

For periodic boundary conditions (bc[a] == False) the index $x_a$ is taken modulo $L_s[a]$ and runs through range($L_s[a]$). For open boundary conditions, $x_a$ is limited to $0 \leq x_a < L_s[a]$ and $0 \leq x_a+dx[a] < \text{lat.Ls[a]}$.

**Parameters**

- **u1** *(int)* – Indices within the unit cell; the $u1$ and $u2$ of add_coupling()
- **u2** *(int)* – Indices within the unit cell; the $u1$ and $u2$ of add_coupling()
- **dx** *(array)* – Length $\text{dim}$. The translation in terms of basis vectors for the coupling.

**Returns**

- **mps1, mps2** *(array)* – For each possible two-site coupling the MPS indices for the $u1$ and $u2$.
- **lat_indices** *(2D int array)* – Rows of *lat_indices* correspond to rows of *mps_ijkl* and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** *(tuple of int)* – Length $\text{dim}$. The correct shape for an array specifying the coupling strength. *lat_indices* has only rows within this shape.

**possible_multi_couplings** *(ops)*

Generalization of *possible_couplings()* to couplings with more than 2 sites.

**Parameters**

- **ops** *(list of (opname, dx, u))* – Same as the argument *ops* of add_multi_coupling().

**Returns**

- **mps_ijkl** *(2D int array)* – Each row contains MPS indices $i,j,k,...$ for each of the operators positions. The positions are defined by $dx$ (j,k,... relative to $i$) and boundary boundary conditions of *self* (how much the box for given $dx$ can be shifted around without hitting a boundary - these are the different rows).
- **lat_indices** *(2D int array)* – Rows of *lat_indices* correspond to rows of *mps_ijkl* and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** *(tuple of int)* – Len *dim*. The correct shape for an array specifying the coupling strength. *lat_indices* has only rows within this shape.

**save_hdf5** *(hdf5_saver, h5gr, subpath)*

Export *self* into a HDF5 file.

This method saves all the data it needs to reconstruct *self* with *from_hdf5()*.

Specifically, it saves unit_cell, *Ls*, unit_cell_positions, *basis*, *boundary_conditions*, *pairs* under their name, *bc_MPS* as "boundary_conditions_MPS", and *order* as "order_for_MPS". Moreover, it saves *dim* and *N_sites* as HDF5 attributes.

**Parameters**

- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.
- **h5gr** *(class`Group`)* – HDF5 group which is supposed to represent *self*.
- **subpath** *(str)* – The name of *h5gr* with a '/' in the end.

**site** *(i)*

return *Site* instance corresponding to an MPS index *i*

**test_sanity** ()

Sanity check.

Raises ValueErrors, if something is wrong.

---

**Square**

- full name: tenpy.models.lattice.Square
- parent module: tenpy.models.lattice
- type: class

---

**Inheritance Diagram**

```
Lattice

SimpleLattice

Square
```
## Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>Square.__init__(Lx, Ly, site, **kwargs)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>Square.count_neighbors([u, key])</code></td>
<td>Count e.g.</td>
</tr>
<tr>
<td><code>Square.coupling_shape(dx)</code></td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td><code>Square.enlarge_mps_unit_cell([factor])</code></td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td><code>Square.from_hdf5(hdf5_loader, h5gr, subpath)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>Square.lat2mps_idx(lat_idx)</code></td>
<td>Translate lattice indices ((x_0, ..., x_{D-1}, u)) to MPS index (i).</td>
</tr>
<tr>
<td><code>Square.mps2lat_idx(i)</code></td>
<td>Translate MPS index (i) to lattice indices ((x_0, ..., x_{(dim-1)}, u)).</td>
</tr>
<tr>
<td><code>Square.mps2lat_values(A[, axes, u])</code></td>
<td>same as <code>Lattice.mps2lat_values()</code>, but ignore (u), setting it to 0.</td>
</tr>
<tr>
<td><code>Square.mps2lat_values_masked(A[, axes, ...])</code></td>
<td>Reshape/reorder an array (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td><code>Square.mps_idx_fix_u([u])</code></td>
<td>return an index array of MPS indices for which the site within the unit cell is (u).</td>
</tr>
<tr>
<td><code>Square.mps_lat_idx_fix_u([u])</code></td>
<td>Similar as <code>mps_idx_fix_u()</code>, but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td><code>Square.mps_sites()</code></td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td><code>Square.multi_coupling_shape(dx)</code></td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td><code>Square.number_nearest_neighbors([u])</code></td>
<td>Deprecated.</td>
</tr>
<tr>
<td><code>Square.number_next_nearest_neighbors([u])</code></td>
<td>Deprecated.</td>
</tr>
<tr>
<td><code>Square.ordering(order)</code></td>
<td>Provide possible orderings of the (N) lattice sites.</td>
</tr>
<tr>
<td><code>Square.plot_basis(ax[, origin, shade])</code></td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td><code>Square.plot_bc_identified(ax[, direction, ...])</code></td>
<td>Mark two sites indified by periodic boundary conditions.</td>
</tr>
<tr>
<td><code>Square.plot_coupling(ax[, coupling, wrap])</code></td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
</tr>
<tr>
<td><code>Square.plot_order(ax[, order, textkwargs])</code></td>
<td>Plot a line connecting sites in the specified “order” and text labels enumerating them.</td>
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<td><code>Square.plot_sites(ax[, markers])</code></td>
<td>Plot the sites of the lattice with markers.</td>
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<tr>
<td><code>Square.position(lat_idx)</code></td>
<td>return ‘space’ position of one or multiple sites.</td>
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<td><code>Square.possible_couplings(u1, u2, dx)</code></td>
<td>Find possible MPS indices for two-site couplings.</td>
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<td><code>Square.possible_multi_couplings(ops)</code></td>
<td>Generalization of <code>possible_couplings()</code> to couplings with more than 2 sites.</td>
</tr>
<tr>
<td><code>Square.save_hdf5(hdf5_saver, h5gr, subpath)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>Square.site(i)</code></td>
<td>return Site instance corresponding to an MPS index (i)</td>
</tr>
<tr>
<td><code>Square.test_sanity()</code></td>
<td>Sanity check.</td>
</tr>
</tbody>
</table>

## Class Attributes and Properties

- **Square.Lu**
- **Square.boundary_conditions** Human-readable list of boundary conditions from `bc` and `bc_shift`. |
- **Square.dim** the dimension of the lattice |
- **Square.nearest_neighbors** |
- **Square.next_nearest_neighbors** continues on next page
Table 91 – continued from previous page

| `Square.next_next_nearest_neighbors` | Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain. |

**class** `tenpy.models.lattice.Square(Lx, Ly, site, **kwargs)`

**Bases:** `tenpy.models.lattice.SimpleLattice`

A square lattice.

![Diagram of a square lattice with labeled sites](image)

**Parameters**

- **Lx** *(int)* – The length in each direction.
- **Ly** *(int)* – The length in each direction.
- **site** *(Site)* – The local lattice site. The *unit_cell* of the *Lattice* is just `[site]`.
- ****kwargs** – Additional keyword arguments given to the *Lattice*. *pairs* are set accordingly. If *order* is specified in the form `(standard, snake_winding, priority)`, the *snake_winding* and *priority* should only be specified for the spatial directions. Similarly, *positions* can be specified as a single vector.

**dim = 2**

the dimension of the lattice
**property boundary_conditions**

Human-readable list of boundary conditions from `bc` and `bc_shift`.

**Returns** boundary_conditions – List of "open" or "periodic", one entry for each direction of the lattice.

**Return type** list of str

**count_neighbors** *(u=0, key='nearest_neighbors')*

Count e.g. the number of nearest neighbors for a site in the bulk.

**Parameters**

- **u** *(int)* – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever key specifies).
- **key** *(str)* – Key of pairs to select what to count.

**Returns** number – Number of nearest neighbors (or whatever key specified) for the u-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

**Return type** int

**coupling_shape** *(dx)*

Calculate correct shape of the strengths for a coupling.

**Parameters** dx *(tuple of int)* – Translation vector in the lattice for a coupling of two operators. Corresponds to dx argument of `tenpy.models.model.CouplingModel.add_multi_coupling()`.

**Returns**

- **coupling_shape** *(tuple of int)* – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.
- **shift_lat_indices** *(array)* – Translation vector from origin to the lower left corner of box spanned by `dx`.

**enlarge_mps_unit_cell** *(factor=2)*

Repeat the unit cell for infinite MPS boundary conditions; in place.

**Parameters** factor *(int)* – The new number of sites in the MPS unit cell will be increased from `N_sites` to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

**classmethod from_hdf5** *(hdf5_loader, h5gr, subpath)*

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

**Parameters**

- **hdf5_loader** *(Hdf5Loader)* – Instance of the loading engine.
- **h5gr** *(Group)* – HDF5 group which is represent the object to be constructed.
- **subpath** *(str)* – The name of `h5gr` with a '/' in the end.

**Returns** obj – Newly generated class instance containing the required data.

**Return type** cls

**lat2mps_idx** *(lat_idx)*

Translate lattice indices `(x_0, ..., x_(D-1), u)` to MPS index `i`.
Parameters `lat_idx` (array_like [`, dim+1]) – The last dimension corresponds to lattice indices \((x_0, \ldots, x_{(D-1)}, u)\). All lattice indices should be positive and smaller than the corresponding entry in `self.shape`. Exception: for “infinite” `bc_MPS`, an \(x_0\) outside indicates shifts accross the boundary.

Returns `i` – MPS index/indices corresponding to `lat_idx`. Has the same shape as `lat_idx` without the last dimension.

Return type array_like

mps2lat_idx(i)
 Translate MPS index `i` to lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\).

Parameters `i` (int | array_like of int) – MPS index/indices.

Returns `lat_idx` – First dimensions like `i`, last dimension has len `dim+1` and contains the lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\) corresponding to `i`. For `i` across the MPS unit cell and “infinite” `bc_MPS`, we shift \(x_0\) accordingly.

Return type array

mps2lat_values(A, axes=0, u=None)
 same as `Lattice.mps2lat_values()`, but ignore `u`, setting it to 0.

mps2lat_values_masked(A, axes=-1, mps_inds=None, include_u=None)
 Reshape/reorder an array `A` to replace an MPS index by lattice indices.

This is a generalization of `mps2lat_values()` allowing for the case of an arbitrary set of MPS indices present in each axis of `A`.

Parameters

- `A` (ndarray) – Some values.
- `axes` ((iterable of) int) – Chooses the axis of `A` which should be replaced. If multiple axes are given, you also need to give multiple index arrays as `mps_inds`.
- `mps_inds` ((list of) 1D ndarray) – Specifies for each `axis` in `axes`, for which MPS indices we have values in the corresponding axis of `A`. Defaults to `[np.arange(A.shape[ax]) for ax in axes]`. For indices accross the MPS unit cell and “infinite” `bc_MPS`, we shift \(x_0\) accordingly.
- `include_u` ((list of) bool) – Specifies for each `axis` in `axes`, whether the \(u\) index of the lattice should be included into the output array `res_A`. Defaults to len(`self.unit_cell`) > 1.

Returns `res_A` – Reshaped and reordered copy of `A`. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index `j` maps to lattice site \((x0, x1, x2)\), then `res_A[..., x0, x1, x2, ...] = A[..., mps_inds[j], ...]`.

Return type np.ma.MaskedArray

mps_idx_fix_u(u=None)
 return an index array of MPS indices for which the site within the unit cell is `u`.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This functions returns an index array of the mps indices which belong to sites given by `self.unit_cell[u]`.

Parameters `u` (None | int) – Selects a site of the unit cell. None (default) means all sites.

Returns `mps_idx` – MPS indices for which `self.site(i)` is `self.unit_cell[u]`. Ordered ascending.
Return type  array

\texttt{mps\_lat\_idx\_fix\_u}(u=None)

Similar as \texttt{mps\_idx\_fix\_u()}, but return also the corresponding lattice indices.

Parameters  \texttt{u} (\texttt{None} / \texttt{int}) – Selects a site of the unit cell. \texttt{None} (default) means all sites.

Returns

- \texttt{mps\_idx} (array) – MPS indices \textit{i} for which \texttt{self.site(i) is self.\texttt{unit\_cell}[u]}.
- \texttt{lat\_idx} (2D array) – The row \textit{j} contains the lattice index (without \texttt{u}) corresponding to \texttt{mps\_idx[j]}.

\texttt{mps\_sites}()

Return a list of sites for all MPS indices.

Equivalent to \texttt{[self.site(i) for i in range(self.N\_sites)]}.

This should be used for \textit{sites} of 1D tensor networks (MPS, MPO,…).

\texttt{multi\_coupling\_shape}(dx)

Calculate correct shape of the \textit{strengths} for a \texttt{multi\_coupling}.

Parameters  \texttt{dx} (2D array, shape (N\_ops, \texttt{dim})) – \texttt{dx[i, :]} is the translation vector in the lattice for the \textit{i}-th operator. Corresponds to the \texttt{dx} of each operator given in the argument \texttt{ops} of \texttt{tenpy.models.model.CouplingModel.add\_multi\_coupling()}.

Returns

- \texttt{coupling\_shape} (tuple of int) – \texttt{Len \texttt{dim}}. The correct shape for an array specifying the coupling strength. \texttt{lat\_indices} has only rows within this shape.
- \texttt{shift\_lat\_indices} (array) – Translation vector from origin to the lower left corner of box spanned by \texttt{dx}. (Unlike for \texttt{coupling\_shape()} it can also contain entries > 0)

\texttt{number\_nearest\_neighbors}(u=0)

Deprecated.

Deprecated since version 0.5.0: Use \texttt{count\_neighbors()} instead.

\texttt{number\_next\_nearest\_neighbors}(u=0)

Deprecated.

Deprecated since version 0.5.0: Use \texttt{count\_neighbors()} instead.

\texttt{property order}

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with \texttt{plot\_order()}.

\texttt{ordering}(order)

Provide possible orderings of the \textit{N} lattice sites.

This function can be overwritten by derived lattices to define additional orderings. The following orders are defined in this method:
Note: For lattices with a non-trivial unit cell (e.g. Honeycomb, Kagome), the grouped order might be more appropriate, see `get_order_grouped()`

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<td>'snakeFstyle'</td>
<td>(dim-1, ..., 1, 0, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
</tbody>
</table>

Parameters order (str | ('standard', snake_winding, priority) | ('grouped', groups)) – Specifies the desired ordering using one of the strings of the above tables. Alternatively, an ordering is specified by a tuple with first entry specifying a function, 'standard' for get_order() and 'grouped' for get_order_grouped(), and other arguments in the tuple as specified in the documentation of these functions.

Returns order – the order to be used for order.

Return type array, shape (N, D+1), dtype np.intp
See also:

*get_order* generates the *order* from equivalent *priority* and *snake_winding*.

*get_order_grouped* variant of *get_order*.

*plot_order* visualizes the resulting *order*.

**plot_basis** *(ax, origin=(0.0, 0.0), shade=None, **kwargs)*
Plot arrows indicating the basis vectors of the lattice.

**Parameters**

- `ax` *(matplotlib.axes.Axes)* – The axes on which we should plot.
- `**kwargs` – Keyword arguments for `ax.arrow`.

**plot_bc_identified** *(ax, direction=None, origin=None, cylinder_axis=False, **kwargs)*
Mark two sites identified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

**Parameters**

- `ax` *(matplotlib.axes.Axes)* – The axes on which we should plot.
- `direction` *(int)* – The direction of the lattice along which we should mark the identified sites. If `None`, mark it along all directions with periodic boundary conditions.
- `cylinder_axis` *(bool)* – Whether to plot the cylinder axis as well.
- `origin` *(None | np.ndarray)* – The origin starting from where we mark the identified sites. Defaults to the first entry of `unit_cell_positions`.
- `**kwargs` – Keyword arguments for the used `ax.plot`.

**plot_coupling** *(ax, coupling=None, wrap=False, **kwargs)*
Plot lines connecting nearest neighbors of the lattice.

**Parameters**

- `ax` *(matplotlib.axes.Axes)* – The axes on which we should plot.
- `coupling` *(list of (u1, u2, dx))* – By default (None), use `self.pairs['nearest_neighbors']`. Specifies the connections to be plotted; iterating over lattice indices `(i0, i1, ...), we plot a connection from the site `(i0, i1, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2), taking into account the boundary conditions.
- `wrap` *(bool)* – If True, wrap
- `**kwargs` – Further keyword arguments given to `ax.plot()`.

**plot_order** *(ax, order=None, textkwargs={'color': 'r'}, **kwargs)*
Plot a line connecting sites in the specified “order” and text labels enumerating them.

**Parameters**

- `ax` *(matplotlib.axes.Axes)* – The axes on which we should plot.
- `order` *(None | 2D array (self.N_sites, self.dim+1))* – The order as returned by `ordering()`; by default (None) use `order`.
- `textkwargs` *(None | dict)* – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for `ax.text()`.
plot_sites (ax, markers=['o', 'v', 's', 'p', 'h', 'D'], **kwargs)
Plot the sites of the lattice with markers.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- **markers** (list) – List of values for the keyword marker of ax.plot() to distinguish the different sites in the unit cell, a site \(u\) in the unit cell is plotted with a marker markers[\(u \% \text{len(markers)}\)].
- **kwargs** – Further keyword arguments given to ax.plot().

position (lat_idx)
return ‘space’ position of one or multiple sites.

Parameters

- **lat_idx** (ndarray, (..., dim+1)) – Lattice indices.

Returns

- **pos** – The position of the lattice sites specified by \(\text{lat_idx}\) in real-space.

Return type

ndarray, (..., dim)

possible_couplings (u1, u2, dx)
Find possible MPS indices for two-site couplings.

For periodic boundary conditions (bc[a] == False) the index \(x_a\) is taken modulo \(L_s[a]\) and runs through range(\(L_s[a]\)). For open boundary conditions, \(x_a\) is limited to 0 <= \(x_a\) < \(L_s[a]\) and 0 <= \(x_a+dx[a]\) < lat.Ls[a].

Parameters

- **u1** (int) – Indices within the unit cell; the \(u1\) and \(u2\) of add_coupling()
- **u2** (int) – Indices within the unit cell; the \(u1\) and \(u2\) of add_coupling()
- **dx** (array) – Length \(dim\). The translation in terms of basis vectors for the coupling.

Returns

- **mps1, mps2** (array) – For each possible two-site coupling the MPS indices for the \(u1\) and \(u2\).
- **lat_indices** (2D int array) – Rows of \(\text{lat_indices}\) correspond to rows of \(\text{mps}_{ijkl}\) and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** (tuple of int) – Len \(dim\). The correct shape for an array specifying the coupling strength. \(\text{lat_indices}\) has only rows within this shape.

possible_multi_couplings (ops)
Generalization of possible_couplings() to couplings with more than 2 sites.

Parameters

- **ops** (list of (opname, dx, u)) – Same as the argument \(\text{ops}\) of add_multi_coupling().

Returns

- **mps_{ijkl}** (2D int array) – Each row contains MPS indices \(ijkl,\ldots\) for each of the operators positions. The positions are defined by \(dx\) (j,k,l,... relative to \(i\)) and boundary condition of \(\text{self}\) (how much the box for given \(dx\) can be shifted around without hitting a boundary - these are the different rows).
- **lat_indices** (2D int array) – Rows of \(\text{lat_indices}\) correspond to rows of \(\text{mps}_{ijkl}\) and contain the lattice indices of the “lower left corner” of the box containing the coupling.
• **coupling_shape** *(tuple of int)* – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

### save_hdf5 *(hdf5_saver, h5gr, subpath)*

Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

Specifically, it saves `unit_cell`, `Ls`, `unit_cell_positions`, `basis`, `boundary_conditions`, `pairs` under their name, `bc_MPS` as "boundary_conditions_MPS", and `order` as "order_for_MPS". Moreover, it saves `dim` and `N_sites` as HDF5 attributes.

**Parameters**

- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.
- **h5gr** *(HDF5Group)* – HDF5 group which is supposed to represent `self`.
- **subpath** *(str)* – The name of `h5gr` with a `'/'` in the end.

```python
def site(i):
    return Site instance corresponding to an MPS index `i`
```

test_sanity()

Sanity check.

Raises ValueErrors, if something is wrong.

### Triangular

- **full name**: `tenpy.models.lattice.Triangular`
- **parent module**: `tenpy.models.lattice`
- **type**: class

### Inheritance Diagram

```
Lattice
  ↓
SimpleLattice
  ↓
Triangular
```
# Methods

<table>
<thead>
<tr>
<th>Method Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>Triangular.__init__(Lx, Ly, site, **kwargs)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>Triangular.count_neighbors([u, key])</code></td>
<td>Count e.g.</td>
</tr>
<tr>
<td><code>Triangular.coupling_shape(dx)</code></td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td><code>Triangular.enlarge_mps_unit_cell([factor])</code></td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td><code>Triangular.from_hdf5(hdf5_loader, h5gr, subpath)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>Triangular.lat2mps_idx(lat_idx)</code></td>
<td>Translate lattice indices ((x_0, \ldots, x_{D-1}, u)) to MPS index (i).</td>
</tr>
<tr>
<td><code>Triangular.mps2lat_idx(i)</code></td>
<td>Translate MPS index (i) to lattice indices ((x_0, \ldots, x_{(dim-1)}, u)).</td>
</tr>
<tr>
<td><code>Triangular.mps2lat_values(A[, axes, u])</code></td>
<td>same as <code>lattice.mps2lat_values()</code>, but ignore (u), setting it to 0.</td>
</tr>
<tr>
<td><code>Triangular.mps2lat_values_masked(A[, axes, ...])</code></td>
<td>Reshape/reorder an array (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td><code>Triangular.mps_idx_fix_u([u])</code></td>
<td>return an index array of MPS indices for which the site within the unit cell is (u).</td>
</tr>
<tr>
<td><code>Triangular.mps_lat_idx_fix_u([u])</code></td>
<td>Similar as <code>mps_idx_fix_u()</code>, but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td><code>Triangular.mps_sites()</code></td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td><code>Triangular.multi_coupling_shape(dx)</code></td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td><code>Triangular.number_nearest_neighbors([u])</code></td>
<td>Deprecated.</td>
</tr>
<tr>
<td><code>Triangular.number_next_nearest_neighbors([u])</code></td>
<td>Deprecated.</td>
</tr>
<tr>
<td><code>Triangular.ordering(order)</code></td>
<td>Provide possible orderings of the (N) lattice sites.</td>
</tr>
<tr>
<td><code>Triangular.plot_basis(ax[, origin, shade])</code></td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td><code>Triangular.plot_bc_identified(ax[, ...])</code></td>
<td>Mark two sites indified by periodic boundary conditions.</td>
</tr>
<tr>
<td><code>Triangular.plot_coupling(ax[, coupling, wrap])</code></td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
</tr>
<tr>
<td><code>Triangular.plot_order(ax[, order, textwargs])</code></td>
<td>Plot a line connecting sites in the specified “order” and text labels enumerating them.</td>
</tr>
<tr>
<td><code>Triangular.plot_sites(ax[, markers])</code></td>
<td>Plot the sites of the lattice with markers.</td>
</tr>
<tr>
<td><code>Triangular.position(lat_idx)</code></td>
<td>return ‘space’ position of one or multiple sites.</td>
</tr>
<tr>
<td><code>Triangular.possible_multi_couplings(u1, u2, dx)</code></td>
<td>Find possible MPS indices for two-site couplings.</td>
</tr>
<tr>
<td><code>Triangular.possible_couplings(ops)</code></td>
<td>Generalization of <code>possible_couplings()</code> to couplings with more than 2 sites.</td>
</tr>
<tr>
<td><code>Triangular.save_hdf5(hdf5_saver, h5gr, subpath)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>Triangular.site(i)</code></td>
<td>return Site instance corresponding to an MPS index (i).</td>
</tr>
<tr>
<td><code>Triangular.test_sanity()</code></td>
<td>Sanity check.</td>
</tr>
</tbody>
</table>
Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triangular.Lu</td>
<td></td>
</tr>
<tr>
<td>Triangular.boundary_conditions</td>
<td>Human-readable list of boundary conditions from bc and bc_shift.</td>
</tr>
<tr>
<td>Triangular.dim</td>
<td>the dimension of the lattice</td>
</tr>
<tr>
<td>Triangular.nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Triangular.next_nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Triangular.next_next_nearest_neighbors</td>
<td></td>
</tr>
<tr>
<td>Triangular.order</td>
<td>Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.</td>
</tr>
</tbody>
</table>

```python
class tenpy.models.lattice.Triangular(Lx, Ly, site, **kwargs)
    Bases: tenpy.models.lattice.SimpleLattice

A triangular lattice.
```

Parameters

- **Lx** *(int)* – The length in each direction.
- **Ly** *(int)* – The length in each direction.
• **site** (*Site*) – The local lattice site. The *unit_cell* of the *Lattice* is just *site*.

• **kwargs –** Additional keyword arguments given to the *Lattice*. *pairs* are set accordingly. If *order* is specified in the form (*'standard*', *snake_winding*, *priority*), the *snake_winding* and *priority* should only be specified for the spatial directions. Similarly, *positions* can be specified as a single vector.

dim = 2
the dimension of the lattice

**property boundary_conditions**
Human-readable list of boundary conditions from *bc* and *bc_shift*.

Returns *boundary_conditions* – List of "open" or "periodic", one entry for each direction of the lattice.

Return type list of str

count_neighbors(*u=0, key='nearest_neighbors'*)
Count e.g. the number of nearest neighbors for a site in the bulk.

Parameters

• *u* (*int*) – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever *key* specifies).

• *key* (*str*) – Key of *pairs* to select what to count.

Returns *number* – Number of nearest neighbors (or whatever *key* specified) for the *u*-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

Return type int

coupling_shape(*dx*)
Calculate correct shape of the *strengths* for a coupling.

Parameters *dx* (*tuple of int*) – Translation vector in the lattice for a coupling of two operators. Corresponds to *dx* argument of *tenpy.models.model.CouplingModel.add_multi_coupling()*.

Returns

• coupling_shape (*tuple of int*) – Len *dim*. The correct shape for an array specifying the coupling strength. *lat_indices* has only rows within this shape.

• shift_lat_indices (*array*) – Translation vector from origin to the lower left corner of box spanned by *dx*.

enlarge_mps_unit_cell(*factor=2*)
Repeat the unit cell for infinite MPS boundary conditions; in place.

Parameters *factor* (*int*) – The new number of sites in the MPS unit cell will be increased from *N_sites* to *factor*\**N_sites_per_ring*. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from (*Lx*, *Ly*, ..., *Lu*) to (*Lx*\*factor, *Ly*, ..., *Lu*).

classmethod from_hdf5(*hdf5_loader, h5gr, subpath*)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with *save_hdf5()*.

Parameters
• **hdf5_loader** (*Hdf5Loader*) – Instance of the loading engine.

• **h5gr** (*Group*) – HDF5 group which is represent the object to be constructed.

• **subpath** (*str*) – The name of **h5gr** with a '/' in the end.

Returns **obj** – Newly generated class instance containing the required data.

Return type **cls**

**lat2mps_idx** (*lat_idx*)

Translate lattice indices \((x_0, \ldots, x_{D-1}, u)\) to MPS index \(i\).

Parameters

**lat_idx** (*array_like [.., dim+1]*) – The last dimension corresponds to lattice indices \((x_0, \ldots, x_{D-1}, u)\). All lattice indices should be positive and smaller than the corresponding entry in **self.shape**. Exception: for “infinite” **bc_MPS**, an \(x_0\) outside indicates shifts across the boundary.

Returns **i** – MPS index/indices corresponding to **lat_idx**. Has the same shape as **lat_idx** without the last dimension.

Return type **array_like**

**mps2lat_idx** (*i*)

Translate MPS index \(i\) to lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\).

Parameters

**i** (*int | array_like of int*) – MPS index/indices.

Returns **lat_idx** – First dimensions like \(i\), last dimension has len \(dim+1\) and contains the lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\) corresponding to \(i\). For \(i\) accross the MPS unit cell and “infinite” **bc_MPS**, we shift \(x_0\) accordingly.

Return type **array**

**mps2lat_values** (*A, axes=0, u=None*)

same as **Lattice.mps2lat_values()**, but ignore \(u\), setting it to 0.

**mps2lat_values_masked** (*A, axes=-1, mps_inds=None, include_u=None*)

Reshape/reorder an array \(A\) to replace an MPS index by lattice indices.

This is a generalization of **mps2lat_values()** allowing for the case of an arbitrary set of MPS indices present in each axis of \(A\).

Parameters

• **A** (*ndarray*) – Some values.

• **axes** (*iterable of int*) – Chooses the axis of \(A\) which should be replaced. If multiple axes are given, you also need to give multiple index arrays as **mps_inds**.

• **mps inds** (*list of 1D ndarray*) – Specifies for each **axis** in **axes**, for which MPS indices we have values in the corresponding **axis** of **A**. Defaults to [np.arange(A.shape[ax]) for ax in axes]. For indices accross the **MPS** unit cell and “infinite” **bc_MPS**, we shift \(x_0\) accordingly.

• **include_u** (*list of bool*) – Specifies for each **axis** in **axes**, whether the **u** index of the lattice should be included into the output array **res_A**. Defaults to len(**self.unit_cell**) > 1.

Returns **res_A** – Reshaped and reordered copy of \(A\). Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index \(j\) maps to lattice site \((x0, x1, x2)\), then \(res_A[\ldots, x0, x1, x2, \ldots] = A[\ldots, mps inds[j], \ldots]\).

Return type **np.ma.MaskedArray**
mps_idx_fix_u(u=None)
return an index array of MPS indices for which the site within the unit cell is u.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites.
This function returns an index array of the mps indices which belong to sites given by self.unit_cell[u].

**Parameters**

- **u** (*None* / *int*) – Selects a site of the unit cell. *None* (default) means all sites.

**Returns**

- **mps_idx** (*array*) – MPS indices for which self.site(i) is self.unit_cell[u]. Ordered ascending.

**Return type**

array

mps_lat_idx_fix_u(u=None)
Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.

**Parameters**

- **u** (*None* / *int*) – Selects a site of the unit cell. *None* (default) means all sites.

**Returns**

- **mps_idx** (*array*) – MPS indices i for which self.site(i) is self.unit_cell[u].
- **lat_idx** (*2D array*) – The row j contains the lattice index (without u) corresponding to mps_idx[j].

mps_sites()
Return a list of sites for all MPS indices.
Equivalent to [self.site(i) for i in range(self.N_sites)].
This should be used for sites of 1D tensor networks (MPS, MPO...).

multi_coupling_shape(dx)
Calculate correct shape of the strengths for a multi_coupling.

**Parameters**

- **dx** (*2D array, shape (N_ops, dim)) – dx[i, :] is the translation vector in the lattice for the i-th operator. Corresponds to the dx of each operator given in the argument ops of tenpy.models.model.CouplingModel.add_multi_coupling().

**Returns**

- **coupling_shape** (*tuple of int*) – Len dim. The correct shape for an array specifying the coupling strength. lat_indices has only rows within this shape.
- **shift_lat_indices** (*array*) – Translation vector from origin to the lower left corner of box spanned by dx. (Unlike for coupling_shape() it can also contain entries > 0)

number_nearest_neighbors(u=0)
Deprecated.
Deprecation since version 0.5.0: Use count_neighbors() instead.

number_next_nearest_neighbors(u=0)
Deprecated.
Deprecation since version 0.5.0: Use count_neighbors() instead.

**property order**

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with plot_order().

---

7.11. models
ordering (order)
Provide possible orderings of the $N$ lattice sites.

This function can be overwritten by derived lattices to define additional orderings. The following orders are defined in this method:

<table>
<thead>
<tr>
<th>order</th>
<th>equivalent priority</th>
<th>equivalent snake_winding</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Cstyle'</td>
<td>(0, 1, ..., dim-1, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'default'</td>
<td>(0, 1, ..., dim-1, dim)</td>
<td>(True, ..., True, True)</td>
</tr>
<tr>
<td>'snake'</td>
<td>(0, 1, ..., dim-1, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'snakeCstyle'</td>
<td>(dim-1, ..., 1, 0, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'snakeFstyle'</td>
<td>(dim-1, ..., 1, 0, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
</tbody>
</table>

Note: For lattices with a non-trivial unit cell (e.g. Honeycomb, Kagome), the grouped order might be more appropriate, see get_order_grouped()

Parameters

order (str | ('standard', snake_winding, priority) | ('grouped', groups)) – Specifies the desired ordering using one of the strings of the above tables. Alternatively, an ordering is specified by a tuple with first entry specifying a function, 'standard' for get_order() and 'grouped' for
get_order_grouped(), and other arguments in the tuple as specified in the documentation of these functions.

Returns order – the order to be used for order.

Return type array, shape (N, D+1), dtype np.intp

See also:

generate_order generates the order from equivalent priority and snake_winding.
generate_order_grouped variant of get_order.
plot_order visualizes the resulting order.

plot_basis(ax, origin=(0.0, 0.0), shade=None, **kwargs)
Plot arrows indicating the basis vectors of the lattice.

Parameters

• ax (matplotlib.axes.Axes) – The axes on which we should plot.

• **kwargs – Keyword arguments for ax.arrow.

plot_bc_identified(ax, direction=-1, origin=None, cylinder_axis=False, **kwargs)
Mark two sites indies by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

Parameters

• ax (matplotlib.axes.Axes) – The axes on which we should plot.

• direction (int) – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.

• cylinder_axis (bool) – Whether to plot the cylinder axis as well.

• origin (None | np.ndarray) – The origin starting from where we mark the identified sites. Defaults to the first entry of unit_cell_positions.

• **kwargs – Keyword arguments for the used ax.plot.

plot_coupling(ax, coupling=None, wrap=False, **kwargs)
Plot lines connecting nearest neighbors of the lattice.

Parameters

• ax (matplotlib.axes.Axes) – The axes on which we should plot.

• coupling (list of (u1, u2, dx)) – By default (None), use self.pairs['nearest_neighbors']. Specifies the connections to be plotted; iterating over lattice indices (i0, i1, ...), we plot a connection from the site (i0, i1, ... u1) to the site (i0+dx[0], i1+dx[1], ..., u2), taking into account the boundary conditions.

• wrap (bool) – If True, wrap

• **kwargs – Further keyword arguments given to ax.plot().

plot_order(ax, order=None, textkwargs={'color': 'r'}, **kwargs)
Plot a line connecting sites in the specified “order” and text labels enumerating them.

Parameters

• ax (matplotlib.axes.Axes) – The axes on which we should plot.
• `order` (None | 2D array (self.N_sites, self.dim+1)) – The order as returned by `ordering()`; by default (None) use `order`.

• `textkwargs` (None | dict) – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for `ax.text()`.

• `**kwargs` – Further keyword arguments given to `ax.plot()`.

Plot the sites of the lattice with markers.

Parameters

• `ax` (matplotlib.axes.Axes) – The axes on which we should plot.

• `markers` (list) – List of values for the keyword `marker` of `ax.plot()` to distinguish the different sites in the unit cell, a site `u` in the unit cell is plotted with a marker `markers[u % len(markers)]`.

• `**kwargs` – Further keyword arguments given to `ax.plot()`.

`position`(lat_idx)
return ‘space’ position of one or multiple sites.

Parameters `lat_idx` (ndarray, (..., dim+1)) – Lattice indices.

Returns `pos` – The position of the lattice sites specified by `lat_idx` in real-space.

Return type ndarray, (..., dim)

`possible_couplings`(u1, u2, dx)
Find possible MPS indices for two-site couplings.

For periodic boundary conditions (bc[a] == False) the index x_a is taken modulo Ls[a] and runs through range(Ls[a]). For open boundary conditions, x_a is limited to 0 <= x_a < Ls[a] and 0 <= x_a+dx[a] < lat.Ls[a].

Parameters

• `u1` (int) – Indices within the unit cell; the `u1` and `u2` of `add_coupling()`

• `u2` (int) – Indices within the unit cell; the `u1` and `u2` of `add_coupling()`

• `dx` (array) – Length `dim`. The translation in terms of basis vectors for the coupling.

Returns

• `mps1, mps2` (array) – For each possible two-site coupling the MPS indices for the `u1` and `u2`.

• `lat_indices` (2D int array) – Rows of `lat_indices` correspond to rows of `mps_ijkl` and contain the lattice indices of the “lower left corner” of the box containing the coupling.

• `coupling_shape` (tuple of int) – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.

`possible_multi_couplings`(ops)
Generalization of `possible_couplings()` to couplings with more than 2 sites.

Parameters `ops` (list of (opname, dx, u)) – Same as the argument `ops` of `add_multi_coupling()`.

Returns

• `mps_ijkl` (2D int array) – Each row contains MPS indices i,j,k,l,... for each of the operators positions. The positions are defined by `dx` (j,k,l,... relative to `i`) and boundary
boundary conditions of self (how much the box for given \(dx\) can be shifted around without hitting a boundary - these are the different rows).

- **lat_indices** (2D int array) – Rows of lat_indices correspond to rows of \(mps_{ijkl}\) and contain the lattice indices of the “lower left corner” of the box containing the coupling.

- **coupling_shape** (tuple of int) – Len \(dim\). The correct shape for an array specifying the coupling strength. lat_indices has only rows within this shape.

**save_hdf5** (hdf5_saver, h5gr, subpath)

Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5(). Specifically, it saves \(unit\_cell\), \(Ls\), \(unit\_cell\_positions\), \(basis\), boundary_conditions, pairs under their name, \(bc\_MPS\) as "boundary_conditions_MPS", and \(order\) as "order_for_MPS". Moreover, it saves \(dim\) and \(N\_sites\) as HDF5 attributes.

**Parameters**

- **hdf5_saver** (Hdf5Saver) – Instance of the saving engine.

- **h5gr** (:class:`Group`) – HDF5 group which is supposed to represent self.

- **subpath** (str) – The name of h5gr with a '/' in the end.

**site** (i)

return Site instance corresponding to an MPS index \(i\)

**test_sanity** ()

Sanity check.

Raises ValueErrors, if something is wrong.

**TrivialLattice**

- full name: tenpy.models.lattice.TrivialLattice

- parent module: tenpy.models.lattice

- type: class

**Inheritance Diagram**

```
      Lattice
       ▼
       TrivialLattice
```

7.11. models
Methods

<table>
<thead>
<tr>
<th>Method Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>TrivialLattice.<strong>init</strong></td>
<td>Initialize self.</td>
</tr>
<tr>
<td>TrivialLattice.count_neighbors</td>
<td>Count e.g.</td>
</tr>
<tr>
<td>TrivialLattice.coupling_shape</td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td>TrivialLattice.enlarge_mps_unit_cell</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>TrivialLattice.from_hdf5</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>TrivialLattice.lat2mps_idx</td>
<td>Translate lattice indices (x_0, \ldots, x_{(D-1)}, u) to MPS index (i).</td>
</tr>
<tr>
<td>TrivialLattice.mps2lat_idx</td>
<td>Translate MPS index (i) to lattice indices (x_0, \ldots, x_{(\dim-1)}, u).</td>
</tr>
<tr>
<td>TrivialLattice.mps2lat_values</td>
<td>Reshape/reorder (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>TrivialLattice.mps2lat_values_masked</td>
<td>Reshape/reorder an array (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td>TrivialLattice.mps_idx_fix_u</td>
<td>Return an index array of MPS indices for which the site within the unit cell is (u).</td>
</tr>
<tr>
<td>TrivialLattice.mps_lat_idx_fix_u</td>
<td>Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td>TrivialLattice.mps_sites</td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td>TrivialLattice.multi_coupling_shape</td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td>TrivialLattice.number_nearest_neighbors</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>TrivialLattice.number_next_nearest_neighbors</td>
<td>Deprecated.</td>
</tr>
<tr>
<td>TrivialLattice.ordering</td>
<td>Provide possible orderings of the (N) lattice sites.</td>
</tr>
<tr>
<td>TrivialLattice.plot_basis</td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td>TrivialLattice.plot_bc_identified</td>
<td>Mark two sites indified by periodic boundary conditions.</td>
</tr>
<tr>
<td>TrivialLattice.plot_coupling</td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
</tr>
<tr>
<td>TrivialLattice.plot_order</td>
<td>Plot a line connecting sites in the specified “order” and text labels enumerating them.</td>
</tr>
<tr>
<td>TrivialLattice.plot_sites</td>
<td>Plot the sites of the lattice with markers.</td>
</tr>
<tr>
<td>TrivialLattice.position</td>
<td>Return ‘space’ position of one or multiple sites.</td>
</tr>
<tr>
<td>TrivialLattice.possible_multi_couplings</td>
<td>Find possible MPS indices for two-site couplings.</td>
</tr>
<tr>
<td>TrivialLattice.possible_multi_couplings</td>
<td>Generalization of possible_couplings() to couplings with more than 2 sites.</td>
</tr>
<tr>
<td>TrivialLattice.save_hdf5</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>TrivialLattice.site</td>
<td>Return Site instance corresponding to an MPS index (i).</td>
</tr>
<tr>
<td>TrivialLattice.test_sanity</td>
<td>Sanity check.</td>
</tr>
</tbody>
</table>
Class Attributes and Properties

<table>
<thead>
<tr>
<th>TrivialLattice.Lu</th>
<th>Human-readable list of boundary conditions from bc and bc_shift.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TrivialLattice.boundary_conditions</td>
<td>Human-readable list of boundary conditions from bc and bc_shift.</td>
</tr>
<tr>
<td>TrivialLattice.dim</td>
<td>The dimension of the lattice.</td>
</tr>
<tr>
<td>TrivialLattice.nearest_neighbors</td>
<td>Trivial lattice consisting of a single (possibly large) unit cell in 1D.</td>
</tr>
<tr>
<td>TrivialLattice.next_nearest_neighbors</td>
<td>This is useful if you need a valid Lattice with given mps_sites() and don’t care about the actual geometry, e.g. because you don’t intend to use the CouplingModel.</td>
</tr>
<tr>
<td>TrivialLattice.next_next_nearest_neighbors</td>
<td>Parameters</td>
</tr>
<tr>
<td>TrivialLattice.order</td>
<td>Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.</td>
</tr>
</tbody>
</table>

```python
class tenpy.models.lattice.TrivialLattice(mps_sites, **kwargs)
    Bases: tenpy.models.lattice.Lattice

    Trivial lattice consisting of a single (possibly large) unit cell in 1D.

    This is useful if you need a valid Lattice with given mps_sites() and don’t care about the actual geometry, e.g. because you don’t intend to use the CouplingModel.
```

**Parameters**

- `mps_sites` (list of Site) – The sites making up a unit cell of the lattice.
- `**kwargs` – Further keyword arguments given to Lattice.

**property boundary_conditions**

Human-readable list of boundary conditions from bc and bc_shift.

```python
Returns boundary_conditions – List of "open" or "periodic", one entry for each direction of the lattice.

Return type list of str
```

**count_neighbors** `u=0, key='nearest_neighbors'`

Count e.g. the number of nearest neighbors for a site in the bulk.

```python
Parameters

- `u (int)` – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever key specifies).
- `key (str)` – Key of pairs to select what to count.

Returns number – Number of nearest neighbors (or whatever key specified) for the `u`-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

Return type int
```

**coupling_shape** `dx`

Calculate correct shape of the strengths for a coupling.

```python
Parameters dx (tuple of int) – Translation vector in the lattice for a coupling of two operators. Corresponds to dx argument of tenpy.models.model.CouplingModel.add_multi_coupling().

Returns

- `coupling_shape (tuple of int)` – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.
```
• `shift_lat_indices (array)` – Translation vector from origin to the lower left corner of box spanned by \( dx \).

**property dim**

The dimension of the lattice.

**enlarge_mps_unit_cell (factor=2)**

Repeat the unit cell for infinite MPS boundary conditions; in place.

**Parameters**

- `factor (int)` – The new number of sites in the MPS unit cell will be increased from \( N_{sites} \) to \( factor*N_{sites\_per\_ring} \). Since MPS unit cells are repeated in the \( x \)-direction in our convention, the lattice shape goes from \((L_x, L_y, \ldots, L_u)\) to \((L_x*factor, L_y, \ldots, L_u)\).

**classmethod from_hdf5 (hdf5_loader, h5gr, subpath)**

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

**Parameters**

- `hdf5_loader (Hdf5Loader)` – Instance of the loading engine.
- `h5gr (Group)` – HDF5 group which is represent the object to be constructed.
- `subpath (str)` – The name of `h5gr` with a ‘/’ in the end.

**Returns**

- `obj` – Newly generated class instance containing the required data.

**Return type**

`cls`

**lat2mps_idx (lat_idx)**

Translate lattice indices \((x_0, \ldots, x_{D-1}, u)\) to MPS index \( i \).

**Parameters**

- `lat_idx (array_like [..., dim+1])` – The last dimension corresponds to lattice indices \((x_0, \ldots, x_{D-1}, u)\). All lattice indices should be positive and smaller than the corresponding entry in `self.shape`. Exception: for “infinite” \( bc\_MPS \), an \( x_0 \) outside indicates shifts across the boundary.

**Returns**

- `i` – MPS index/indices corresponding to `lat_idx`. Has the same shape as `lat_idx` without the last dimension.

**Return type**

`array_like`

**mps2lat_idx (i)**

Translate MPS index \( i \) to lattice indices \((x_0, \ldots, x_{(D-1)}, u)\).

**Parameters**

- `i (int | array_like of int)` – MPS index/indices.

**Returns**

- `lat_idx` – First dimensions like \( i \), last dimension has `len` \( dim+1 \) and contains the lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\) corresponding to \( i \). For \( i \) across the MPS unit cell and “infinite” \( bc\_MPS \), we shift \( x_0 \) accordingly.

**Return type**

`array`

**mps2lat_values (A, axes=0, u=None)**

Reshape/reorder \( A \) to replace an MPS index by lattice indices.

**Parameters**

- `A (ndarray)` – Some values. Must have `A.shape[axes] = self.N_sites` if \( u \) is None, or `A.shape[axes] = self.N_cells` if \( u \) is an int.
- `axes ((iterable of) int)` – chooses the axis which should be replaced.
• \(u\) (None or int) – Optionally choose a subset of MPS indices present in the axes of \(A\), namely the indices corresponding to \(\text{self.unit.cell}[u]\), as returned by \(\text{mps.idx.fix.u()}\). The resulting array will not have the additional dimension(s) of \(u\).

Returns **res** \(A\) – Reshaped and reordered versions of \(A\). Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index \(j\) maps to lattice site \((x_0, x_1, x_2)\), then \(\text{res} \_A[\ldots, x_0, x_1, x_2, \ldots] = A[\ldots, j, \ldots]\).

Return type **ndarray**

Examples

Say you measure expectation values of an onsite term for an MPS, which gives you an 1D array \(A\), where \(A[i]\) is the expectation value of the site given by \(\text{self.mps2lat.idx}(i)\). Then this function gives you the expectation values ordered by the lattice:

```python
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[tuple(lat.mps2lat_idx(5))] == A[5]
True
```

If you have a correlation function \(C[i, j]\), it gets just slightly more complicated:

```python
>>> print(lat.shape, C.shape)
(10, 3, 2) (60, 60)
>>> lat.mps2lat_values(C, axes=[0, 1]).shape
(10, 3, 2, 10, 3, 2)
```

If the unit cell consists of different physical sites, an onsite operator might be defined only on one of the sites in the unit cell. Then you can use \(\text{mps.idx.fix.u()}\) to get the indices of sites it is defined on, measure the operator on these sites, and use the argument \(u\) of this function.

```python
>>> u = 0
>>> idx_subset = lat.mps.idx.fix.u(u)
>>> A_u = A[idx_subset]
>>> A_u_res = lat.mps2lat_values(A_u, u=u)
>>> A_u_res.shape
(10, 3)
>>> np.all(A_res[:, :, u] == A_u_res[:, :])
True
```

### mps2lat_values_masked

\(\text{A, axes=}-1, \text{mpsmods=None, include_u=None})\)

Reshape/reorder an array \(A\) to replace an MPS index by lattice indices.

This is a generalization of \(\text{mps2lat_values()}\) allowing for the case of an arbitrary set of MPS indices present in each axis of \(A\).

Parameters

- **\(A\)** (**ndarray**) – Some values.
- **axes** (**iterable of int**) – Chooses the axis of \(A\) which should be replaced. If multiple axes are given, you also need to give multiple index arrays as \(\text{mps.mods}\).
• **mps_inds** *(list of 1D ndarray)* – Specifies for each axis in axes, for which
  MPS indices we have values in the corresponding axis of A. Defaults to 
  [np.arange(A.shape[ax]) for ax in axes]. For indices across the MPS unit cell and “infinite” 
  bc_MPS, we shift $x_0$ accordingly.

• **include_u** *(list of bool)* – Specifies for each axis in axes, whether the $u$ index 
  of the lattice should be included into the output array res_A. Defaults to len(self.
  unit_cell) > 1.

Returns **res_A** – Reshaped and reordered copy of A. Such that MPS indices along the specified 
  axes are replaced by lattice indices, i.e., if MPS index $j$ maps to lattice site $(x_0, x_1, x_2)$, then 
  res_A[... , x0, x1, x2, ...] = A[... , mps_inds[j], ...].

Return type np.ma.MaskedArray

mps_idx_fix_u *(u=None)*

return an index array of MPS indices for which the site within the unit cell is $u$.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. 
This functions returns an index array of the mps indices which belong to sites given by self.
unit_cell[u].

Parameters **u** *(None | int)* – Selects a site of the unit cell. None (default) means all sites.

Returns **mps_idx** – MPS indices for which self.site(i) is self.unit_cell[u]. 
Ordered ascending.

Return type array

mps_lat_idx_fix_u *(u=None)*

Similar as mps_idx_fix_u(), but return also the corresponding lattice indices.

Parameters **u** *(None | int)* – Selects a site of the unit cell. None (default) means all sites.

Returns

• **mps_idx** *(array)* – MPS indices $i$ for which self.site(i) is self.
  unit_cell[u].

• **lat_idx** *(2D array)* – The row $j$ contains the lattice index (without $u$) corresponding to 
  mps_idx[j].

mps_sites() 

Return a list of sites for all MPS indices.

Equivalent to [self.site(i) for i in range(self.N_sites)].

This should be used for sites of 1D tensor networks (MPS, MPO, ...).

multi_coupling_shape *(dx)*

Calculate correct shape of the strengths for a multi_coupling.

Parameters **dx** *(2D array, shape (N_ops, dim))* – dx[i, :] is the translation vector in the 
  lattice for the $i$-th operator. Corresponds to the dx of each operator given in the argument ops 
  of tenpy.models.model.CouplingModel.add_multi_coupling().

Returns

• **coupling_shape** *(tuple of int)* – Len dim. The correct shape for an array specifying the 
  coupling strength. lat_indices has only rows within this shape.

• **shift_lat_indices** *(array)* – Translation vector from origin to the lower left corner of box 
  spanned by $dx$. (Unlike for coupling_shape() it can also contain entries > 0)
number_nearest_neighbors \((u=0)\)

Deprecated.

Deprecated since version 0.5.0: Use `count_neighbors()` instead.

number_next_nearest_neighbors \((u=0)\)

Deprecated.

Deprecated since version 0.5.0: Use `count_neighbors()` instead.

**property order**

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with `plot_order()`.

**ordering** \((order)\)

Provide possible orderings of the \(N\) lattice sites.

This function can be overwritten by derived lattices to define additional orderings. The following orders are defined in this method:

<table>
<thead>
<tr>
<th>order</th>
<th>equivalent priority</th>
<th>equivalent snake_winding</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Cstyle'</td>
<td>(0, 1, ..., dim-1, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'default'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>'snake'</td>
<td>(0, 1, ..., dim-1, dim)</td>
<td>(True, ..., True, True)</td>
</tr>
<tr>
<td>'snakeCstyle'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>'Fstyle'</td>
<td>(dim-1, ..., 1, 0, dim)</td>
<td>(False, ..., False, False)</td>
</tr>
<tr>
<td>'snakeFstyle'</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Note:** For lattices with a non-trivial unit cell (e.g. Honeycomb, Kagome), the grouped order might be more appropriate, see `get_order_grouped()`

**Parameters**

- **order** (str | (‘standard’, snake_winding, priority) | (‘grouped’, groups)) — Specifies the desired ordering using one of the strings of the above tables. Alternatively, an ordering is specified by a tuple with first entry specifying a function, ‘standard’ for `get_order()` and ‘grouped’ for `get_order_grouped()`, and other arguments in the tuple as specified in the documentation of these functions.

**Returns**

- **order** – the order to be used for `order`.

**Return type**

array, shape (N, D+1), dtype np.intp

See also:

- `get_order` generates the order from equivalent `priority` and `snake_winding`.
- `get_order_grouped` variant of `get_order`.
- `plot_order` visualizes the resulting order.

**plot_basis** \((ax, origin=(0.0, 0.0), shade=None, **kwargs)\)

Plot arrows indicating the basis vectors of the lattice.

**Parameters**
• *ax* (matplotlib.axes.Axes) – The axes on which we should plot.

• **kwargs – Keyword arguments for *ax.arrow*.

**plot_bc_identified** (*ax*, *direction*=- 1, *origin*=None, *cylinder_axis*=False, **kwargs)
Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

**Parameters**

• *ax* (matplotlib.axes.Axes) – The axes on which we should plot.

• *direction* (*int*) – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.

• *cylinder_axis* (*bool*) – Whether to plot the cylinder axis as well.

• *origin* (*None | np.ndarray*) – The origin starting from where we mark the identified sites. Defaults to the first entry of *unit_cell_positions*.

• **kwargs – Keyword arguments for the used *ax.plot*.

**plot_coupling** (*ax*, *coupling*=None, *wrap*=False, **kwargs)
Plot lines connecting nearest neighbors of the lattice.

**Parameters**

• *ax* (matplotlib.axes.Axes) – The axes on which we should plot.

• *coupling* (*list of (u1, u2, dx]*) – By default (None), use *self.pairs[‘nearest_neighbors’]*. Specifies the connections to be plotted; iterating over lattice indices (*i0, il, ...*), we plot a connection from the site (*i0, il, ..., u1*) to the site (*i0+dx[0], il+dx[1], ..., u2*), taking into account the boundary conditions.

• *wrap* (*bool*) – If True, wrap

• **kwargs – Further keyword arguments given to *ax.plot()*.

**plot_order** (*ax*, *order*=None, *textkwargs*={<’color’: ‘r’}, **kwargs)
Plot a line connecting sites in the specified “order” and text labels enumerating them.

**Parameters**

• *ax* (matplotlib.axes.Axes) – The axes on which we should plot.

• *order* (*None | 2D array (self.N_sites, self.dim+1))* – The order as returned by *ordering()*; by default (None) use *order*.

• *textkwargs* (*None | dict*) – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for *ax.text()*.

• **kwargs – Further keyword arguments given to *ax.plot()*.

**plot_sites** (*ax*, *markers*=['o', 'v', 's', 'p', 'h', 'D'], **kwargs)
Plot the sites of the lattice with markers.

**Parameters**

• *ax* (matplotlib.axes.Axes) – The axes on which we should plot.

• *markers* (*list*) – List of values for the keyword *marker* of *ax.plot()* to distinguish the different sites in the unit cell, a site *u* in the unit cell is plotted with a marker *markers[u % len(markers)]*.

• **kwargs – Further keyword arguments given to *ax.plot()*.
position (lat_idx)
    return 'space' position of one or multiple sites.
    Parameters lat_idx (ndarray, (... , dim+1)) – Lattice indices.
    Returns pos – The position of the lattice sites specified by lat_idx in real-space.
    Return type ndarray, (... , dim)

possible_couplings (u1, u2, dx)
    Find possible MPS indices for two-site couplings.
    For periodic boundary conditions (bc[a] == False) the index x_a is taken modulo Ls[a] and runs through range(Ls[a]). For open boundary conditions, x_a is limited to 0 <= x_a < Ls[a] and 0 <= x_a+dx[a] < lat.Ls[a].
    Parameters
        • u1 (int) – Indices within the unit cell; the u1 and u2 of add_coupling()
        • u2 (int) – Indices within the unit cell; the u1 and u2 of add_coupling()
        • dx (array) – Length dim. The translation in terms of basis vectors for the coupling.
    Returns
        • mps1, mps2 (array) – For each possible two-site coupling the MPS indices for the u1 and u2.
        • lat_indices (2D int array) – Rows of lat_indices correspond to rows of mps_ijkl and contain the lattice indices of the "lower left corner" of the box containing the coupling.
        • coupling_shape (tuple of int) – Len dim. The correct shape for an array specifying the coupling strength. lat_indices has only rows within this shape.

possible_multi_couplings (ops)
    Generalization of possible_couplings() to couplings with more than 2 sites.
    Parameters ops (list of (opname, dx, u)) – Same as the argument ops of add_multi_coupling().
    Returns
        • mps_ijkl (2D int array) – Each row contains MPS indices i,j,k,l,... for each of the operators positions. The positions are defined by dx (j,k,l,... relative to i) and boundary boundary conditions of self (how much the box for given dx can be shifted around without hitting a boundary - these are the different rows).
        • lat_indices (2D int array) – Rows of lat_indices correspond to rows of mps_ijkl and contain the lattice indices of the “lower left corner” of the box containing the coupling.
        • coupling_shape (tuple of int) – Len dim. The correct shape for an array specifying the coupling strength. lat_indices has only rows within this shape.

save_hdf5 (hdf5_saver, h5gr, subpath)
    Export self into a HDF5 file.
    This method saves all the data it needs to reconstruct self with from_hdf5().
    Specifically, it saves unit_cell, Ls, unit_cell_positions, basis, boundary_conditions, pairs under their name, bc_MPS as "boundary_conditions_MPS", and order as "order_for_MPS". Moreover, it saves dim and N_sites as HDF5 attributes.
    Parameters
        • hdf5_saver (Hdf5Saver) – Instance of the saving engine.
• **h5gr** (:class:`Group`) – HDF5 group which is supposed to represent self.

• **subpath** (str) – The name of h5gr with a ‘/’ in the end.

```python
def site(i):
    return Site instance corresponding to an MPS index i
```

```python
def test_sanity():
    Sanity check.
    Raises ValueErrors, if something is wrong.
```

### Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>get_lattice(lattice_name)</code></td>
<td>Given the name of a Lattice class, get the lattice class itself.</td>
</tr>
<tr>
<td><code>get_order(shape, snake_winding[, priority])</code></td>
<td>Built the Lattice.order in (Snake-) C-Style for a given lattice shape.</td>
</tr>
<tr>
<td><code>get_order_grouped(shape, groups)</code></td>
<td>Variant of get_order(), grouping some sites of the unit cell.</td>
</tr>
</tbody>
</table>

#### get_lattice

- full name: tenpy.models.lattice.get_lattice
- parent module: tenpy.models.lattice
- type: function

```python
def tenpy.models.lattice.get_lattice(lattice_name):
    Given the name of a Lattice class, get the lattice class itself.
```

Parameters:
- **lattice_name** (str) – Name of a Lattice class defined in the module lattice, for example "Chain", "Square", "Honeycomb", ...

Returns:
- **LatticeClass** – The lattice class (type, not instance) specified by lattice_name.

Return type: Lattice

#### get_order

- full name: tenpy.models.lattice.get_order
- parent module: tenpy.models.lattice
- type: function

```python
def tenpy.models.lattice.get_order(shape, snake_winding[, priority=None]):
    Built the Lattice.order in (Snake-) C-Style for a given lattice shape.
```

Note: In this doc-string, the word ‘direction’ refer to a physical direction of the lattice or the index $u$ of the unit cell as an “artificial direction”.

Parameters:
- **shape** (tuple of int) – The shape of the lattice, i.e., the length in each direction.
• **snake_winding** *(tuple of bool)* – For each direction one bool, whether we should wind as a “snake” (True) in that direction (i.e., going forth and back) or simply repeat ascending (False)

• **priority** *(None | tuple of float)* – If None (default), use C-Style ordering. Otherwise, this defines the priority along which direction to wind first; the direction with the highest priority increases fastest. For example, “C-Style” order is enforced by `priority=(0, 1, 2, ...)` and Fortrans F-style order is enforced by `priority=(dim, dim-1, ..., 1, 0)`

• **group** *(None | tuple of tuple)* – If None (default), ignore it. Otherwise, it specifies that we group the fastests changing dimension

**Returns order** – An order of the sites for `Lattice.order` in the specified ordering.

**Return type** `ndarray (np.prod(shape), len(shape))`

See also:

- `Lattice.ordering` method in `Lattice` to obtain the order from parameters.
- `Lattice.plot_order` visualizes the resulting order in a `Lattice`.
- `get_order_grouped` a variant grouping sites of the unit cell.

### get_order_grouped

- full name: `tenpy.models.lattice.get_order_grouped`
- parent module: `tenpy.models.lattice`
- type: function

`tenpy.models.lattice.get_order_grouped(shape, groups)`

Variant of `get_order()`, grouping some sites of the unit cell.

This function is useful for lattices with a unit cell of more than 2 sites (e.g., Kagome). For 2D lattices with a unit cell, the ordering goes first within a group, then along y, then the next group (for the same x-value), again along y, and finally along x when all groups are done.

As an example, consider the Kagome lattice.

**Note:** In this doc-string, the word ‘direction’ refer to a physical direction of the lattice or the index $u$ of the unit cell as an “artificial direction”.

**Parameters**

- **shape** *(tuple of int)* – The shape of the lattice, i.e., the length in each direction.

- **groups** *(tuple of tuple of int)* – A partition and reordering of `range(shape[-1])` into smaller groups. The ordering goes first within a group, then along the last spatial dimensions, then changing between different groups and finally in C-style order along the remaining spatial dimensions.

**Returns order** – An order of the sites for `Lattice.order` in the specified ordering.

**Return type** `ndarray (np.prod(shape), len(shape))`

See also:
7.11. models
Module description

Classes to define the lattice structure of a model.

The base class `Lattice` defines the general structure of a lattice, you can subclass this to define your own lattice. The `SimpleLattice` is a slight simplification for lattices with a single-site unit cell. Further, we have some predefined lattices, namely `Chain`, `Ladder` in 1D and `Square`, `Triangular`, `Honeycomb`, and `Kagome` in 2D.

The `IrregularLattice` provides a way to remove or add sites to an existing, regular lattice.

See also the `Models`.

### 7.11.2 model

- full name: `tenpy.models.model`
- parent module: `tenpy.models`
- type: module

#### Classes

```
Hdf5Exportable

Model

MPOModel
CouplingModel
NearestNeighborModel

CouplingMPOModel
MultiCouplingModel
```

<table>
<thead>
<tr>
<th>CouplingMPOModel(model_params)</th>
<th>Combination of the <code>CouplingModel</code> and <code>MPOModel</code>.</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>CouplingModel(lattice, bc_coupling, ...)</code></td>
<td>Base class for a general model of a Hamiltonian consisting of two-site couplings.</td>
</tr>
</tbody>
</table>

continues on next page
Table 97 – continued from previous page

<table>
<thead>
<tr>
<th>Class Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPOModel(lattice, H_MPO)</td>
<td>Base class for a model with an MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td>Model(lattice)</td>
<td>Base class for all models.</td>
</tr>
<tr>
<td>MultiCouplingModel(lattice[, bc_coupling, ...])</td>
<td>Deprecated class which was a generalization of the CouplingModel.</td>
</tr>
<tr>
<td>NearestNeighborModel(lattice, H_bond)</td>
<td>Base class for a model of nearest neighbor interactions w.r.t.</td>
</tr>
</tbody>
</table>

**CouplingModel**

- full name: tenpy.models.model.CouplingModel
- parent module: tenpy.models.model
- type: class

**Inheritance Diagram**

```
Hdf5Exportable
   ↓
Model
   ↓
CouplingModel
```

**Methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CouplingModel.<strong>init</strong>(lattice[,...])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>CouplingModel.add_coupling(strength, u1, ...</td>
<td>Add two-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>CouplingModel.add_coupling_term(strength, i,...)</td>
<td>Add a two-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>CouplingModel.add_exponentially_decaying_coupling(...</td>
<td>Add an exponentially decaying long-range coupling.</td>
</tr>
<tr>
<td>CouplingModel.add_local_term(strength, term)</td>
<td>Add a single term to self.</td>
</tr>
<tr>
<td>CouplingModel.add_multi_coupling(strength, ops)</td>
<td>Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
</tbody>
</table>
Table 98 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>CouplingModel.add_multi_coupling_term(...)</code></td>
<td>Add a general M-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td><code>CouplingModel.add_onsite(strength, u, op_name)</code></td>
<td>Add onsite terms to <code>onsite_terms</code>.</td>
</tr>
<tr>
<td><code>CouplingModel.add_onsite_term(strength, i, op)</code></td>
<td>Add an onsite term on a given MPS site.</td>
</tr>
<tr>
<td><code>CouplingModel.all_coupling_terms()</code></td>
<td>Sum of all <code>coupling_terms</code>.</td>
</tr>
<tr>
<td><code>CouplingModel.all_onsite_terms()</code></td>
<td>Sum of all <code>onsite_terms</code>.</td>
</tr>
<tr>
<td><code>CouplingModel.calc_H_MPO([tol_zero])</code></td>
<td>Calculate MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td><code>CouplingModel.calc_H_bond([tol_zero])</code></td>
<td>Calculate $H_{bond}$ from <code>coupling_terms</code> and <code>onsite_terms</code>.</td>
</tr>
<tr>
<td><code>CouplingModel.calc_H_onsite([tol_zero])</code></td>
<td>Calculate $H_{onsite}$ from <code>self.onsite_terms</code>.</td>
</tr>
<tr>
<td><code>CouplingModel.coupling_strength_add_ext_flux()</code></td>
<td>Add an external flux to the coupling strength.</td>
</tr>
<tr>
<td><code>CouplingModel.enlarge_mps_unit_cell([factor])</code></td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td><code>CouplingModel.from_hdf5(hdf5_loader, h5grp, ...)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>CouplingModel.group_sites([n, grouped_sites])</code></td>
<td>Modify <code>self</code> in place to group sites.</td>
</tr>
<tr>
<td><code>CouplingModel.save_hdf5(hdf5_saver, h5grp, ...)</code></td>
<td>Export <code>self</code> into a HDF5 file.</td>
</tr>
<tr>
<td><code>CouplingModel.test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
</tbody>
</table>

```python
class tenpy.models.model.CouplingModel(lattice, bc_coupling=None, explicit_plus_hc=False)
```

Base class for a general model of a Hamiltonian consisting of two-site couplings.

In this class, the terms of the Hamiltonian are specified explicitly as `OnsiteTerms` or `CouplingTerms`.

Deprecated since version 0.4.0: `bc_coupling` will be removed in 1.0.0. To specify the full geometry in the lattice, use the `bc` parameter of the `Lattice`.

Parameters

- `lattice` (Lattice) – The lattice defining the geometry and the local Hilbert space(s).
- `bc_coupling` ((iterable of) {'open' | 'periodic' | int}) – Boundary conditions of the couplings in each direction of the lattice. Defines how the couplings are added in `add_coupling()`. A single string holds for all directions. An integer `shift` means that we have periodic boundary conditions along this direction, but shift/tilt by `-shift*lattice.basis[0]` (cylinder axis for `bc_MPS='infinite'`) when going around the boundary along this direction.
- `explicit_plus_hc` (bool) – If True, the Hermitian conjugate of the MPO is computed at runtime, rather than saved in the MPO.

`onsite_terms`

The `OnsiteTerms` ordered by category.

Type `{'category': OnsiteTerms}`

`coupling_terms`

The `CouplingTerms` ordered by category. In case we’ve added terms with more than 2 operators, e.g. with `add_multi_coupling()`, the values of the dictionary may also be `MultiCouplingTerms`.

Type `{'category': CouplingTerms}`
**exp_decaying_terms**
Collection of coupling terms with exponentially decaying long-range interactions. Filled by `add_exponentially_decaying_coupling()`.

Type `ExponentiallyDecayingTerms`

**explicit_plus_hc**
If `True`, `self` represents the terms in `onsite_terms`, `coupling_terms` and `exp_decaying_terms` plus their hermitian conjugate added. The flag will be carried on to the MPO, which will have a reduced bond dimension if `self.add_coupling(..., plus_hc=True)` was used. Note that `add_onsite()`, `add_coupling()`, `add_multi_coupling()` and `add_exponentially_decaying_coupling()` respect this flag, ensuring that the represented Hamiltonian is independent of the `explicit_plus_hc` flag.

Type `bool`

**test_sanity()**
Sanity check, raises ValueErrors, if something is wrong.

**add_local_term(strength, term, category=None, plus_hc=False)**
Add a single term to `self`.

The represented term is `strength` times the product of the operators given in `terms`. Each operator is specified by the name and the site it acts on; the latter given by a lattice index, see `Lattice`.

Depending on the length of `term`, it can add an onsite term or a coupling term to `onsite_terms` or `coupling_terms`, respectively.

Parameters

- **strength** (float/complex) – The prefactor of the term.
- **term** (list of (str, array_like)) – List of tuples (opname, lat_idx) where opname is a string describing the operator acting on the site given by the lattice index lat_idx. Here, lat_idx is for example \([x, y, u]\) for a 2D lattice, with \(u\) being the index within the unit cell.
- **category** – Descriptive name used as key for `onsite_terms` or `coupling_terms`.
- **plus_hc** (bool) – If `True`, the hermitian conjugate of the terms is added automatically.

**add_onsite(strength, u, opname, category=None, plus_hc=False)**
Add onsite terms to `onsite_terms`.

Adds \(\sum_{x} strength[x] \cdot OP\) to the represented Hamiltonian, where the operator \(OP=lat.unit_cell[u].get_op(opname)\) acts on the site given by a lattice index \((x_0, \ldots, x_{(dim-1)}, u)\).

The necessary terms are just added to `onsite_terms`; doesn’t rebuild the MPO.

Parameters

- **strength** (scalar | array) – Prefactor of the onsite term. May vary spatially. If an array of smaller size is provided, it gets tiled to the required shape.
- **u** (int) – Picks a Site `lat.unit_cell[u]` out of the unit cell.
- **opname** (str) – valid operator name of an onsite operator in `lat.unit_cell[u]`.
- **category** (str) – Descriptive name used as key for `onsite_terms`. Defaults to opname.
- **plus_hc** (bool) – If `True`, the hermitian conjugate of the terms is added automatically.
See also:

**add_coupling** Add a terms acting on two sites.

**add_onsite_term** Add a single term without summing over vecx.

### add_onsite_term

**add_onsite_term** *(strength, i, op, category=None, plus hc=False)*

Add an onsite term on a given MPS site.

Wrapper for `self.onsite_terms[category].add_onsite_term(...)`.

**Parameters**

- **strength** *(float)* – The strength of the term.
- **i** *(int)* – The MPS index of the site on which the operator acts. We require `0 <= i < L`.
- **op** *(str)* – Name of the involved operator.
- **category** *(str)* – Descriptive name used as key for `onsite_terms`. Defaults to `op`.
- **plus hc** *(bool)* – If `True`, the hermitian conjugate of the term is added automatically.

### all_onsite_terms()

Sum of all `onsite_terms`.

### add_coupling

**add_coupling** *(strength, u1, op1, u2, op2, dx, op_string=None, str_on_first=True, raise_op2_left=False, category=None, plus hc=False)*

Add twosite coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \( \sum_{x_0, \ldots, x_{\text{dim}-1}} \text{strength}[\text{shift}(\vec{x})] * \text{OP}_0 * \text{OP}_1 \), where \( \text{OP}_0 := \text{lat.unit_cell[u0]}.\text{get_op}(\text{op0}) \) acts on the site \((x_0, \ldots, x_{\text{dim}-1}, u1)\), and \( \text{OP}_1 := \text{lat.unit_cell[u1]}.\text{get_op}(\text{op1}) \) acts on the site \((x_0+dx[0], \ldots, x_{\text{dim}-1}+dx[\text{dim}-1], u1)\). Possible combinations \(x_0, \ldots, x_{\text{dim}-1}\) are determined from the boundary conditions in `possible_couplings()`.

The coupling `strength` may vary spatially if the given `strength` is a numpy array. The correct shape of this array is the `coupling_shape` returned by `tenpy.models.lattice.possible_couplings()` and depends on the boundary conditions. The `shift(...)` depends on `dx`, and is chosen such that the first entry `strength[0, 0, \ldots]` of `strength` is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to `coupling_terms`; this function does not rebuild the MPO.

Deprecated since version 0.4.0: The arguments `str_on_first` and `raise_op2_left` will be removed in version 1.0.0.

**Parameters**

- **strength** *(scalar / array)* – Prefactor of the coupling. May vary spatially (see above). If an array of smaller size is provided, it gets tiled to the required shape.
- **u1** *(int)* – Picks the site \(\text{lat.unit_cell[u1]}\) for OP1.
- **op1** *(str)* – Valid operator name of an onsite operator in \(\text{lat.unit_cell[u1]}\) for OP1.
- **u2** *(int)* – Picks the site \(\text{lat.unit_cell[u2]}\) for OP2.
- **op2** *(str)* – Valid operator name of an onsite operator in \(\text{lat.unit_cell[u2]}\) for OP2.
- **dx** *(iterable of int)* – Translation vector (of the unit cell) between OP1 and OP2. For a 1D lattice, a single int is also fine.
• **op_string** *(str | None)* – Name of an operator to be used between the OP1 and OP2 sites. Typical use case is the phase for a Jordan-Wigner transformation. The operator should be defined on all sites in the unit cell. If None, auto-determine whether a Jordan-Wigner string is needed, using `op_needs_JW()`.

• **str_on_first** *(bool)* – Whether the provided `op_string` should also act on the first site. This option should be chosen as True for Jordan-Wigner strings. When handling Jordan-Wigner strings we need to extend the `op_string` to also act on the ‘left’, first site (in the sense of the MPS ordering of the sites given by the lattice). In this case, there is a well-defined ordering of the operators in the physical sense (i.e. which of `op1` or `op2` acts first on a given state). We follow the convention that `op2` acts first (in the physical sense), independent of the MPS ordering. Deprecated.

• **raise_op2_left** *(bool)* – Raise an error when `op2` appears left of `op1` (in the sense of the MPS ordering given by the lattice). Deprecated.

• **category** *(str)* – Descriptive name used as key for `coupling_terms`. Defaults to a string of the form "\(\{\text{op1}\}_i \{\text{op2}\}_j\)".

• **plus hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

### Examples

When initializing a model, you can add a term \(J \sum_{<i,j>} S_i^z S_j^z\) on all nearest-neighbor bonds of the lattice like this:

```python
>>> J = 1. # the strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(J, u1, 'Sz', u2, 'Sz', dx)
```

The strength can be an array, which gets tiled to the correct shape. For example, in a 1D Chain with an even number of sites and periodic (or infinite) boundary conditions, you can add alternating strong and weak couplings with a line like:

```python
>>> self.add_coupling([1.5, 1.], u1, 'Sz', u2, 'Sz', dx)
```

Make sure to use the **plus hc** argument if necessary, e.g. for hoppings:

```python
>>> t = 1. # hopping strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(t, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```

Alternatively, you can add the hermitian conjugate terms explicitly. The correct way is to complex conjugate the strength, take the hermitian conjugate of the operators and swap the order (including a swap \(u1 \leftrightarrow u2\)), and use the opposite direction \(-dx\), i.e. the h.c. of `add_coupling(t, u1, 'A', u2, 'B', dx)` is `add_coupling(np.conj(t), u2, hc('B'), u1, hc('A'), -dx)`, where `hc` takes the hermitian conjugate of the operator names, see `get_hc_op_name()`. For spin-less fermions (`FermionSite`), this would be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(t, u1, 'Cd', u2, 'C', dx)
...    self.add_coupling(np.conj(t), u2, 'Cd', u1, 'C', -dx) # h.c.
```

With spin-full fermions (`SpinHalfFermions`), it could be:
Note that the Jordan-Wigner strings for the fermions are added automatically!

See also:

add_onsite Add terms acting on one site only.

add_multi_coupling_term for terms on more than two sites.

add_coupling_term Add a single term without summing over \(\mathbf{v}_\mathbf{c}x\).

add_coupling_term(strength, i, op_i, op_j, op_string='Id', category=None, plus_hc=False)

Add a two-site coupling term on given MPS sites.

Wrapper for self.coupling_terms[category].add_coupling_term(...).

Warning: This function does not handle Jordan-Wigner strings! You might want to use add_local_term() instead.

Parameters

- **strength** (float) – The strength of the coupling term.
- **i** (int) – The MPS indices of the two sites on which the operator acts. We require \(0 \leq i < N_{\text{sites}}\) and \(i < j\), i.e., \(op_i\) acts “left” of \(op_j\). If \(j \geq N_{\text{sites}}\), it indicates couplings between unit cells of an infinite MPS.
- **j** (int) – The MPS indices of the two sites on which the operator acts. We require \(0 \leq i < N_{\text{sites}}\) and \(i < j\), i.e., \(op_i\) acts “left” of \(op_j\). If \(j \geq N_{\text{sites}}\), it indicates couplings between unit cells of an infinite MPS.
- **op1** (str) – Names of the involved operators.
- **op2** (str) – Names of the involved operators.
- **op_string** (str) – The operator to be inserted between \(i\) and \(j\).
- **category** (str) – Descriptive name used as key for coupling_terms. Defaults to a string of the form "\(\{op1\}_i \{op2\}_j\)".
- **plus_hc** (bool) – If True, the hermitian conjugate of the term is added automatically.

all_coupling_terms()

Sum of all coupling_terms.

add_multi_coupling(strength, ops, _deprecate_1='DEPRECATED', _deprecate_2='DEPRECATED', op_string=None, category=None, plus_hc=False)

Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \(\sum_2 \text{strength}[\text{shift}(\vec{x})] \ast OP_0 \ast OP_1 \ast \ldots \ast OP_{M-1}\), involving \(M\) operators. Here, \(OP_m\) stands for the operator defined by the \(m\)-th tuple \((\text{opname}, \ dx, \ u)\) given in the argument \(ops\), which determines the position \(\vec{x} + \vec{d}x\) and unit-cell index \(u\) of the site it acts on; the actual operator is given by self.lat.unit_cell[u].get_op(opname).
The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_multi_couplings() and depends on the boundary conditions. The shift(...) depends on the dx entries of ops and is chosen such that the first entry strength[0, 0, ...] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to coupling_terms; this function does not rebuild the MPO.

Deprecated since version 0.6.0: We switched from the three arguments u0, op0 and other_op with other_ops=[(u1, op1, dx1), (op2, u2, dx2), ...] to a single, equivalent argument ops which should now read ops=[(op0, dx0, u0), (op1, dx1, u1), (op2, dx2, u2), ...], where dx0 = [0]*self.lat.dim. Note the changed order inside the tuples!

Parameters

- **strength** (scalar | array) – Prefactor of the coupling. May vary spatially, and is tiled to the required shape.

- **ops** (list of (opname, dx, u)) – Each tuple determines one operator of the coupling, see the description above. opname (str) is the name of the operator, dx (list of length lat.dim) is a translation vector, and u (int) is the index of lat.unit_cell on which the operator acts. The first entry of ops corresponds to OP0 and acts last in the physical sense.

- **op_string** (str | None) – If a string is given, we use this as the name of an operator to be used inbetween the operators, excluding the sites on which any operators act. This operator should be defined on all sites in the unit cell.

  If None, auto-determine whether a Jordan-Wigner string is needed (using op_needs_JW()) for each of the segments inbetween the operators and also on the sites of the left operators.

- **category** (str) – Descriptive name used as key for coupling_terms. Defaults to a string of the form "\(\{\text{op0}\}_i \{\text{other_ops[0]}\}_j \{\text{other_ops[1]}\}_k \ldots\)".

- **plus_hc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

Examples

A call to add_coupling() with arguments add_coupling(strength, u1, 'A', u2, 'B', dx) is equivalent to the following:

```python
>>> dx_0 = [0] * self.lat.dim  # = [0] for a 1D lattice, [0, 0] in 2D
>>> self.add_multi_coupling(strength, [('A', dx_0, u1), ('B', dx, u2)])
```

To explicitly add the hermitian conjugate (instead of simply using plus_hc = True), you need to take the complex conjugate of the strength, reverse the order of the operators and take the hermitian conjugates of the individual operator names (indicated by the hc(...), see get_hc_op_name()):

```python
>>> self.add_multi_coupling(np.conj(strength), [(hc('B'), dx, u2), (hc('A'), u1, -dx_0, u1)])
```

See also:

- **add_onsite** Add terms acting on one site only.
- **add_coupling** Add terms acting on two sites.
- **add_multi_coupling_term** Add a single term, not summing over the possible \(\vec{x}\).
add_multi_coupling_term (strength, iijkl, ops_iijkl, op_string, category=None, plus_hc=False)
Add a general M-site coupling term on given MPS sites.
Wrapper for self.coupling_terms[category].add_multi_coupling_term(...).

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use add_local_term() instead.

**Parameters**

- **strength (float)** – The strength of the coupling term.
- **ijkl (list of int)** – The MPS indices of the sites on which the operators acts. With i, j, k, ... = iijkl, we require that they are ordered ascending, i < j < k < ... and that 0 <= i < N_sites. Indices >= N_sites indicate couplings between different unit cells of an infinite MPS.
- **ops_iijkl (list of str)** – Names of the involved operators on sites i, j, k, ....
- **op_string (list of str)** – Names of the operator to be inserted between the operators, e.g., op_string[0] is inserted between i and j.
- **category (str)** – Descriptive name used as key for coupling_terms. Defaults to a string of the form "{op0}_i {op1}_j {op2}_k ...".
- **plus_hc (bool)** – If True, the hermitian conjugate of the term is added automatically.

add_exponentially_decaying_coupling (strength, lambda_, op_i, op_j, subsites=None, op_string=None, plus_hc=False)
Add an exponentially decaying long-range coupling.

\[
\text{strength} \sum_{i<j} \lambda^{i-j} A_{\text{subsites}[i]} B_{\text{subsites}[j]}
\]

Where the operator A is given by op_i, and B is given by op_j. Note that the sum over i,j is long-range, for infinite systems going beyond the MPS unit cell. Moreover, note that the distance in the exponent is the distance within subsites.

**Parameters**

- **strength (float)** – Overall prefactor.
- **lambda (float)** – Decay-rate
- **op_i (string)** – Names for the operators.
- **op_j (string)** – Names for the operators.
- **subsites (None / 1D array)** – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. None selects all sites.
- **op_string (None / str)** – The operator to be inserted between A and B; If None, this function checks whether a fermionic "JW" string is needed for the given operators; in this case the right op_j acts first.
- **plus_hc (bool)** – If True, the hermitian conjugate of the term is added automatically.

**Examples**

At least for simple enough 1D chains (or ladders), you can use fit_with_sum_of_exp() to approximate a long-range function with a few sum of exponentials and then add them with this function.
```python
>>> def decay(x):
...     return np.exp(-0.1*x) / x**2
>>> from tenpy.tools.fit import fit_with_sum_of_exp, sum_of_exp

>>> n_exp = 5
>>> fit_range = 50
>>> lam, pref = fit_with_sum_of_exp(decay, n_exp, fit_range)
>>> x = np.arange(1, fit_range + 1)
>>> print('error in fit: {0:.3e}'.format(np.sum(np.abs(decay(x) - sum_of_exp(lam, pref, x)))))
error in fit: 1.073e-04
>>> for pr, la in zip(pref, lam):
...     self.add_exponentially_decaying_coupling(pr, la, 'N', 'N')
```

calc_H_onsite (tol_zero=1e-15)

Calculate $H_{\text{onsite}}$ from self.onsite_terms.

Deprecated since version 0.4.0: This function will be removed in 1.0.0. Replace calls to this function by self.all_onsite_terms().remove_zeros(tol_zero).to_Arrays(self.lat.mps_sites()). You might also want to take explicit_plus hc into account.

**Parameters**

- tol_zero (float) – prefactors with abs(strength) < tol_zero are considered to be zero.

**Returns**

- $H_{\text{onsite}}$ (list of npc.Array)

- onsite terms of the Hamiltonian. If explicit_plus hc is True, – Hermitian conjugates of the onsite terms will be included.

calc_H_bond (tol_zero=1e-15)

calculate $H_{\text{bond}}$ from coupling_terms and onsite_terms.

**Parameters**

- tol_zero (float) – prefactors with abs(strength) < tol_zero are considered to be zero.

**Returns**

- $H_{\text{bond}}$ – Bond terms as required by the constructor of NearestNeighborModel. Legs are ['p0', 'p0*', 'p1', 'p1*']

**Return type**

list of Array

:raises ValueError : if the Hamiltonian contains longer-range terms:

calc_H_MPO (tol_zero=1e-15)

Calculate MPO representation of the Hamiltonian.

Uses onsite_terms and coupling_terms to build an MPOGraph (and then an MPO).

**Parameters**

- tol_zero (float) – Prefactors with abs(strength) < tol_zero are considered to be zero.

**Returns**

- $H_{\text{MPO}}$ – MPO representation of the Hamiltonian.

**Return type**

MPO

coupling_strength_add_ext_flux (strength, dx, phase)

Add an external flux to the coupling strength.

When performing DMRG on a “cylinder” geometry, it might be useful to put an “external flux” through the cylinder. This means that a particle hopping around the cylinder should pick up a phase given by the external flux [resta1998]. This is also called “twisted boundary conditions” in literature. This function...
adds a complex phase to the strength array on some bonds, such that particles hopping in positive direction around the cylinder pick up \( \exp(+i \text{ phase}) \).

**Warning:** For the sign of phase it is important that you consistently use the creation operator as \( \text{op}1 \) and the annihilation operator as \( \text{op}2 \) in \text{add_coupling}().

**Parameters**

- **strength** (scalar | array) – The strength to be used in \text{add_coupling}(), when no external flux would be present.
- **dx** (iterable of int) – Translation vector (of the unit cell) between \( \text{op}1 \) and \( \text{op}2 \) in \text{add_coupling}().
- **phase** (iterable of float) – The phase of the external flux for hopping in each direction of the lattice. E.g., if you want flux through the cylinder on which you have an infinite MPS, you should give phase=[0, \phi] such that particles pick up a phase \( \phi \) when hopping around the cylinder.

**Returns** strength – The strength array to be used as strength in \text{add_coupling}() with the given dx.

**Return type** complex array

**Examples**

Let’s say you have an infinite MPS on a cylinder, and want to add nearest-neighbor hopping of fermions with the FermionSite. The cylinder axis is the \( x \)-direction of the lattice, so to put a flux through the cylinder, you want particles hopping around the cylinder to pick up a phase \( \phi \) given by the external flux.

```python
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0, phi])
...    self.add_coupling(strength_with_flux, u1, 'Cd', u2, 'C', dx)
...    self.add_coupling(np.conj(strength_with_flux), u2, 'Cd', u1, 'C', -dx)
```

**enlarge_mps_unit_cell** (factor=2)

Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and cannot be reverted.

**Parameters** factor (int) – The new number of sites in the MPS unit cell will be increased from \( N_\text{sites} \) to \( \text{factor} \times N_\text{sites}_\text{per_ring} \). Since MPS unit cells are repeated in the \( x \)-direction in our convention, the lattice shape goes from \((L_x, L_y, \ldots, L_u)\) to \((L_x \times \text{factor}, L_y, \ldots, L_u)\).

**classmethod** from_hdf5 (hdf5_loader, h5gr, subpath)

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with \text{save_hdf5}().

**Parameters**

- hdf5_loader (Hdf5Loader) – Instance of the loading engine.
- h5gr (Group) – HDF5 group which is represent the object to be constructed.
• **subpath** (*str*) – The *name* of *h5gr* with a *' / '* in the end.

Returns **obj** – Newly generated class instance containing the required data.

Return type **cls**

**group_sites** (*n=2, grouped_sites=None*)

Modify *self* in place to group sites.

Group each *n* sites together using the *GroupedSite*. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and can not be reverted.

Parameters

• **n** (*int*) – Number of sites to be grouped together.

• **grouped_sites** (None | list of *GroupedSite*) – The sites grouped together.

Returns **grouped_sites** – The sites grouped together.

Return type list of *GroupedSite*

**save_hdf5** (*hdf5_saver, h5gr, subpath*)

Export *self* into a HDF5 file.

This method saves all the data it needs to reconstruct *self* with *from_hdf5()*.

This implementation saves the content of *__dict__* with *save_dict_content()* , storing the format under the attribute *'format'*.

Parameters

• **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.

• **h5gr** (class `Group`) – HDF5 group which is supposed to represent *self*.

• **subpath** (*str*) – The *name* of *h5gr* with a *' / '* in the end.

**MPOModel**

• full name: tenpy.models.model.MPOModel

• parent module: tenpy.models.model

• type: class
Inheritance Diagram

```
<table>
<thead>
<tr>
<th>Hdf5Exportable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
</tr>
<tr>
<td>MPOModel</td>
</tr>
</tbody>
</table>
```

Methods

- `MPOModel.__init__(lattice, H_MPO)`: Initialize self.
- `MPOModel.calc_H_bond_from_MPO([tol_zero])`: Calculate the bond Hamiltonian from the MPO Hamiltonian.
- `MPOModel.enlarge_mps_unit_cell([factor])`: Repeat the unit cell for infinite MPS boundary conditions; in place.
- `MPOModel.from_hdf5(hdf5_loader, h5gr, subpath)`: Load instance from a HDF5 file.
- `MPOModel.group_sites([n, grouped_sites])`: Modify `self` in place to group sites.
- `MPOModel.save_hdf5(hdf5_saver, h5gr, subpath)`: Export `self` into a HDF5 file.
- `MPOModel.test_sanity()`

```python
class tenpy.models.model.MPOModel(lattice, H_MPO)
    Bases: tenpy.models.model.Model

    Base class for a model with an MPO representation of the Hamiltonian.

    In this class, the Hamiltonian gets represented by an MPO. Thus, instances of this class are suitable for MPO-based algorithms like DMRG `dmrg` and MPO time evolution.

    **Todo:** implement MPO for time evolution...
```

**Parameters**

- `H_MPO`: The Hamiltonian rewritten as an MPO.

  - **H_MPO**
    - MPO representation of the Hamiltonian. If the `explicit_plus_hc` flag of the MPO is `True`, the represented Hamiltonian is `H_MPO + hermitian_conjugate(H_MPO)`.

    - **Type**: `tenpy.networks.mpo.MPO`
**enlarge_mps_unit_cell** *(factor=2)*

Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and cannot be reverted.

**Parameters**

- **factor** *(int)* – The new number of sites in the MPS unit cell will be increased from \( N\_\text{sites} \) to \( \text{factor}\times N\_\text{sites\_per\_ring} \). Since MPS unit cells are repeated in the \( x \)-direction in our convention, the lattice shape goes from \((L_x, L_y, \ldots, L_u)\) to \((L_x\times\text{factor}, L_y, \ldots, L_u)\).

**group_sites** *(n=2, grouped_sites=None)*

Modify **self** in place to group sites.

Group each \( n \) sites together using the **GroupedSite**. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and cannot be reverted.

**Parameters**

- **n** *(int)* – Number of sites to be grouped together.
- **grouped_sites** *(None | list of GroupedSite)* – The sites grouped together.

**Returns**

- **grouped_sites** – The sites grouped together.

**Return type**

- list of GroupedSite

**calc_H_bond_from_MPO** *(tol_zero=1e-15)*

Calculate the bond Hamiltonian from the MPO Hamiltonian.

**Parameters**

- **tol_zero** *(float)* – Arrays with norm < \( \text{tol\_zero} \) are considered to be zero.

**Returns**

- **H_bond** – Bond terms as required by the constructor of **NearestNeighborModel**.
  - Legs are ['p0', 'p0*', 'p1', 'p1*']

**Return type**

- list of Array

:raises ValueError: if the Hamiltonian contains longer-range terms.

**classmethod** **from_hdf5** *(hdf5_loader, h5gr, subpath)*

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with **save_hdf5()**.

**Parameters**

- **hdf5_loader** *(Hdf5Loader)* – Instance of the loading engine.
- **h5gr** *(Group)* – HDF5 group which is represent the object to be constructed.
- **subpath** *(str)* – The name of \( h5gr \) with a '/' in the end.

**Returns**

- **obj** – Newly generated class instance containing the required data.

**Return type**

- cls

**save_hdf5** *(hdf5_saver, h5gr, subpath)*

Export **self** into a HDF5 file.

This method saves all the data it needs to reconstruct **self** with **from_hdf5()**.

This implementation saves the content of **__dict__** with **save_dict_content()**, storing the format under the attribute 'format'.

**Parameters**

- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.
• **h5gr (`class` `Group`)** – HDF5 group which is supposed to represent `self`.
• **subpath** (**str**) – The name of `h5gr` with a `/` in the end.

**Model**

• full name: `tenpy.models.model.Model`
• parent module: `tenpy.models.model`
• type: class

**Inheritance Diagram**

```
    Hdf5Exportable
    ↓               ↓
  Model      Model
```

**Methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>Model.__init__(lattice)</code></td>
<td>Initialize <code>self</code>.</td>
</tr>
<tr>
<td><code>Model.enlarge_mps_unit_cell([factor])</code></td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td><code>Model.from_hdf5(hdf5_loader, h5gr, subpath)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>Model.group_sites([n, grouped_sites])</code></td>
<td>Modify <code>self</code> in place to group sites.</td>
</tr>
<tr>
<td><code>Model.save_hdf5(hdf5_saver, h5gr, subpath)</code></td>
<td>Export <code>self</code> into a HDF5 file.</td>
</tr>
</tbody>
</table>

**class** `tenpy.models.model.Model(lattice)`

Bases: `tenpy.tools.hdf5_io.Hdf5Exportable`

Base class for all models.

The common base to all models is the underlying Hilbert space and geometry, specified by a `Lattice`.

**Parameters**

- **lattice** (**Lattice**) – The lattice defining the geometry and the local Hilbert space(s).
- **lat**
  The lattice defining the geometry and the local Hilbert space(s).
  Type **Lattice**
- **enlarge_mps_unit_cell** (**factor=2**)
  Repeat the unit cell for infinite MPS boundary conditions; in place.
This has to be done after finishing initialization and can not be reverted.

Parameters

**factor** (*int*) – The new number of sites in the MPS unit cell will be increased from \(N_{\text{sites}}\) to \(\text{factor} \times N_{\text{sites\_per\_ring}}\). Since MPS unit cells are repeated in the \(x\)-direction in our convention, the lattice shape goes from \((L_x, L_y, \ldots, L_u)\) to \((L_x \times \text{factor}, L_y, \ldots, L_u)\).

**group_sites** *(n=2, grouped_sites=None)*

Modify `self` in place to group sites.

Group each \(n\) sites together using the `GroupedSite`. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and can not be reverted.

Parameters

- **n** (*int*) – Number of sites to be grouped together.
- **grouped_sites** (*None | list of GroupedSite*) – The sites grouped together.

Returns **grouped_sites** – The sites grouped together.

Return type list of GroupedSite

classmethod **from_hdf5** *(hdf5_loader, h5gr, subpath)*

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

Parameters

- **hdf5_loader** (*Hdf5Loader*) – Instance of the loading engine.
- **h5gr** (*Group*) – HDF5 group which is represent the object to be constructed.
- **subpath** (*str*) – The name of `h5gr` with a '/' in the end.

Returns **obj** – Newly generated class instance containing the required data.

Return type cls

**save_hdf5** *(hdf5_saver, h5gr, subpath)*

Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute 'format'.

Parameters

- **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.
- **h5gr** (*class `Group`*) – HDF5 group which is supposed to represent `self`.
- **subpath** (*str*) – The name of `h5gr` with a '/' in the end.
MultiCouplingModel

- full name: tenpy.models.model.MultiCouplingModel
- parent module: tenpy.models.model
- type: class

Inheritance Diagram

![Inheritance Diagram]

Methods

- **MultiCouplingModel.__init__(lattice[, ...])** Initialize self.
- **MultiCouplingModel.add_coupling(strength, ...)** Add two-site coupling terms to the Hamiltonian, summing over lattice sites.
- **MultiCouplingModel.add_coupling_term(...[, ...])** Add a two-site coupling term on given MPS sites.
- **MultiCouplingModel.add_exponentially_decaying_coupling(...)** Add an exponentially decaying long-range coupling.
- **MultiCouplingModel.add_local_term(strength, term)** Add a single term to self.
- **MultiCouplingModel.add_multi_coupling(...)** Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.
- **MultiCouplingModel.add_multi_coupling_term(...)** Add a general M-site coupling term on given MPS sites.
- **MultiCouplingModel.add_onsite(strength, u, ...)** Add onsite terms to onsite_terms.

continues on next page
<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>add_onsite_term(strength, ...)</code></td>
<td>Add an onsite term on a given MPS site.</td>
</tr>
<tr>
<td><code>all_coupling_terms()</code></td>
<td>Sum of all coupling_terms.</td>
</tr>
<tr>
<td><code>all_onsite_terms()</code></td>
<td>Sum of all onsite_terms.</td>
</tr>
<tr>
<td><code>calc_H_MPO([tol_zero])</code></td>
<td>Calculate MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td><code>calc_H_bond([tol_zero])</code></td>
<td>Calculate $H_{bond}$ from coupling_terms and onsite_terms.</td>
</tr>
<tr>
<td><code>calc_H_onsite([tol_zero])</code></td>
<td>Calculate $H_{onsite}$ from self.onsite_terms.</td>
</tr>
<tr>
<td><code>coupling_strength_add_ext_flux(...)</code></td>
<td>Add an external flux to the coupling strength.</td>
</tr>
<tr>
<td><code>enlarge_mps_unit_cell(...)</code></td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td><code>from_hdf5(hdf5_loader, ...)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>group_sites([n, ...])</code></td>
<td>Modify self in place to group sites.</td>
</tr>
<tr>
<td><code>save_hdf5(hdf5_saver, ...)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
</tbody>
</table>

**class tenpy.models.model.MultiCouplingModel** (lattice, bc_coupling=None, explicit_plus hc=False)

Bases: tenpy.models.model.CouplingModel

Deprecated class which was a generalization of the CouplingModel.

Deprecated since version 0.7.2: In earlier versions of TeNPy, this class contained the methods `add_multi_coupling()` and `add_multi_coupling_term()`. However, since we introduced the MultiCouplingTerms, this separation within the Model class is no longer necessary. We hence merged the MultiCouplingModel with the CouplingModel.

**add_coupling**(strength, ul, op1, u2, op2, dx, op_string=None, str_on_first=True, raise_op2_left=False, category=None, plus_hc=False)

Add two-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form $\sum_{\vec{x}_0, \ldots, \vec{x}_{dim-1}} strength[shift(\vec{x})] \cdot OP0 \cdot OP1$, where $OP0 := \text{lat}.\text{unit_cell}[ul].\text{get_op}(op0)$ acts on the site $(x_0, \ldots, x_{(dim-1)}, ul)$, and $OP1 := \text{lat}.\text{unit_cell}[ul].\text{get_op}(op1)$ acts on the site $(x_0+dx[0], \ldots, x_{(dim-1)}+dx[dim-1], ul)$. Possible combinations $x_0, \ldots, x_{(dim-1)}$ are determined from the boundary conditions in `possible_couplings()`.

The coupling `strength` may vary spatially if the given `strength` is a numpy array. The correct shape of this array is the `coupling_shape` returned by `tenpy.models.lattice.possible_couplings()` and depends on the boundary conditions. The `shift(...)` depends on `dx`, and is chosen such that the first entry `strength[0, 0, ...]` of `strength` is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to `coupling_terms`; this function does not rebuild the MPO.

Deprecated since version 0.4.0: The arguments `str_on_first` and `raise_op2_left` will be removed in version 1.0.0.

**Parameters**

- `strength` (scalar / array) – Prefactor of the coupling. May vary spatially (see above). If an array of smaller size is provided, it gets tiled to the required shape.
• **u1** (*int*) – Picks the site `lat.unit_cell[u1]` for OP1.

• **op1** (*str*) – Valid operator name of an onsite operator in `lat.unit_cell[u1]` for OP1.

• **u2** (*int*) – Picks the site `lat.unit_cell[u2]` for OP2.

• **op2** (*str*) – Valid operator name of an onsite operator in `lat.unit_cell[u2]` for OP2.

• **dx** (*iterable of int*) – Translation vector (of the unit cell) between OP1 and OP2. For a 1D lattice, a single int is also fine.

• **op_string** (*str | None*) – Name of an operator to be used between the OP1 and OP2 sites. Typical use case is the phase for a Jordan-Wigner transformation. The operator should be defined on all sites in the unit cell. If None, auto-determine whether a Jordan-Wigner string is needed, using `op_needs_JW()`.

• **str_on_first** (*bool*) – Whether the provided `op_string` should also act on the first site. This option should be chosen as `True` for Jordan-Wigner strings. When handling Jordan-Wigner strings we need to extend the `op_string` to also act on the ‘left’, first site (in the sense of the MPS ordering of the sites given by the lattice). In this case, there is a well-defined ordering of the operators in the physical sense (i.e. which of `op1` or `op2` acts first on a given state). We follow the convention that `op2` acts first (in the physical sense), independent of the MPS ordering. Deprecated.

• **raise_op2_left** (*bool*) – Raise an error when `op2` appears left of `op1` (in the sense of the MPS ordering given by the lattice). Deprecated.

• **category** (*str*) – Descriptive name used as key for `coupling_terms`. Defaults to a string of the form `{op1}_i {op2}_j`.

• **plus hc** (*bool*) – If `True`, the hermitian conjugate of the terms is added automatically.

### Examples

When initializing a model, you can add a term $J \sum_{<i,j>} S^z_i S^z_j$ on all nearest-neighbor bonds of the lattice like this:

```python
>>> J = 1.0  # the strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(J, u1, 'Sz', u2, 'Sz', dx)
```

The strength can be an array, which gets tiled to the correct shape. For example, in a 1D *Chain* with an even number of sites and periodic (or infinite) boundary conditions, you can add alternating strong and weak couplings with a line like:

```python
>>> self.add_coupling([1.5, 1.0], u1, 'Sz', u2, 'Sz', dx)
```

Make sure to use the **plus hc** argument if necessary, e.g. for hoppings:

```python
>>> t = 1.0  # hopping strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```

Alternatively, you can add the hermitian conjugate terms explicitly. The correct way is to complex conjugate the strength, take the hermitian conjugate of the operators and swap the order (including a swap `u1 <-> u2`), and use the opposite direction `-dx`, i.e. the `h.c.` of `add_coupling(t, u1, 'A', u2, 'B', dx)` is `add_coupling(np.conj(t), u2, 'hc('B'), u1, 'hc('A), -dx)`, where
hc takes the hermitian conjugate of the operator names, see get_hc_op_name(). For spin-less fermions (FermionSite), this would be

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx)
...     self.add_coupling(np.conj(t), u2, 'Cd', u1, 'C', -dx)  # h.c.
```

With spin-full fermions (SpinHalfFermions), it could be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cdu', u2, 'Cd', dx)  # Cdagger_up C_down
...     self.add_coupling(np.conj(t), u2, 'Cdd', u1, 'Cu', -dx)  # h.c._

→ C dagger_down C up
```

Note that the Jordan-Wigner strings for the fermions are added automatically!

See also:

- **add_onsite** Add terms acting on one site only.
- **add_multi_coupling_term** for terms on more than two sites.
- **add_coupling_term** Add a single term without summing over vecx.

**add_coupling_term** *(strength, i, j, op_j, op_string='Id', category=None, plus_hc=False)*

Add a two-site coupling term on given MPS sites.

Wrapper for self.coupling_terms[category].add_coupling_term(...).

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use add_local_term() instead.

**Parameters**

- **strength** *(float)* – The strength of the coupling term.
- **i** *(int)* – The MPS indices of the two sites on which the operator acts. We require 0 <= i < N_sites and i < j, i.e., op_i acts “left” of op_j. If j >= N_sites, it indicates couplings between unit cells of an infinite MPS.
- **j** *(int)* – The MPS indices of the two sites on which the operator acts. We require 0 <= i < N_sites and i < j, i.e., op_i acts “left” of op_j. If j >= N_sites, it indicates couplings between unit cells of an infinite MPS.
- **op1** *(str)* – Names of the involved operators.
- **op2** *(str)* – Names of the involved operators.
- **op_string** *(str)* – The operator to be inserted between i and j.
- **category** *(str)* – Descriptive name used as key for coupling_terms. Defaults to a string of the form "{op1}_i {op2}_j".
- **plus_hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.
add_exponentially_decaying_coupling(strength, lambda_, op_i, op_j, subsites=None, op_string=None, plus_hc=False)

Add an exponentially decaying long-range coupling.

\[
\text{strength} \sum_{i<j} \lambda^{i-j} A_{\text{subsites}[i]} B_{\text{subsites}[j]}
\]

Where the operator \( A \) is given by \( op_i \), and \( B \) is given by \( op_j \). Note that the sum over \( i,j \) is long-range, for infinite systems going beyond the MPS unit cell. Moreover, note that the distance in the exponent is the distance within \( \text{subsites} \).

Parameters

- **strength** (float) – Overall prefactor.
- **lambda** (float) – Decay-rate.
- **op_i** (string) – Names for the operators.
- **op_j** (string) – Names for the operators.
- **subsites** (None | 1D array) – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. None selects all sites.
- **op_string** (None | str) – The operator to be inserted between \( A \) and \( B \); If None, this function checks whether a fermionic "JW" string is needed for the given operators; in this case the right \( op_j \) acts first.
- **plus_hc** (bool) – If True, the hermitian conjugate of the term is added automatically.

Examples

At least for simple enough 1D chains (or ladders), you can use \code{fit_with_sum_of_exp()} to approximate a long-range function with a few sum of exponentials and then add them with this function.

```python
>>> def decay(x):
...     return np.exp(-0.1*x) / x**2
... from tenpy.tools.fit import fit_with_sum_of_exp, sum_of_exp
... n_exp = 5
... fit_range = 50
... lam, pref = fit_with_sum_of_exp(decay, n_exp, fit_range)
... x = np.arange(1, fit_range + 1)
... print('error in fit: {0:.3e}'.format(np.sum(np.abs(decay(x) - sum_of_exp(lam, pref, x)))))
error in fit: 1.073e-04
>>> for pr, la in zip(pref, lam):
...     self.add_exponentially_decaying_coupling(pr, la, 'N', 'N')
```

add_local_term(strength, term, category=None, plus_hc=False)

Add a single term to \code{self}.

The represented term is \( \text{strength} \) times the product of the operators given in \code{terms}. Each operator is specified by the name and the site it acts on; the latter given by a lattice index, see \code{Lattice}.

Depending on the length of \code{term}, it can add an onsite term or a coupling term to \code{onsite_terms} or \code{coupling_terms}, respectively.

Parameters

- **strength** (float/complex) – The prefactor of the term.
• **term** *(list of \((str, array_like)\)) – List of tuples \((opname, lat_idx)\) where \(opname\) is a string describing the operator acting on the site given by the lattice index \(lat_idx\). Here, \(lat_idx\) is for example \([x, y, u]\) for a 2D lattice, with \(u\) being the index within the unit cell.

• **category** – Descriptive name used as key for `onsite_terms` or `coupling_terms`.

• **plus_hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

### add_multi_coupling *(strength, ops, _deprecate_1=’DEPRECATED’, _deprecate_2=’DEPRECATED’, op_string=None, category=None, plus_hc=False)*

Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \(\sum_{\vec{x}} strength[\text{shift}(\vec{x})] \cdot OP_0 \cdot OP_1 \cdot \ldots \cdot OP_{M-1}\), involving \(M\) operators. Here, \(OP_m\) stands for the operator defined by the \(m\)-th tuple \((opname, dx, u)\) given in the argument \(ops\), which determines the position \(\vec{x} + \vec{dx}\) and unit-cell index \(u\) of the site it acts on; the actual operator is given by \(self.lat.unit_cell[u].get_op(opname)\).

The coupling \(strength\) may vary spatially if the given \(strength\) is a numpy array. The correct shape of this array is the `coupling_shape` returned by \(tenpy.models.lattice.possible_multi_couplings()\) and depends on the boundary conditions. The \(\text{shift}(\ldots)\) depends on the \(dx\) entries of \(ops\) and is chosen such that the first entry \(strength[0, 0, \ldots]\) of \(strength\) is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to `coupling_terms`; this function does not rebuild the MPO.

Deprecated since version 0.6.0: We switched from the three arguments \(u0, op0\) and \(other_op\) with \(other_ops=\[(u1, op1, dx1), (op2, u2, dx2), \ldots\]\) to a single, equivalent argument \(ops\) which should now read \(ops=\[(op0, dx0, u0), (op1, dx1, u1), (op2, dx2, u2), \ldots\]\), where \(dx0 = [0] \ast self.lat.dim\). Note the changed order inside the tuples!

#### Parameters

• **strength** *(scalar | array)* – Prefactor of the coupling. May vary spatially, and is tiled to the required shape.

• **ops** *(list of \((opname, dx, u)\)) – Each tuple determines one operator of the coupling, see the description above. \(opname\) *(str)* is the name of the operator, \(dx\) *(list of length \(lat.dim)\)* is a translation vector, and \(u\) *(int)* is the index of \(lat.unit_cell\) on which the operator acts. The first entry of \(ops\) corresponds to \(OP_0\) and acts last in the physical sense.

• **op_string** *(str | None)* – If a string is given, we use this as the name of an operator to be used inbetween the operators, excluding the sites on which any operators act. This operator should be defined on all sites in the unit cell.

If \(None\), auto-determine whether a Jordan-Wigner string is needed (using \(op_needs_JW()\)) for each of the segments inbetween the operators and also on the sites of the left operators.

• **category** *(str)* – Descriptive name used as key for `coupling_terms`. Defaults to a string of the form "\(\{op0\}_i \{other_ops[0]\}_j \{other_ops[1]\}_k \ldots\)".

• **plus_hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

### Examples

A call to `add_coupling()` with arguments `add_coupling(strength, u1, 'A', u2, 'B', dx)` is equivalent to the following:
dx_0 = [0] * self.lat.dim  # = {0} for a 1D lattice, {0, 0} in 2D
self.add_multi_coupling(strength, [('A', dx_0, u1), ('B', dx, u2)])

To explicitly add the hermitian conjugate (instead of simply using plus_hc = True), you need to take the complex conjugate of the strength, reverse the order of the operators and take the hermitian conjugates of the individual operator names (indicated by the hc(...), see get_hc_op_name()):

self.add_multi_coupling(np.conj(strength), [(hc('B'), dx, u2), (hc('A'), dx_0, u1)])

See also:

- **add_onsite** Add terms acting on one site only.
- **add_coupling** Add terms acting on two sites.
- **add_multi_coupling_term** Add a single term, not summing over the possible $\vec{x}$.

**add_multi_coupling_term** *(strength, i j k l, ops_i j k l, op_string=None, category=None, plus_hc=None)*

Add a general M-site coupling term on given MPS sites.

Wrapper for self.coupling_terms[category].add_multi_coupling_term(...).

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use add_local_term() instead.

**Parameters**

- **strength** *(float)* - The strength of the coupling term.
- **ijkl** *(list of int)* - The MPS indices of the sites on which the operators acts. With $i, j, k, \ldots = i j k l$, we require that they are ordered ascending, $i < j < k < \ldots$ and that $0 \leq i < N_{-}sites$. Indices $>= N_{-}sites$ indicate couplings between different unit cells of an infinite MPS.
- **ops_i j k l** *(list of str)* - Names of the involved operators on sites $i, j, k, \ldots$.
- **op_string** *(list of str)* - Names of the operator to be inserted between the operators, e.g., op_string[0] is inserted between $i$ and $j$.
- **category** *(str)* - Descriptive name used as key for coupling_terms. Defaults to a string of the form "(op0)_i (op1)_j (op2)_k \ldots".
- **plus_hc** *(bool)* - If True, the hermitian conjugate of the term is added automatically.

**add_onsite** *(strength, u, opname, category=None, plus_hc=None)*

Add onsite terms to onsite_terms.

Adds $\sum_{\vec{x}} strength[\vec{x}] \ast OP$ to the represented Hamiltonian, where the operator OP=lat.unit_cell[u].get_op(opname) acts on the site given by a lattice index $(x_0, \ldots, x_{(dim-1)}, u)$.

The necessary terms are just added to onsite_terms; doesn’t rebuild the MPO.

**Parameters**

- **strength** *(scalar | array)* - Prefactor of the onsite term. May vary spatially. If an array of smaller size is provided, it gets tiled to the required shape.
• \(u(int)\) – Picks aSite \(lat.unit_cell[u]\) out of the unit cell.
• \(opname(str)\) – valid operator name of an onsite operator in \(lat.unit_cell[u]\).
• \(category(str)\) – Descriptive name used as key for \(onsite_terms\). Defaults to \(opname\).
• \(plus_hc(bool)\) – If True, the hermitian conjugate of the terms is added automatically.

See also:

- \texttt{add_coupling} Add a terms acting on two sites.
- \texttt{add_onsite_term} Add a single term without summing over \(vecx\).

\textbf{add_onsite_term}(strength, i, op, category=None, plus_hc=False)

Add an onsite term on a given MPS site.

Wrapper for \(self.onsite_terms[category].add_onsite_term(...\).

Parameters

• \texttt{strength(float)} – The strength of the term.
• \texttt{i(int)} – The MPS index of the site on which the operator acts. We require \(0 \leq i < L\).
• \texttt{op(str)} – Name of the involved operator.
• \texttt{category(str)} – Descriptive name used as key for \(onsite_terms\). Defaults to \(op\).
• \texttt{plus_hc(bool)} – If True, the hermitian conjugate of the term is added automatically.

\textbf{all_coupling_terms}()
Sum of all \(coupling_terms\).

\textbf{all_onsite_terms}()
Sum of all \(onsite_terms\).

\textbf{calc_H_MPO}(tol_zero=1e-15)

Calculate MPO representation of the Hamiltonian.

Uses \(onsite_terms\) and \(coupling_terms\) to build an MPOGraph (and then an MPO).

Parameters \texttt{tol_zero(float)} – Prefactors with \(abs(strength) < tol_zero\) are considered to be zero.

Returns \(H\_MPO\) – MPO representation of the Hamiltonian.

Return type \(MPO\)

\textbf{calc_H_bond}(tol_zero=1e-15)

calculate \(H\_bond\) from \(coupling_terms\) and \(onsite_terms\).

Parameters \texttt{tol_zero(float)} – prefactors with \(abs(strength) < tol_zero\) are considered to be zero.

Returns \(H\_bond\) – Bond terms as required by the constructor of \texttt{NearestNeighborModel}. Legs are ['p0', 'p0*', 'p1', 'p1*']

Return type list of \texttt{Array}

:raises ValueError : if the Hamiltonian contains longer-range terms.
calc_H_onsite (tol_zero=1e-15)
Calculate $H_{on site}$ from self.onsite_terms.

Deprecated since version 0.4.0: This function will be removed in 1.0.0. Replace calls to this function by self.all_onsite_terms().remove_zeros(tol_zero).to_Arrays(self.lat.mps_sites()). You might also want to take explicit_plus_hc into account.

**Parameters**

- **tol_zero** *(float)* - prefactors with abs(strength) < tol_zero are considered to be zero.

**Returns**

- **H_onsite** *(list of npc.Array)*
- onsite terms of the Hamiltonian. If explicit_plus_hc is True, – Hermitian conjugates of the onsite terms will be included.

coupling_strength_add_ext_flux (strength, dx, phase)
Add an external flux to the coupling strength.

When performing DMRG on a “cylinder” geometry, it might be useful to put an “external flux” through the cylinder. This means that a particle hopping around the cylinder should pick up a phase given by the external flux [resta1998]. This is also called “twisted boundary conditions” in literature. This function adds a complex phase to the strength array on some bonds, such that particles hopping in positive direction around the cylinder pick up exp($+i \phi$).

**Warning:** For the sign of phase it is important that you consistently use the creation operator as $op1$ and the annihilation operator as $op2$ in add_coupling().

**Parameters**

- **strength** *(scalar | array)* - The strength to be used in add_coupling(), when no external flux would be present.
- **dx** *(iterable of int)* - Translation vector (of the unit cell) between $op1$ and $op2$ in add_coupling().
- **phase** *(iterable of float)* - The phase of the external flux for hopping in each direction of the lattice. E.g., if you want flux through the cylinder on which you have an infinite MPS, you should give phase=[0, phi] such that particles pick up a phase $\phi$ when hopping around the cylinder.

**Returns**

- **strength** - The strength array to be used as strength in add_coupling() with the given dx.

**Return type** complex array

**Examples**

Let’s say you have an infinite MPS on a cylinder, and want to add nearest-neighbor hopping of fermions with the FermionSite. The cylinder axis is the x-direction of the lattice, so to put a flux through the cylinder, you want particles hopping around the cylinder to pick up a phase $\phi$ given by the external flux.

```python
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0, phi])
```
(continues on next page)
.. self.add_coupling(strength_with_flux, u1, 'Cd', u2, 'C', dx)

.. self.add_coupling(np.conj(strength_with_flux), u2, 'Cd', u1, 'C', -dx)

**enlarge_mps_unit_cell**(factor=2)
Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and can not be reverted.

**Parameters**

- **factor** *(int)* – The new number of sites in the MPS unit cell will be increased from \(N_{\text{sites}}\) to \(\text{factor} \times N_{\text{sites\_per\_ring}}\). Since MPS unit cells are repeated in the \(x\)-direction in our convention, the lattice shape goes from \((L_x, L_y, \ldots, L_u)\) to \((L_x \times \text{factor}, L_y, \ldots, L_u)\).

**classmethod from_hdf5**(hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

**Parameters**

- **hdf5_loader** *(Hdf5Loader)* – Instance of the loading engine.
- **h5gr** *(Group)* – HDF5 group which is represent the object to be constructed.
- **subpath** *(str)* – The name of h5gr with a '/ ' in the end.

**Returns**

- **obj** – Newly generated class instance containing the required data.

**Return type**

- **cls**

**group_sites**(n=2, grouped_sites=None)
Modify self in place to group sites.

Group each \(n\) sites together using the `GroupedSite`. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and can not be reverted.

**Parameters**

- **n** *(int)* – Number of sites to be grouped together.
- **grouped_sites** *(None | list of GroupedSite)* – The sites grouped together.

**Returns**

- **grouped_sites** – The sites grouped together.

**Return type**

- **list of GroupedSite**

**save_hdf5**(hdf5_saver, h5gr, subpath)
Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with `from_hdf5()`.

This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute 'format'.

**Parameters**

- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.
- **h5gr** *(:class`Group`)* – HDF5 group which is supposed to represent self.
- **subpath** *(str)* – The name of h5gr with a '/ ' in the end.
test_sanity()
Sanity check, raises ValueErrors, if something is wrong.

NearestNeighborModel

- full name: tenpy.models.model.NearestNeighborModel
- parent module: tenpy.models.model
- type: class

Inheritance Diagram

Methods

NearestNeighborModel.__init__(lattice, H_bond) Initialize self.

NearestNeighborModel.bond_energies(psi) Calculate bond energies \langle \psi | H_{bond} | \psi \rangle .

NearestNeighborModel.calc_H_MPO_from_bond(…) Calculate the MPO Hamiltonian from the bond Hamiltonian.

NearestNeighborModel.enlarge_mps_unit_cell(…) Repeat the unit cell for infinite MPS boundary conditions; in place.

NearestNeighborModel.from_MPOModel(mpo_model) Initialize a NearestNeighborModel from a model class defining an MPO.

NearestNeighborModel.from_hdf5(hdf5_loader, …) Load instance from a HDF5 file.

NearestNeighborModel.group_sites([n, …]) Modify self in place to group sites.

NearestNeighborModel.save_hdf5(hdf5_saver, …) Export self into a HDF5 file.

NearestNeighborModel.test_sanity() continues on next page
NearestNeighborModel.

trivial_like_NNModel()

Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

class tenpy.models.model.NearestNeighborModel(lattice, H_bond)

    Bases: tenpy.models.model.Model

    Base class for a model of nearest neigbor interactions w.r.t. the MPS index.

    In this class, the Hamiltonian \( H = \sum_i H_{i,i+1} \) is represented by "bond terms" \( H_{i,i+1} \) acting only on two neighboring sites \( i \) and \( i+1 \), where \( i \) is an integer. Instances of this class are suitable for tebd.

    Note that the “nearest-neighbor” in the name refers to the MPS index, not the lattice. In short, this works only for 1-dimensional (1D) nearest-neighbor models: A 2D lattice is internally mapped to a 1D MPS “snake”, and even a nearest-neighbor coupling in 2D becomes long-range in the MPS chain.

    Parameters

    - **lattice** (tenpy.model.lattice.Lattice) -- The lattice defining the geometry and the local Hilbert space(s).

    - **H_bond** (list of {Array | None}) -- The Hamiltonian rewritten as \( \sum_i H_{\text{bond}[i]} \) for MPS indices \( i \). \( H_{\text{bond}[i]} \) acts on sites \( (i-1, i) \); we require \( \text{len}(H_{\text{bond}}) == \text{lat.N_sites} \). Legs of each \( H_{\text{bond}[i]} \) are \[ \{'p0', 'p0*', 'p1', 'p1*'\} \].

    - **H_bond** (list of {Array | None}) -- The Hamiltonian rewritten as \( \sum_i H_{\text{bond}[i]} \) for MPS indices \( i \). \( H_{\text{bond}[i]} \) acts on sites \( (i-1, i) \). None represents 0. Legs of each \( H_{\text{bond}[i]} \) are \[ \{'p0', 'p0*', 'p1', 'p1*'\} \]. \( H_{\text{bond}} \) is not affected by the \text{explicit_plus_hc} flag of a CouplingModel.

    Type list of {Array | None}

    classmethod from_MPOModel(mpo_model)

    Initialize a NearestNeighborModel from a model class defining an MPO.

    This is especially usefull in combination with MPOModel.group_sites().

    Parameters **mpo_model** (MPOModel) -- A model instance implementing the MPO. Does not need to be a NearestNeighborModel, but should only have nearest-neighbor couplings.

    Examples

    The SpinChainNNN2 has next-nearest-neighbor couplings and thus only implements an MPO:

    >>> from tenpy.models.spins_nnn import SpinChainNNN2
    >>> nnn_chain = SpinChainNNN2({'L': 20, 'verbose': 0})
    >>> print(isinstance(nnn_chain, NearestNeighborModel))
    False
    >>> print("range before grouping:", nnn_chain.H_MPO.max_range)
    range before grouping: 2

    By grouping each two neighboring sites, we can bring it down to nearest neighbors.

    >>> grouped_sites = nnn_chain.group_sites(2)
    >>> print("range after grouping:", nnn_chain.H_MPO.max_range)
    range after grouping: 1

    Yet, TEBD will not yet work, as the model doesn’t define \( H_{\text{bond}} \). However, we can initialize a Nearest-NeighborModel from the MPO:
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
>>> isinstance(nnn_chain_for_tebd, NearestNeighborModel)
True

trivial_like_NNModel()
Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

bond_energies(psi)
Calculate bond energies $\langle \psi|H_bond|\psi\rangle$.

Parameters
psi (MPS) -- The MPS for which the bond energies should be calculated.

Returns E_bond -- List of bond energies: for finite bc, $E_{Bond}[i]$ is the energy of bond $i$, $i+1$. (i.e. we omit bond 0 between sites L-1 and 0); for infinite bc $E_{bond}[i]$ is the energy of bond $i-1$, $i$.

Return type 1D ndarray

enlarge_mps_unit_cell(factor=2)
Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and can not be reverted.

Parameters
factor (int) -- The new number of sites in the MPS unit cell will be increased from $N_{sites}$ to $factor \times N_{sites\_per\_ring}$. Since MPS unit cells are repeated in the $x$-direction in our convention, the lattice shape goes from $(L_x, L_y, ..., L_u)$ to $(L_x \times factor, L_y, ..., L_u)$.

group_sites(n=2, grouped_sites=None)
Modify self in place to group sites.

Group each $n$ sites together using the GroupedSite. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and can not be reverted.

Parameters
• n (int) -- Number of sites to be grouped together.
• grouped_sites (None | list of GroupedSite) -- The sites grouped together.

Returns grouped_sites -- The sites grouped together.

Return type list of GroupedSite

calc_H_MPO_from_bond(tol_zero=1e-15)
Calculate the MPO Hamiltonian from the bond Hamiltonian.

Parameters
tol_zero (float) -- Arrays with norm < tol_zero are considered to be zero.

Returns H_MPO -- MPO representation of the Hamiltonian.

Return type MPO

classmethod from_hdf5(hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

Parameters
• hdf5_loader (Hdf5Loader) -- Instance of the loading engine.
• h5gr (Group) -- HDF5 group which is represent the object to be constructed.
• **subpath** *(str)* – The *name* of `h5gr` with a '/' in the end.

**Returns**  `obj` – Newly generated class instance containing the required data.

**Return type**  `cls`

**save_hdf5** *(hdf5_saver, h5gr, subpath)*

Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute 'format'.

**Parameters**

• **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.

• **h5gr** *(class:`Group`)* – HDF5 group which is supposed to represent `self`.

• **subpath** *(str)* – The *name* of `h5gr` with a '/' in the end.

**Module description**

This module contains some base classes for models.

A ‘model’ is supposed to represent a Hamiltonian in a generalized way. The `Lattice` specifies the geometry and underlying Hilbert space, and is thus common to all models. It is needed to initialize the common base class `Model` of all models.

Different algorithms require different representations of the Hamiltonian. For example for DMRG, the Hamiltonian needs to be given as an MPO, while TEBD needs the Hamiltonian to be represented by ‘nearest neighbor’ bond terms. This module contains the base classes defining these possible representations, namely the `MPOModel` and `NearestNeighborModel`.

A particular model like the `XXZChain` should then yet another class derived from these classes. In it’s `__init__`, it needs to explicitly call the `MPOModel.__init__(self, lattice, H_MPO)`, providing an MPO representation of `H`, and also the `NearestNeighborModel.__init__(self, lattice, H_bond)`, providing a representation of `H` by bond terms `H_bond`.

The `CouplingModel` is the attempt to generalize the representation of `H` by explicitly specifying the couplings in a general way, and providing functionality for converting them into `H_MPO` and `H_bond`. This allows to quickly generate new model classes for a very broad class of Hamiltonians.

The `CouplingMPOModel` aims at structuring the initialization for most models and is used as base class in (most of) the predefined models in TeNPy.

See also the introduction in *Models*.

**Specific models**

<table>
<thead>
<tr>
<th>Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>tf_ising</code></td>
<td>Prototypical example of a quantum model: the transverse field Ising model.</td>
</tr>
<tr>
<td><code>xxz_chain</code></td>
<td>Prototypical example of a 1D quantum model: the spin-1/2 XXZ chain.</td>
</tr>
<tr>
<td><code>spins</code></td>
<td>Nearest-neighbour spin-S models.</td>
</tr>
<tr>
<td><code>spins_nnn</code></td>
<td>Next-Nearest-neighbour spin-S models.</td>
</tr>
<tr>
<td><code>fermions_spinless</code></td>
<td>Spinless fermions with hopping and interaction.</td>
</tr>
</tbody>
</table>

continues on next page
Table 103 – continued from previous page

<table>
<thead>
<tr>
<th>Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>hubbard</td>
<td>Bosonic and fermionic Hubbard models.</td>
</tr>
<tr>
<td>hofstadter</td>
<td>Cold atomic (Harper-)Hofstadter model on a strip or cylinder.</td>
</tr>
<tr>
<td>haldane</td>
<td>Bosonic and fermionic Haldane models.</td>
</tr>
<tr>
<td>toric_code</td>
<td>Kitaev’s exactly solvable toric code model.</td>
</tr>
</tbody>
</table>

7.11.3 tf_ising

- full name: tenpy.models.tf_ising
- parent module: tenpy.models
- type: module

Classes

```
Hdf5Exportable
  Model
    CouplingModel
    MPOModel
      CouplingMPOModel
      NearestNeighborModel
        TFIModel
          TFIChain
```

<table>
<thead>
<tr>
<th>TFIChain(model_params)</th>
<th>The TFIModel on a Chain, suitable for TEBD.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TFIModel(model_params)</td>
<td>Transverse field Ising model on a general lattice.</td>
</tr>
</tbody>
</table>
TFIChain

- full name: tenpy.models.tf_ising.TFIChain
- parent module: tenpy.models.tf_ising
- type: class

Inheritance Diagram

![Inheritance Diagram]

Methods

<table>
<thead>
<tr>
<th>Method Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>TFIChain.<strong>init</strong> (model_params)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>TFIChain.add_coupling(strength, u1, op1, u2, ...)</td>
<td>Add two site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>TFIChain.add_coupling_term(strength, i, j, ...)</td>
<td>Add a two-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>TFIChain.add_exponentially_decaying_coupling(...)</td>
<td>Add an exponentially decaying long-range coupling.</td>
</tr>
<tr>
<td>Method</td>
<td>Description</td>
</tr>
<tr>
<td>------------------------------------------------------------------------</td>
<td>-------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>TFIChain.add_local_term(strength, term[,])</td>
<td>Add a single term to self.</td>
</tr>
<tr>
<td>TFIChain.add_multi_coupling(strength, ops[,])</td>
<td>Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>TFIChain.add_multi_coupling_term(strength, ...)</td>
<td>Add a general M-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>TFIChain.add_onsite(strength, u, opname[,])</td>
<td>Add onsite terms to onsite_terms.</td>
</tr>
<tr>
<td>TFIChain.add_onsite_term(strength, i, op[,])</td>
<td>Add an onsite term on a given MPS site.</td>
</tr>
<tr>
<td>TFIChain.all_coupling_terms()</td>
<td>Sum of all coupling_terms.</td>
</tr>
<tr>
<td>TFIChain.all_onsite_terms()</td>
<td>Sum of all onsite_terms.</td>
</tr>
<tr>
<td>TFIChain.bond_energies(psi)</td>
<td>Calculate bond energies &lt;psi</td>
</tr>
<tr>
<td>TFIChain.calc_H_MPO([tol_zero])</td>
<td>Calculate MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td>TFIChain.calc_H_MPO_from_bond([tol_zero])</td>
<td>Calculate the MPO Hamiltonian from the bond Hamiltonian.</td>
</tr>
<tr>
<td>TFIChain.calc_H_onsite([tol_zero])</td>
<td>Calculate H_onsite from self.onsite_terms.</td>
</tr>
<tr>
<td>TFIChain.coupling_strength_add_ext_flux()</td>
<td>Add an external flux to the coupling strength.</td>
</tr>
<tr>
<td>TFIChain.enlarge_mps_unit_cell([factor])</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>TFIChain.from_MPOModel(mpo_model)</td>
<td>Initialize a NearestNeighborModel from a model class defining an MPO.</td>
</tr>
<tr>
<td>TFIChain.from_hdf5(hdf5_loader, h5gr, subpath)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>TFIChain.group_sites(n, grouped_sites)</td>
<td>Modify self in place to group sites.</td>
</tr>
<tr>
<td>TFIChain.init_lattice(model_params)</td>
<td>Initialize a lattice for the given model parameters.</td>
</tr>
<tr>
<td>TFIChain.init_sites(model_params)</td>
<td>Define the local Hilbert space and operators; needs to be implemented in subclasses.</td>
</tr>
<tr>
<td>TFIChain.init_terms(model_params)</td>
<td>Add the onsite and coupling terms to the model; subclasses should implement this.</td>
</tr>
<tr>
<td>TFIChain.save_hdf5(hdf5_saver, h5gr, subpath)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>TFIChain.test_sanity()</td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td>TFIChain.trivial_like_NNModel()</td>
<td>Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.</td>
</tr>
</tbody>
</table>

class tenpy.models.tf_ising.TFIChain(model_params)

    The TFIModel on a Chain, suitable for TEBD.

    See the TFIModel for the documentation of parameters.

    add_coupling(strength, ul, op1, u2, op2, dx, op_string=None, str_on_first=True, raise_op2_left=False, category=None, plus_hc=False)

        Add two-site coupling terms to the Hamiltonian, summing over lattice sites.

        Represents couplings of the form \[ \sum_{x_0, \ldots, x_{dim-1}} \text{strength} [\text{shift}(\vec{x})] * \text{OP0} * \text{OP1}, \] where \text{OP0} := \text{lat}.unit_cell[u0].get_op(op0) acts on the site \( (x_0, \ldots, x_{(dim-1)}, u1) \), and \text{OP1} := \text{lat}.unit_cell[u1].get_op(op1) acts on the site \( (x_0+dx[0], \ldots, x_{(dim-1)}+dx[\text{dim-1}], u1) \). Possible combinations \( x_0, \ldots, x_{(dim-1)} \) are determined from the boundary conditions in possible_couplings().
The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_couplings() and depends on the boundary conditions. The shift(...) depends on dx, and is chosen such that the first entry strength[0, 0, ...] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to coupling_terms; this function does not rebuild the MPO.

Deprecated since version 0.4.0: The arguments str_on_first and raise_op2_left will be removed in version 1.0.0.

Parameters

- **strength** *(scalar / array)* – Prefactor of the coupling. May vary spatially (see above). If an array of smaller size is provided, it gets tiled to the required shape.
- **u1** *(int)* – Picks the site lat.unit_cell[u1] for OP1.
- **op1** *(str)* – Valid operator name of an onsite operator in lat.unit_cell[u1] for OP1.
- **u2** *(int)* – Picks the site lat.unit_cell[u2] for OP2.
- **op2** *(str)* – Valid operator name of an onsite operator in lat.unit_cell[u2] for OP2.
- **dx** *(iterable of int)* – Translation vector (of the unit cell) between OP1 and OP2. For a 1D lattice, a single int is also fine.
- **op_string** *(str / None)* – Name of an operator to be used between the OP1 and OP2 sites. Typical use case is the phase for a Jordan-Wigner transformation. The operator should be defined on all sites in the unit cell. If None, auto-determine whether a Jordan-Wigner string is needed, using op_needs_JW().
- **str_on_first** *(bool)* – Whether the provided op_string should also act on the first site. This option should be chosen as True for Jordan-Wigner strings. When handling Jordan-Wigner strings we need to extend the op_string to also act on the ‘left’, first site (in the sense of the MPS ordering of the sites given by the lattice). In this case, there is a well-defined ordering of the operators in the physical sense (i.e. which of op1 or op2 acts first on a given state). We follow the convention that op2 acts first (in the physical sense), independent of the MPS ordering. Deprecated.
- **raise_op2_left** *(bool)* – Raise an error when op2 appears left of op1 (in the sense of the MPS ordering given by the lattice). Deprecated.
- **category** *(str)* – Descriptive name used as key for coupling_terms. Defaults to a string of the form "(op1)_i (op2)_j".
- **plus_hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

Examples

When initializing a model, you can add a term $J \sum_{<i,j>} S_i^z S_j^z$ on all nearest-neighbor bonds of the lattice like this:

```python
>>> J = 1.  # the strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(J, u1, 'Sz', u2, 'Sz', dx)
```
The strength can be an array, which gets tiled to the correct shape. For example, in a 1D Chain with an even number of sites and periodic (or infinite) boundary conditions, you can add alternating strong and weak couplings with a line like:

```python
>>> self.add_coupling([1.5, 1.], u1, 'Sz', u2, 'Sz', dx)
```

Make sure to use the `plus_hc` argument if necessary, e.g. for hoppings:

```python
>>> t = 1. # hopping strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```

Alternatively, you can add the hermitian conjugate terms explicitly. The correct way is to complex conjugate the strength, take the hermitian conjugate of the operators and swap the order (including a swap `u1 <-> u2`), and use the opposite direction `-dx`, i.e. the h.c. of `add_coupling(t, u1, 'A', u2, 'B', dx)` is `add_coupling(np.conj(t), u2, hc('B'), u1, hc('A'), -dx)`, where `hc` takes the hermitian conjugate of the operator names, see `get_hc_op_name()`. For spin-less fermions (FermionSite), this would be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx)
...     self.add_coupling(np.conj(t), u2, 'Cd', u1, 'C', -dx) # h.c.
```

With spin-full fermions (SpinHalfFermions), it could be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cdu', u2, 'Cd', dx) # Cdagger_up C_down
...     self.add_coupling(np.conj(t), u2, 'Cdd', u1, 'Cu', -dx) # h.c.
```

Note that the Jordan-Wigner strings for the fermions are added automatically!

See also:

- `add_onsite` Add terms acting on one site only.
- `add_multi_coupling_term` for terms on more than two sites.
- `add_coupling_term` Add a single term without summing over `vecx`.

**add_coupling_term** *(strength, i, j, op_i, op_j, op_string='Id', category=None, plus_hc=False)*

Add a two-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_coupling_term(...)`. Wrap around `self.add_coupling_term(...)`. This function does not handle Jordan-Wigner strings! You might want to use `add_local_term()` instead.

**Parameters**

- `strength` *(float)* – The strength of the coupling term.
- `i` *(int)* – The MPS indices of the two sites on which the operator acts. We require `0 <= i < N_sites` and `i < j`, i.e., `op_i` acts “left” of `op_j`. If `j >= N_sites`, it indicates couplings between unit cells of an infinite MPS.
• **j** *(int)* – The MPS indices of the two sites on which the operator acts. We require $0 \leq i < \text{N\_sites}$ and $i < j$, i.e., $\text{op}_i$ acts “left” of $\text{op}_j$. If $j \geq \text{N\_sites}$, it indicates couplings between unit cells of an infinite MPS.

• **op1** *(str)* – Names of the involved operators.

• **op2** *(str)* – Names of the involved operators.

• **op\_string** *(str)* – The operator to be inserted between $i$ and $j$.

• **category** *(str)* – Descriptive name used as key for coupling_terms. Defaults to a string of the form "\(\text{op}_1\)_i \(\text{op}_2\)_j".

• **plus\_hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.

### add\_exponentially\_decaying\_coupling

(strength, lambda\_, op\_i, op\_j, subsites=None, op\_string=None, plus\_hc=False)

Add an exponentially decaying long-range coupling.

$$\text{strength} \sum_{i<j} \lambda^{i-j} A_{\text{subsites}[i]} B_{\text{subsites}[j]}$$

Where the operator $A$ is given by $\text{op}_i$, and $B$ is given by $\text{op}_j$. Note that the sum over $i,j$ is long-range, for infinite systems going beyond the MPS unit cell. Moreover, note that the distance in the exponent is the distance within **subsites**.

**Parameters**

• **strength** *(float)* – Overall prefactor.

• **lambda** *(float)* – Decay-rate

• **op\_i** *(string)* – Names for the operators.

• **op\_j** *(string)* – Names for the operators.

• **subsites** *(None | 1D array)* – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. None selects all sites.

• **op\_string** *(None | str)* – The operator to be inserted between $A$ and $B$; If None, this function checks whether a fermionic "JW" string is needed for the given operators; in this case the right $\text{op}_j$ acts first.

• **plus\_hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.

**Examples**

At least for simple enough 1D chains (or ladders), you can use `fit\_with\_sum\_of\_exp()` to approximate a long-range function with a few sum of exponentials and then add them with this function.

```python
def decay(x):
    ... return np.exp(-0.1*x) / x**2

from tenpy.tools.fit import fit_with_sum_of_exp, sum_of_exp

n_exp = 5
fit_range = 50
lam, pref = fit_with_sum_of_exp(decay, n_exp, fit_range)
x = np.arange(1, fit_range + 1)
print('error in fit: {0:.3e}'.format(np.sum(np.abs(decay(x) - sum_of_exp(lam, pref, x))))))
error in fit: 1.073e-04
for pr, la in zip(pref, lam):
    ... self.add_exponentially_decaying_coupling(pr, la, 'N', 'N')
```
add_local_term(strength, term, category=None, plushc=False)
Add a single term to self.

The represented term is `strength` times the product of the operators given in `term`. Each operator is specified by the name and the site it acts on; the latter given by a lattice index, see `Lattice`.

Depending on the length of `term`, it can add an onsite term or a coupling term to `onsite_terms` or `coupling_terms`, respectively.

Parameters

- **strength** ([float/complex]) – The prefactor of the term.
- **term** ([list of (str, array_like)]) – List of tuples (opname, lat_idx) where `opname` is a string describing the operator acting on the site given by the lattice index `lat_idx`. Here, `lat_idx` is for example `[x, y, u]` for a 2D lattice, with `u` being the index within the unit cell.
- **category** – Descriptive name used as key for `onsite_terms` or `coupling_terms`.
- **plushc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

add_multi_coupling(strength, ops, _deprecate_1='DEPRECATED', _deprecate_2='DEPRECATED', op_string=None, category=None, plushc=False)
Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \( \sum_x \text{strength}[\text{shift}(\vec{x})] \cdot O_{P_0} \cdot O_{P_1} \cdot \ldots \cdot O_{P_{M-1}} \), involving \( M \) operators. Here, \( O_{P_m} \) stands for the operator defined by the \( m \)-th tuple \((\text{opname}, \text{dx}, u)\) given in the argument `ops`, which determines the position \( \vec{x} + \vec{dx} \) and unit-cell index \( u \) of the site it acts on; the actual operator is given by `self.lat.unit_cell[u].get_op(opname)`.

The coupling `strength` may vary spatially if the given `strength` is a numpy array. The correct shape of this array is the `coupling_shape` returned by `tenpy.models.lattice.possible_multi_couplings()` and depends on the boundary conditions. The `shift(...)` depends on the `dx` entries of `ops` and is chosen such that the first entry `strength[0, 0, \ldots]` of `strength` is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to `coupling_terms`; this function does not rebuild the MPO.

Deprecated since version 0.6.0: We switched from the three arguments \( u_0, \text{op0} \) and `other_op` with `other_ops`=[\( (u_1, \text{op1}, \text{dx1}), (\text{op2}, u_2, \text{dx2}), \ldots) \)] to a single, equivalent argument `ops` which should now read `ops`=[\( (\text{op0}, \text{dx0}, u_0), (\text{op1}, \text{dx1}, u_1), (\text{op2}, \text{dx2}, u_2), \ldots) \)], where `dx0 = [0]*self.lat.dim`. Note the changed order inside the tuples!

Parameters

- **strength** ([scalar | array]) – Prefactor of the coupling. May vary spatially, and is tiled to the required shape.
- **ops** ([list of (opname, dx, u)]) – Each tuple determines one operator of the coupling, see the description above. `opname` (str) is the name of the operator, `dx` (list of length `lat.dim`) is a translation vector, and `u` (int) is the index of `lat.unit_cell` on which the operator acts. The first entry of `ops` corresponds to `OP_0` and acts last in the physical sense.
- **op_string** (str | None) – If a string is given, we use this as the name of an operator to be used inbetween the operators, **excluding** the sites on which any operators act. This operator should be defined on all sites in the unit cell.
If None, auto-determine whether a Jordan-Wigner string is needed (using op_needs_JW()) for each of the segments inbetween the operators and also on the sites of the left operators.

- **category** *(str)* – Descriptive name used as key for coupling_terms. Defaults to a string of the form "{op0}_i {other_ops[0]}_j {other_ops[1]}_k ...".

- **plus_hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

### Examples

A call to add_coupling() with arguments add_coupling(strength, u1, 'A', u2, 'B', dx) is equivalent to the following:

```python
def add_multi_coupling(strength, ops_ijkl, op_string, category=None, plus_hc=False):
    # ... (implementation)
```

To explicitly add the hermitian conjugate (instead of simply using plus_hc = True), you need to take the complex conjugate of the strength, reverse the order of the operators and take the hermitian conjugates of the individual operator names (indicated by the hc(...), see get_hc_op_name()):

```python
def add_multi_coupling(np.conj(strength), (hc('B'), dx, u2), (hc('A'), dx_0, u1))
```

---

**See also:**

- **add_onsite** Add terms acting on one site only.
- **add_coupling** Add terms acting on two sites.
- **add_multi_coupling_term** Add a single term, not summing over the possible ĭ.

### add_multi_coupling_term *(strength, ijk, ops_ijk, op_string, category=None, plus_hc=False)*

Add a general M-site coupling term on given MPS sites.

Wrapper for self.coupling_terms[category].add_multi_coupling_term(...).

---

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use add_local_term() instead.

### Parameters

- **strength** *(float)* – The strength of the coupling term.

- **ijkl** *(list of int)* – The MPS indices of the sites on which the operators acts. With i, j, k, ... = ijk, we require that they are ordered ascending, i < j < k < ... and that 0 <= i < N_sites. Inidces >= N_sites indicate couplings between different unit cells of an infinite MPS.

- **ops_ijk** *(list of str)* – Names of the involved operators on sites i, j, k,....

- **op_string** *(list of str)* – Names of the operator to be inserted between the operators, e.g., op_string[0] is inserted between i and j.

- **category** *(str)* – Descriptive name used as key for coupling_terms. Defaults to a string of the form "{op0}_i {op1}_j {op2}_k ...".

- **plus_hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.
add_onsite (strength, u, opname, category=None, plus_hc=False)
Add onsite terms to onsite_terms.

Adds $\sum_x strength[x] \cdot OP$ to the represented Hamiltonian, where the operator OP=lat.unit_cell[u].get_op(opname) acts on the site given by a lattice index ($x_0, \ldots, x_{(dim-1)}$, u).

The necessary terms are just added to onsite_terms; doesn’t rebuild the MPO.

Parameters

- **strength** *(scalar / array)* – Prefactor of the onsite term. May vary spatially. If an array of smaller size is provided, it gets tiled to the required shape.
- **u** *(int)* – Picks a Site lat.unit_cell[u] out of the unit cell.
- **opname** *(str)* – valid operator name of an onsite operator in lat.unit_cell[u].
- **category** *(str)* – Descriptive name used as key for onsite_terms. Defaults to opname.
- **plus_hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

See also:

add_coupling Add a terms acting on two sites.
add_onsite_term Add a single term without summing over vecx.

add_onsite_term (strength, i, op, category=None, plus_hc=False)
Add an onsite term on a given MPS site.

Wrapper for self.onsite_terms[category].add_onsite_term(...).

Parameters

- **strength** *(float)* – The strength of the term.
- **i** *(int)* – The MPS index of the site on which the operator acts. We require $0 \leq i < L$.
- **op** *(str)* – Name of the involved operator.
- **category** *(str)* – Descriptive name used as key for onsite_terms. Defaults to op.
- **plus_hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.

all_coupling_terms ()
Sum of all coupling_terms.

all_onsite_terms ()
Sum of all onsite_terms.

bond_energies (psi)
Calculate bond energies $\langle \psi | H_{\text{bond}} | \psi \rangle$.

Parameters psi *(MPS)* – The MPS for which the bond energies should be calculated.

Returns E_bond – List of bond energies: for finite bc, $E_{\text{Bond}}[i]$ is the energy of bond $i$, $i+1$. (i.e. we omit bond 0 between sites L-1 and 0); for infinite bc $E_{\text{Bond}}[i]$ is the energy of bond $i-1$, $i$.

Return type 1D ndarray
calc_H_MPO \( (\text{tol}_\text{zero}=1e^{-15}) \)
Calculate MPO representation of the Hamiltonian.

Uses onsite_terms and coupling_terms to build an MPOGraph (and then an MPO).

Parameters
\begin{itemize}
  \item \textbf{tol\_zero} (\textit{float}) – Prefactors with \( \text{abs(strength)} < \text{tol\_zero} \) are considered to be zero.
\end{itemize}

Returns
\begin{itemize}
  \item \textbf{H\_MPO} – MPO representation of the Hamiltonian.
\end{itemize}

Return type
\textit{MPO}

\begin{itemize}
\end{itemize}

calc_H_MPO\_from\_bond \( (\text{tol}_\text{zero}=1e^{-15}) \)
Calculate the MPO Hamiltonian from the bond Hamiltonian.

Parameters
\begin{itemize}
  \item \textbf{tol\_zero} (\textit{float}) – Arrays with norm < \text{tol\_zero} are considered to be zero.
\end{itemize}

Returns
\begin{itemize}
  \item \textbf{H\_MPO} – MPO representation of the Hamiltonian.
\end{itemize}

Return type
\textit{MPO}

\begin{itemize}
\end{itemize}

calc_H\_bond \( (\text{tol}_\text{zero}=1e^{-15}) \)
calculate \( H\_bond \) from coupling_terms and onsite_terms.

Parameters
\begin{itemize}
  \item \textbf{tol\_zero} (\textit{float}) – prefactors with \( \text{abs(strength)} < \text{tol\_zero} \) are considered to be zero.
\end{itemize}

Returns
\begin{itemize}
  \item \textbf{H\_bond} – Bond terms as required by the constructor of NearestNeighborModel.
    Legs are \['\text{p0}', '\text{p0}^\ast', '\text{p1}', '\text{p1}^\ast']\]
\end{itemize}

Return type
\textit{list of Array}

:raises \text{ValueError} : if the Hamiltonian contains longer-range terms.

\begin{itemize}
\end{itemize}

calc_H\_bond\_from\_MPO \( (\text{tol}_\text{zero}=1e^{-15}) \)
Calculate the bond Hamiltonian from the MPO Hamiltonian.

Parameters
\begin{itemize}
  \item \textbf{tol\_zero} (\textit{float}) – Arrays with norm < \text{tol\_zero} are considered to be zero.
\end{itemize}

Returns
\begin{itemize}
  \item \textbf{H\_bond} – Bond terms as required by the constructor of NearestNeighborModel.
    Legs are \['\text{p0}', '\text{p0}^\ast', '\text{p1}', '\text{p1}^\ast']\]
\end{itemize}

Return type
\textit{list of Array}

:raises \text{ValueError} : if the Hamiltonian contains longer-range terms.

\begin{itemize}
\end{itemize}

calc_H\_onsite \( (\text{tol}_\text{zero}=1e^{-15}) \)
Calculate \( H\_onsite \) from \( self.\text{onsite\_terms} \).

Deprecated since version 0.4.0: This function will be removed in 1.0.0. Replace calls to this function by \( \text{self.all\_onsite\_terms()}\).\text{remove\_zeros(tol\_zero)}\).\text{to\_Arrays}(\text{self.\_lat.mps\_sites()}). You might also want to take explicit\_plus\_hc into account.

Parameters
\begin{itemize}
  \item \textbf{tol\_zero} (\textit{float}) – prefactors with \( \text{abs(strength)} < \text{tol\_zero} \) are considered to be zero.
\end{itemize}

Returns
\begin{itemize}
  \item \textbf{H\_onsite} \( (\text{list of npc.Array}) \)
    onsite terms of the Hamiltonian. If explicit\_plus\_hc is True, – Hermitian conjugates of the onsite terms will be included.
\end{itemize}

\begin{itemize}
\end{itemize}

coupling\_strength\_add\_ext\_flux \( (\text{strength, dx, phase}) \)
Add an external flux to the coupling strength.
When performing DMRG on a “cylinder” geometry, it might be useful to put an “external flux” through the cylinder. This means that a particle hopping around the cylinder should pick up a phase given by the external flux [resta1998]. This is also called “twisted boundary conditions” in literature. This function adds a complex phase to the strength array on some bonds, such that particles hopping in positive direction around the cylinder pick up $exp(+i \text{phase})$.

**Warning:** For the sign of phase it is important that you consistently use the creation operator as op1 and the annihilation operator as op2 in add_coupling().

**Parameters**

- **strength** (*scalar | array*) – The strength to be used in add_coupling(), when no external flux would be present.
- **dx** (*iterable of int*) – Translation vector (of the unit cell) between op1 and op2 in add_coupling().
- **phase** (*iterable of float*) – The phase of the external flux for hopping in each direction of the lattice. E.g., if you want flux through the cylinder on which you have an infinite MPS, you should give phase=[0, phi] such that particles pick up a phase phi when hopping around the cylinder.

**Returns** strength – The strength array to be used as strength in add_coupling() with the given dx.

**Return type** complex array

**Examples**

Let’s say you have an infinite MPS on a cylinder, and want to add nearest-neighbor hopping of fermions with the FermionSite. The cylinder axis is the x-direction of the lattice, so to put a flux through the cylinder, you want particles hopping around the cylinder to pick up a phase phi given by the external flux.

```python
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0, phi])
...    self.add_coupling(strength_with_flux, u1, 'Cd', u2, 'C', dx)
...    self.add_coupling(np.conj(strength_with_flux), u2, 'Cd', u1, 'C', -dx)
```

**enlarge_mps_unit_cell** (*factor=2*)

Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and can not be reverted.

**Parameters** factor (*int*) – The new number of sites in the MPS unit cell will be increased from N_sites to factor*N_sites_per_ring. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from (Lx, Ly, ..., Lu) to (Lx*factor, Ly, ..., Lu).

**classmethod from_MPOModel** (*mpo_model*)

Initialize a NearestNeighborModel from a model class defining an MPO.

This is especially usefull in combination with MPOModel.group_sites().
**Parameters**

Parameters `mpo_model` (MPOModel) – A model instance implementing the MPO. Does not need to be a NearestNeighborModel, but should only have nearest-neighbor couplings.

**Examples**

The SpinChainNNN2 has next-nearest-neighbor couplings and thus only implements an MPO:

```python
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20, 'verbose': 0})
>>> print(isinstance(nnn_chain, NearestNeighborModel))
False
>>> print("range before grouping:", nnn_chain.H_MPO.max_range)
range before grouping: 2
```

By grouping each two neighboring sites, we can bring it down to nearest neighbors.

```python
>>> grouped_sites = nnn_chain.group_sites(2)
>>> print("range after grouping:", nnn_chain.H_MPO.max_range)
range after grouping: 1
```

Yet, TEBD will not yet work, as the model doesn’t define $H_{\text{bond}}$. However, we can initialize a NearestNeighborModel from the MPO:

```python
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
>>> isinstance(nnn_chain_for_tebd, NearestNeighborModel)
True
```

**classmethod** `from_hdf5`(hdf5_loader, h5gr, subpath)

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

Parameters

- `hdf5_loader` (Hdf5Loader) – Instance of the loading engine.
- `h5gr` (Group) – HDF5 group which is represent the object to be constructed.
- `subpath` (str) – The name of `h5gr` with a `'/` in the end.

Returns `obj` – Newly generated class instance containing the required data.

Return type `cls`

**group_sites** (n=2, grouped_sites=None)

Modify `self` in place to group sites.

Group each $n$ sites together using the GroupedSite. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and can not be reverted.

Parameters

- `n` (int) – Number of sites to be grouped together.
- `grouped_sites` (None | list of GroupedSite) – The sites grouped together.

Returns `grouped_sites` – The sites grouped together.

Return type list of GroupedSite
**init_lattice** (*model_params*)

Initialize a lattice for the given model parameters.

This function reads out the model parameter *lattice*. This can be a full *Lattice* instance, in which case it is just returned without further action. Alternatively, the *lattice* parameter can be a string giving the name of one of the predefined lattices, which then gets initialized. Depending on the dimensionality of the lattice, this requires different model parameters.

**Parameters**

- **model_params** (*dict*) – The model parameters given to *__init____.

**Returns**

- **lat** – An initialized lattice.

**Return type**

*Lattice*

**Options**

- **option** *CouplingMPOModel.lattice: str | Lattice*
  
  The name of a lattice pre-defined in TeNPy to be initialized. Alternatively, a (possibly self-defined) Lattice instance. In the latter case, no further parameters are read out.

- **option** *CouplingMPOModel.bc_MPS: str*
  
  Boundary conditions for the MPS.

- **option** *CouplingMPOModel.order: str*
  
  The order of sites within the lattice for non-trivial lattices, e.g., 'default', 'snake', see *ordering()*.

  Only used if *lattice* is a string.

- **option** *CouplingMPOModel.L: int*
  
  The length in x-direction; only read out for 1D lattices. For an infinite system the length of the unit cell.

- **option** *CouplingMPOModel.Lx: int*

  **option** *CouplingMPOModel.Ly: int*
  
  The length in x- and y-direction; only read out for 2D lattices. For "infinite" *bc_MPS*, the system is infinite in x-direction and \( L_x \) is the number of "rings" in the infinite MPS unit cell, while \( Ly \) gives the circumference around the cylinder or width of th the rung for a ladder (depending on *bc_y*).

- **option** *CouplingMPOModel.bc_y: str*
  
  "cylinder" | "ladder"; only read out for 2D lattices. The boundary conditions in y-direction.

- **option** *CouplingMPOModel.bc_x: str*
  
  "open" | "periodic". Can be used to force “periodic” boundaries for the lattice, i.e., for the couplings in the Hamiltonian, even if the MPS is finite. Defaults to "open" for bc_MPS="finite" and "periodic" for bc_MPS="infinite". If you are not aware of the consequences, you should probably not use “periodic” boundary conditions. (The MPS is still “open”, so this will introduce long-range couplings between the first and last sites of the MPS!)

**init_sites** (*model_params*)

Define the local Hilbert space and operators; needs to be implemented in subclasses.

This function gets called by *init_lattice()* to get the *Site* for the lattice unit cell.

**Note:** Initializing the sites requires to define the conserved quantum numbers. All pre-defined sites accept *conserve=None* to disable using quantum numbers. Many models in TeNPy read out the *conserve* model parameter, which can be set to "best" to indicate the optimal parameters.

If you need to initialize more than one site, the function *tenpy.networks.site.set_common_charges()* should be helpful.
Parameters `model_params (dict) – The model parameters given to __init__.

Returns `sites – The local sites of the lattice, defining the local basis states and operators.

Return type (tuple of) `Site

`init_terms (model_params)
Add the onsite and coupling terms to the model; subclasses should implement this.

`save_hdf5 (hdf5_saver, h5gr, subpath)
Export `self into a HDF5 file.

This method saves all the data it needs to reconstruct `self with `from_hdf5()

This implementation saves the content of `__dict__ with `save_dict_content(), storing the format under the attribute 'format'.

Parameters

• `hdf5_saver (Hdf5Saver) – Instance of the saving engine.
• `h5gr (:class:`Group`) – HDF5 group which is supposed to represent `self.
• `subpath (str) – The name of `h5gr with a ' / ' in the end.

`test_sanity ()
Sanity check, raises ValueErrors, if something is wrong.

`trivial_like_NNModel ()
Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

Module description

Prototypical example of a quantum model: the transverse field Ising model.

Like the `XXZChain, the transverse field ising chain `TFIChain is contained in the more general `SpinChain; the idea is more to serve as a pedagogical example for a 'model'.

We choose the field along z to allow to conserve the parity, if desired.

7.11.4 `xxz_chain

• full name: tenpy.models.xxz_chain
• parent module: `tenpy.models
• type: module
Classes

**XXZChain**(model_params)  Spin-1/2 XXZ chain with Sz conservation.

**XXZChain2**(model_params)  Another implementation of the Spin-1/2 XXZ chain with Sz conservation.

**XXZChain2**

- full name: tenpy.models.xxz_chain.XXZChain2
- parent module: tenpy.models.xxz_chain
- type: class
Inheritance Diagram

Methods

\texttt{XXZChain2.__init__}(model\_params) \quad Initialize self.

\texttt{XXZChain2.add\_coupling}(strength, u1, \ldots) \quad Add two site coupling terms to the Hamiltonian, summing over lattice sites.

\texttt{XXZChain2.add\_coupling\_term}(strength, i, j, \ldots) \quad Add a two site coupling term on given MPS sites.

\texttt{XXZChain2.add\_exponentially\_decaying\_coupling}(\ldots) \quad Add an exponentially decaying long-range coupling.

\texttt{XXZChain2.add\_local\_term}(strength, term[, \ldots]) \quad Add a single term to \texttt{self}.

\texttt{XXZChain2.add\_multi\_coupling}(strength, ops) \quad Add multi site coupling terms to the Hamiltonian, summing over lattice sites.

\texttt{XXZChain2.add\_multi\_coupling\_term}(strength, Add a general M site coupling term on given MPS sites.

\texttt{XXZChain2.add\_onsite}(strength, u, \texttt{opname}[, \texttt{\ldots}]) \quad Add onsite terms to \texttt{onsite\_terms}.

\texttt{XXZChain2.add\_onsite\_term}(strength, i, \texttt{op[, \texttt{\ldots}]) \quad Add an onsite term on a given MPS site.

\texttt{XXZChain2.all\_coupling\_terms}() \quad Sum of all \texttt{coupling\_terms}.

\texttt{XXZChain2.all\_onsite\_terms}() \quad Sum of all \texttt{onsite\_terms}.

\texttt{XXZChain2.bond\_energies}(\psi) \quad Calculate bond energies \langle\psi\vert H\vert\psi\rangle.

continues on next page

7.11. models
Table 107 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>XXZChain2.calc_H_MPO([tol_zero])</code></td>
<td>Calculate MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td><code>XXZChain2.calc_H_MPO_from_bond([tol_zero])</code></td>
<td>Calculate the MPO Hamiltonian from the bond Hamiltonian.</td>
</tr>
<tr>
<td><code>XXZChain2.calc_H_bond([tol_zero])</code></td>
<td>Calculate ( H_{\text{bond}} ) from ( \text{coupling_terms} ) and ( \text{onsite_terms} ).</td>
</tr>
<tr>
<td><code>XXZChain2.calc_H_bond_from_MPO([tol_zero])</code></td>
<td>Calculate the bond Hamiltonian from the MPO Hamiltonian.</td>
</tr>
<tr>
<td><code>XXZChain2.calc_H_onsite([tol_zero])</code></td>
<td>Calculate ( H_{\text{onsite}} ) from ( \text{self.onsite_terms} ).</td>
</tr>
<tr>
<td><code>XXZChain2.coupling_strength_add_ext_flux</code></td>
<td>Add an external flux to the coupling strength.</td>
</tr>
<tr>
<td><code>XXZChain2.enlarge_mps_unit_cell([factor])</code></td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td><code>XXZChain2.from_MPOModel(mpo_model)</code></td>
<td>Initialize a NearestNeighborModel from a model class defining an MPO.</td>
</tr>
<tr>
<td><code>XXZChain2.from_hdf5(hdf5_loader, h5gr, sub-path)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>XXZChain2.group_sites([n, grouped_sites])</code></td>
<td>Modify ( \text{self} ) in place to group sites.</td>
</tr>
<tr>
<td><code>XXZChain2.init_lattice(model_params)</code></td>
<td>Initialize a lattice for the given model parameters.</td>
</tr>
<tr>
<td><code>XXZChain2.init_sites(model_params)</code></td>
<td>Define the local Hilbert space and operators; needs to be implemented in subclasses.</td>
</tr>
<tr>
<td><code>XXZChain2.init_terms(model_params)</code></td>
<td>Add the onsite and coupling terms to the model; subclasses should implement this.</td>
</tr>
<tr>
<td><code>XXZChain2.save_hdf5(hdf5_saver, h5gr, sub-path)</code></td>
<td>Export ( \text{self} ) into a HDF5 file.</td>
</tr>
<tr>
<td><code>XXZChain2.test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td><code>XXZChain2.trivial_like_NNModel()</code></td>
<td>Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.</td>
</tr>
</tbody>
</table>

class tenpy.models.xxz_chain.XXZChain2(model_params)

Another implementation of the Spin-1/2 XXZ chain with Sz conservation.

This implementation takes the same parameters as the `XXZChain`, but is implemented based on the CouplingMPOModel.

Parameters model_params (dict | Config) – See `XXZChain`

init_sites (model_params)
Define the local Hilbert space and operators; needs to be implemented in subclasses.

This function gets called by `init_lattice()` to get the Site for the lattice unit cell.

Note: Initializing the sites requires to define the conserved quantum numbers. All pre-defined sites accept conserve=None to disable using quantum numbers. Many models in TeNPy read out the conserve model parameter, which can be set to "best" to indicate the optimal parameters.

If you need to initialize more than one site, the function tenpy.networks.site.set_common_charges() should be helpful.

Parameters model_params (dict) – The model parameters given to __init__.

Returns sites – The local sites of the lattice, defining the local basis states and operators.

Return type (tuple of) Site
\texttt{init}\_\texttt{terms}(\texttt{model}\_\texttt{params})

Add the onsite and coupling terms to the model; subclasses should implement this.

\texttt{add}\_\texttt{coupling}(\texttt{strength}, \texttt{u1}, \texttt{op1}, \texttt{u2}, \texttt{op2}, \texttt{dx}, \texttt{op_string=\texttt{None}}, \texttt{str\_on\_first=\texttt{True}}, \texttt{raise_op2\_left=\texttt{False}}, \texttt{category=\texttt{None}}, \texttt{plus_hc=\texttt{False}})

Add twosite coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \( \sum_{x_0, \ldots, x_{\text{dim}-1}} \text{strength}[\text{shift}(\vec{x})] \ast \text{OP0} \ast \text{OP1} \), where \( \text{OP0} := \text{lat.unit}\_\text{cell}[\text{u0}].\text{get}\_\text{op}(\text{op0}) \) acts on the site \( (x_0, \ldots, x_{(\text{dim}-1)}, \text{u1}) \), and \( \text{OP1} := \text{lat.unit}\_\text{cell}[\text{u1}].\text{get}\_\text{op}(\text{op1}) \) acts on the site \( (x_0 + \text{dx}[0], \ldots, x_{(\text{dim}-1)} + \text{dx}[\text{dim}-1], \text{u1}) \). Possible combinations \( x_0, \ldots, x_{(\text{dim}-1)} \) are determined from the boundary conditions in \texttt{possible}\_\texttt{couplings}().

The coupling \texttt{strength} may vary spatially if the given \texttt{strength} is a numpy array. The correct shape of this array is the \texttt{coupling}\_\texttt{shape} returned by \texttt{tenpy.models.lattice.possible}\_\texttt{couplings}() and depends on the boundary conditions. The \texttt{shift}(\ldots) depends on \texttt{dx}, and is chosen such that the first entry \texttt{strength}[0, 0, \ldots] of \texttt{strength} is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to \texttt{coupling}\_\texttt{terms}; this function does not rebuild the MPO.

Deprecated since version 0.4.0: The arguments \texttt{str\_on\_first} and \texttt{raise_op2\_left} will be removed in version 1.0.0.

Parameters

- **\texttt{strength}** (\texttt{scalar} | \texttt{array}) – Prefactor of the coupling. May vary spatially (see above). If an array of smaller size is provided, it gets tiled to the required shape.
- **\texttt{u1}** (\texttt{int}) – Picks the site \texttt{lat.unit}\_\texttt{cell}[\texttt{u1}] for \texttt{OP1}.
- **\texttt{op1}** (\texttt{str}) – Valid operator name of an onsite operator in \texttt{lat.unit}\_\texttt{cell}[\texttt{u1}] for \texttt{OP1}.
- **\texttt{u2}** (\texttt{int}) – Picks the site \texttt{lat.unit}\_\texttt{cell}[\texttt{u2}] for \texttt{OP2}.
- **\texttt{op2}** (\texttt{str}) – Valid operator name of an onsite operator in \texttt{lat.unit}\_\texttt{cell}[\texttt{u2}] for \texttt{OP2}.
- **\texttt{dx}** (\texttt{iterable of int}) – Translation vector (of the unit cell) between \texttt{OP1} and \texttt{OP2}. For a 1D lattice, a single int is also fine.
- **\texttt{op_string}** (\texttt{str} | \texttt{None}) – Name of an operator to be used between the \texttt{OP1} and \texttt{OP2} sites. Typical use case is the phase for a Jordan-Wigner transformation. The operator should be defined on all sites in the unit cell. If \texttt{None}, auto-determine whether a Jordan-Wigner string is needed, using \texttt{op_needs_JW}().
- **\texttt{str\_on\_first}** (\texttt{bool}) – Whether the provided \texttt{op_string} should also act on the first site. This option should be chosen as \texttt{True} for Jordan-Wigner strings. When handling Jordan-Wigner strings we need to extend the \texttt{op_string} to also act on the ‘left’ first site (in the sense of the MPS ordering of the sites given by the lattice). In this case, there is a well-defined ordering of the operators in the physical sense (i.e. which of \texttt{op1} or \texttt{op2} acts first on a given state). We follow the convention that \texttt{op2} acts first (in the physical sense), independent of the MPS ordering. Deprecated.
- **\texttt{raise_op2\_left}** (\texttt{bool}) – Raise an error when \texttt{op2} appears left of \texttt{op1} (in the sense of the MPS ordering given by the lattice). Deprecated.
- **\texttt{category}** (\texttt{str}) – Descriptive name used as key for \texttt{coupling}\_\texttt{terms}. Defaults to a string of the form "\texttt{\{op1\}_i \{op2\}_j}".
- **\texttt{plus_hc}** (\texttt{bool}) – If \texttt{True}, the hermitian conjugate of the terms is added automatically.
Examples

When initializing a model, you can add a term \( J \sum_{<i,j>} S_i^z S_j^z \) on all nearest-neighbor bonds of the lattice like this:

```python
>>> J = 1. # the strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(J, u1, 'Sz', u2, 'Sz', dx)
```

The strength can be an array, which gets tiled to the correct shape. For example, in a 1D Chain with an even number of sites and periodic (or infinite) boundary conditions, you can add alternating strong and weak couplings with a line like:

```python
>>> self.add_coupling([1.5, 1.], u1, 'Sz', u2, 'Sz', dx)
```

Make sure to use the `plus_hc` argument if necessary, e.g. for hoppings:

```python
>>> t = 1. # hopping strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(t, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```

Alternatively, you can add the hermitian conjugate terms explicitly. The correct way is to complex conjugate the strength, take the hermitian conjugate of the operators and swap the order (including a swap \( u1 <-> u2 \)), and use the opposite direction \(-dx\), i.e. the \( h.c.\) of `add_coupling(t, u1, 'A', u2, 'B', dx)` is `add_coupling(np.conj(t), u2, hc('B'), u1, hc('A'), -dx)`, where \( hc \) takes the hermitian conjugate of the operator names, see `get_hc_op_name()`. For spin-less fermions (`FermionSite`), this would be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(t, u1, 'Cd', u2, 'C', dx)
...    self.add_coupling(np.conj(t), u2, 'Cd', u1, 'C', -dx) # h.c.
```

With spin-full fermions (`SpinHalfFermions`), it could be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(t, u1, 'Cdu', u2, 'Cd', dx) # Cdagger_up C_down
...    self.add_coupling(np.conj(t), u2, 'Cdd', u1, 'Cu', -dx) # h.c.
```

Note that the Jordan-Wigner strings for the fermions are added automatically!

See also:

`add_onsite` Add terms acting on one site only.

`add_multi_coupling_term` for terms on more than two sites.

`add_coupling_term` Add a single term without summing over \( vecx \).

`add_coupling_term`  

```
add_coupling_term(strength, i, j, op_i, op_j, op_string='Id', category=None, plus_hc=False)  
Add a two-site coupling term on given MPS sites.
Wrapper for self.coupling_terms[category].add_coupling_term(...).
```
Warning: This function does not handle Jordan-Wigner strings! You might want to use `add_local_term()` instead.

Parameters

- **strength (float)** – The strength of the coupling term.
- **i (int)** – The MPS indices of the two sites on which the operator acts. We require \(0 \leq i < N\_sites\) and \(i < j\), i.e., \(op\_i\) acts “left” of \(op\_j\). If \(j \geq N\_sites\), it indicates couplings between unit cells of an infinite MPS.
- **j (int)** – The MPS indices of the two sites on which the operator acts. We require \(0 \leq i < N\_sites\) and \(i < j\), i.e., \(op\_i\) acts “left” of \(op\_j\). If \(j \geq N\_sites\), it indicates couplings between unit cells of an infinite MPS.
- **op1 (str)** – Names of the involved operators.
- **op2 (str)** – Names of the involved operators.
- **op\_string (str)** – The operator to be inserted between \(i\) and \(j\).
- **category (str)** – Descriptive name used as key for coupling_terms. Defaults to a string of the form \("{op1}\_i {op2}\_j\"\).
- **plus_hc (bool)** – If True, the hermitian conjugate of the term is added automatically.

```python
add_exponentially_decaying_coupling(strength, lambda_, op_i, op_j, subsites=None, op\_string=None, plus_hc=False)
```

Add an exponentially decaying long-range coupling.

\[
\text{strength} \sum_{i < j} \lambda^{i-j} A_{\text{subsites}[i]} B_{\text{subsites}[j]}
\]

Where the operator \(A\) is given by \(\text{op}\_i\), and \(B\) is given by \(\text{op}\_j\). Note that the sum over \(ij\) is long-range, for infinite systems going beyond the MPS unit cell. Moreover, note that the distance in the exponent is the distance within \(\text{subsites}\).

Parameters

- **strength (float)** – Overall prefactor.
- **lambda (float)** – Decay-rate
- **op\_i (string)** – Names for the operators.
- **op\_j (string)** – Names for the operators.
- **subsites (None / 1D array)** – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. None selects all sites.
- **op\_string (None / str)** – The operator to be inserted between \(A\) and \(B\). If None, this function checks whether a fermionic "JW" string is needed for the given operators; in this case the right \(\text{op}\_j\) acts first.
- **plus_hc (bool)** – If True, the hermitian conjugate of the term is added automatically.

Examples

At least for simple enough 1D chains (or ladders), you can use `fit_with_sum_of_exp()` to approximate a long-range function with a few sum of exponentials and then add them with this function.
```python
>>> def decay(x):
...     return np.exp(-0.1*x) / x**2
>>> from tenpy.tools.fit import fit_with_sum_of_exp, sum_of_exp
>>> n_exp = 5
>>> fit_range = 50
>>> lam, pref = fit_with_sum_of_exp(decay, n_exp, fit_range)
>>> x = np.arange(1, fit_range + 1)
>>> print('error in fit: {0:.3e}'.format(np.sum(np.abs(decay(x) - sum_of_exp(lam, pref, x)))))
error in fit: 1.073e-04
>>> for pr, la in zip(pref, lam):
...     self.add_exponentially_decaying_coupling(pr, la, 'N', 'N')
```

```python
add_local_term(strength, term, category=None, plus_hc=False)
```

Add a single term to `self`. The represented term is `strength` times the product of the operators given in `term`. Each operator is specified by the name and the site it acts on; the latter given by a lattice index, see `Lattice`

Depending on the length of `term`, it can add an onsite term or a coupling term to `onsite_terms` or `coupling_terms`, respectively.

Parameters

- **strength** *(float/complex)* - The prefactor of the term.
- **term** *(list of (str, array_like))* - List of tuples `(opname, lat_idx)` where `opname` is a string describing the operator acting on the site given by the lattice index `lat_idx`. Here, `lat_idx` is for example `[x, y, u]` for a 2D lattice, with `u` being the index within the unit cell.
- **category** - Descriptive name used as key for `onsite_terms` or `coupling_terms`.
- **plus_hc** *(bool)* - If `True`, the hermitian conjugate of the terms is added automatically.

```python
add_multi_coupling(strength, ops, _deprecate_1='DEPRECATED', _deprecate_2='DEPRECATED', op_string=None, category=None, plus_hc=False)
```

Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form sum_{i} strength[shift](x) * O_{P0} * O_{P1} * ... * O_{PM-1}, involving M operators. Here, O_{Pm} stands for the operator defined by the m-th tuple `(opname, dx, u)` given in the argument `ops`, which determines the position \vec{x} + \vec{dx} and unit-cell index `u` of the site it acts on; the actual operator is given by `self.lat.unit_cell[u].get_op(opname)`.

The coupling `strength` may vary spatially if the given `strength` is a numpy array. The correct shape of this array is the `coupling_shape` returned by `tenpy.models.lattice.possible_multi_couplings()` and depends on the boundary conditions. The `shift(...)` depends on the `dx` entries of `ops` and is chosen such that the first entry `strength[0, 0, ...]` of `strength` is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to `coupling_terms`; this function does not rebuild the MPO.

Deprecated since version 0.6.0: We switched from the three arguments `u0`, `op0` and `other_op` with `other_ops`=[(u1, op1, dx1), (op2, u2, dx2), ...] to a single, equivalent argument `ops` which should now read `ops`=[(op0, dx0, u0), (op1, dx1, u1), (op2, dx2, u2), ...], where `dx0` = [0]*self.lat.dim. Note the changed order inside the tuples!

Parameters
• **strength** (*scalar | array*) – Prefactor of the coupling. May vary spatially, and is
tiled to the required shape.

• **ops** (list of (opname, dx, u)) – Each tuple determines one operator of the coupling,
see the description above. opname (str) is the name of the operator, dx (list of length
lat.dim) is a translation vector, and u (int) is the index of lat.unit_cell on which the operator
acts. The first entry of ops corresponds to OP0 and acts last in the physical sense.

• **op_string** (str | None) – If a string is given, we use this as the name of an operator
to be used inbetween the operators, excluding the sites on which any operators act. This
operator should be defined on all sites in the unit cell.

  If None, auto-determine whether a Jordan-Wigner string is needed (using
  op_needs_JW()) for each of the segments inbetween the operators and also on
  the sites of the left operators.

• **category** (str) – Descriptive name used as key for coupling_terms. Defaults to a
string of the form "\{op0\}_i \{other_ops[0]\}_j \{other_ops[1]\}_k ...".

• **plus_hc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

### Examples

A call to `add_coupling()` with arguments `add_coupling(strength, u1, 'A', u2,
'B', dx)` is equivalent to the following:

```python
>>> dx_0 = [0] * self.lat.dim  # = [0] for a 1D lattice, [0, 0] in 2D
>>> self.add_multi_coupling(strength, [('A', dx_0, u1), ('B', dx, u2)])
```

To explicitly add the hermitian conjugate (instead of simply using `plus_hc = True`), you need to take the
complex conjugate of the strength, reverse the order of the operators and take the hermitian conjugates of
the individual operator names (indicated by the `hc(...), see `get_hc_op_name()`):

```python
>>> self.add_multi_coupling(np.conj(strength), [(hc('B'), dx, u2), (hc('A'),
 → dx_0, u1)])
```

### See also:

- **add_onsite** Add terms acting on one site only.
- **add_coupling** Add terms acting on two sites.
- **add_multi_coupling_term** Add a single term, not summing over the possible \vec{x}.

### add_multi_coupling_term (strength, ijkld, ops_i, op_string, category=None, plus_hc=False)

Add a general M-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_multi_coupling_term(...)`.

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use
`add_local_term()` instead.

### Parameters

- **strength** (*float*) – The strength of the coupling term.
• \textbf{ijkl} (\textit{list of int}) – The MPS indices of the sites on which the operators acts. With \(i, j, k, \ldots = \text{ijkl}\), we require that they are ordered ascending, \(i < j < k < \ldots\) and that \(0 \leq i < N_{\text{sites}}\). Indices \(>= N_{\text{sites}}\) indicate couplings between different unit cells of an infinite MPS.

• \textbf{ops_ijkl} (\textit{list of str}) – Names of the involved operators on sites \(i, j, k, \ldots\).

• \textbf{op_string} (\textit{list of str}) – Names of the operator to be inserted between the operators, e.g., \texttt{op_string}[0] is inserted between \(i\) and \(j\).

• \textbf{category} (\textit{str}) – Descriptive name used as key for \texttt{coupling_terms}. Defaults to a string of the form "\{op0\}_i \{op1\}_j \{op2\}_k \ldots".

• \textbf{plus_hc} (\textit{bool}) – If \(\text{True}\), the hermitian conjugate of the term is added automatically.

\texttt{add_onsite} (\textit{strength, u, opname, category=None, plus_hc=False})

Add onsite terms to \texttt{onsite_terms}.

Adds \(\sum_{\vec{r}} \text{strength}[\vec{r}] \times \text{OP}\) to the represented Hamiltonian, where the operator \texttt{OP}=\texttt{lat.unit_cell}[u].\texttt{get_op(opname)} acts on the site given by a lattice index \((x_0, \ldots, x_{\text{dim}-1}, u)\).

The necessary terms are just added to \texttt{onsite_terms}; doesn’t rebuild the MPO.

\textbf{Parameters}

• \textbf{strength} (\textit{scalar / array}) – Prefactor of the onsite term. May vary spatially. If an array of smaller size is provided, it gets tiled to the required shape.

• \textbf{u} (\textit{int}) – Picks a Site \texttt{lat.unit_cell}[u] out of the unit cell.

• \textbf{opname} (\textit{str}) – valid operator name of an onsite operator in \texttt{lat.unit_cell}[u].

• \textbf{category} (\textit{str}) – Descriptive name used as key for \texttt{onsite_terms}. Defaults to \texttt{opname}.

• \textbf{plus_hc} (\textit{bool}) – If \(\text{True}\), the hermitian conjugate of the terms is added automatically.

See also:

\texttt{add_coupling} Add a terms acting on two sites.

\texttt{add_onsite_term} Add a single term without summing over \texttt{vecx}.

\texttt{add_onsite_term} (\textit{strength, i, op, category=None, plus_hc=False})

Add an onsite term on a given MPS site.

Wrapper for \texttt{self.onsite_terms[category].add_onsite_term(...)}.

\textbf{Parameters}

• \textbf{strength} (\textit{float}) – The strength of the term.

• \textbf{i} (\textit{int}) – The MPS index of the site on which the operator acts. We require \(0 \leq i < L\).

• \textbf{op} (\textit{str}) – Name of the involved operator.

• \textbf{category} (\textit{str}) – Descriptive name used as key for \texttt{onsite_terms}. Defaults to \texttt{op}.

• \textbf{plus_hc} (\textit{bool}) – If \(\text{True}\), the hermitian conjugate of the term is added automatically.

\texttt{all_coupling_terms}()

Sum of all \texttt{coupling_terms}. 

452 Chapter 7. License
all_onsite_terms()
    Sum of all onsite_terms.

bond_energies(\psi)
    Calculate bond energies \langle \psi | H_{\text{bond}} | \psi \rangle.
    Parameters psi (MPS) – The MPS for which the bond energies should be calculated.
    Returns E_bond – List of bond energies: for finite bc, E_Bond[i] is the energy of bond i, i+1.
    (i.e. we omit bond 0 between sites L-1 and 0); for infinite bc E_bond[i] is the
    energy of bond i-1, i.
    Return type 1D ndarray

calc_H_MPO(tol_zero=1e-15)
    Calculate MPO representation of the Hamiltonian.
    Uses onsite_terms and coupling_terms to build an MPOGraph (and then an MPO).
    Parameters tol_zero (float) – Prefactors with abs(strength) < tol_zero are
    considered to be zero.
    Returns H_MPO – MPO representation of the Hamiltonian.
    Return type MPO

calc_H_MPO_from_bond(tol_zero=1e-15)
    Calculate the MPO Hamiltonian from the bond Hamiltonian.
    Parameters tol_zero (float) – Arrays with norm < tol_zero are considered to be zero.
    Returns H_MPO – MPO representation of the Hamiltonian.
    Return type MPO

calc_H_bond(tol_zero=1e-15)
    calculate $H_{\text{bond}}$ from coupling_terms and onsite_terms.
    Parameters tol_zero (float) – prefactors with abs(strength) < tol_zero are
    considered to be zero.
    Returns H_bond – Bond terms as required by the constructor of NearestNeighborModel.
    Legs are ['p0', 'p0*', 'p1', 'p1*']
    Return type list of Array
:raises ValueError : if the Hamiltonian contains longer-range terms.:  

calc_H_bond_from_MPO(tol_zero=1e-15)
    Calculate the bond Hamiltonian from the MPO Hamiltonian.
    Parameters tol_zero (float) – Arrays with norm < tol_zero are considered to be zero.
    Returns H_bond – Bond terms as required by the constructor of NearestNeighborModel.
    Legs are ['p0', 'p0*', 'p1', 'p1*']
    Return type list of Array
:raises ValueError : if the Hamiltonian contains longer-range terms.:  

calc_H_onsite(tol_zero=1e-15)
    Calculate $H_{\text{onsite}}$ from self.onsite_terms.
    Deprecated since version 0.4.0: This function will be removed in 1.0.0. Replace calls to this
    function by self.all_onsite_terms().remove_zeros(tol_zero).to_Arrays(self.
    lat.mps_sites()). You might also want to take explicit_plus_hc into account.
Parameters **tol_zero** (*float*) – prefactors with \( \text{abs(strength)} < \text{tol_zero} \) are considered to be zero.

Returns

- **H_onsite** (list of `np.ndarray`)
  - onsite terms of the Hamiltonian. If `explicit_plus_hc` is True, – Hermitian conjugates of the onsite terms will be included.

`coupling_strength_add_ext_flux` (**strength**, **dx**, **phase**)

Add an external flux to the coupling strength.

When performing DMRG on a “cylinder” geometry, it might be useful to put an “external flux” through the cylinder. This means that a particle hopping around the cylinder should pick up a phase given by the external flux [resta1998]. This is also called “twisted boundary conditions” in literature. This function adds a complex phase to the `strength` array on some bonds, such that particles hopping in positive direction around the cylinder pick up \( \exp(+i \ \text{phase}) \).

**Warning:** For the sign of `phase` it is important that you consistently use the creation operator as `op1` and the annihilation operator as `op2` in `add_coupling()`.

Parameters

- **strength** (*scalar | array*) – The strength to be used in `add_coupling()`, when no external flux would be present.
- **dx** (*iterable of int*) – Translation vector (of the unit cell) between `op1` and `op2` in `add_coupling()`.
- **phase** (*iterable of float*) – The phase of the external flux for hopping in each direction of the lattice. E.g., if you want flux through the cylinder on which you have an infinite MPS, you should give `phase=[0, phi]` such that particles pick up a phase \( \phi \) when hopping around the cylinder.

Returns **strength** – The strength array to be used as `strength` in `add_coupling()` with the given `dx`.

**Return type** complex array

Examples

Let’s say you have an infinite MPS on a cylinder, and want to add nearest-neighbor hopping of fermions with the `FermionSite`. The cylinder axis is the x-direction of the lattice, so to put a flux through the cylinder, you want particles hopping *around* the cylinder to pick up a phase \( \phi \) given by the external flux.

```python
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0, phi])
...     self.add_coupling(strength_with_flux, u1, 'Cd', u2, 'C', dx)
...     self.add_coupling(np.conj(strength_with_flux), u2, 'Cd', u1, 'C', -dx)
```

`enlarge_mps_unit_cell` (**factor=2**)

Repeat the unit cell for infinite MPS boundary conditions; in place.
This has to be done after finishing initialization and can not be reverted.

**Parameters**

`factor (int)` – The new number of sites in the MPS unit cell will be increased from `N_sites` to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

**classmethod from_MPOModel (mpo_model)**

Initialize a NearestNeighborModel from a model class defining an MPO.

This is especially useful in combination with `MPOModel.group_sites()`.

**Parameters**

`mpo_model (MPOModel)` – A model instance implementing the MPO. Does not need to be a `NearestNeighborModel`, but should only have nearest-neighbor couplings.

**Examples**

The `SpinChainNNN2` has next-nearest-neighbor couplings and thus only implements an MPO:

```python
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20, 'verbose': 0})
>>> print(isinstance(nnn_chain, NearestNeighborModel))
False
>>> print("range before grouping:", nnn_chain.H_MPO.max_range)
range before grouping: 2
```

By grouping each two neighboring sites, we can bring it down to nearest neighbors.

```python
>>> grouped_sites = nnn_chain.group_sites(2)
>>> print("range after grouping:", nnn_chain.H_MPO.max_range)
range after grouping: 1
```

Yet, TEBD will not yet work, as the model doesn’t define `H_bond`. However, we can initialize a Nearest-NeighborModel from the MPO:

```python
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
>>> isinstance(nnn_chain_for_tebd, NearestNeighborModel)
True
```

**classmethod from_hdf5 (hdf5_loader, h5gr, subpath)**

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

**Parameters**

- `hdf5_loader (Hdf5Loader)` – Instance of the loading engine.
- `h5gr (Group)` – HDF5 group which is represent the object to be constructed.
- `subpath (str)` – The name of `h5gr` with a `'/'` in the end.

**Returns**

`obj` – Newly generated class instance containing the required data.

**Return type**

`cls`

**group_sites** (`n=2, grouped_sites=None`)

Modify `self` in place to group sites.

Group each `n` sites together using the `GroupedSite`. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).
This has to be done after finishing initialization and can not be reverted.

**Parameters**

- **n** *(int)* – Number of sites to be grouped together.
- **grouped_sites** *(None | list of GroupedSite)* – The sites grouped together.

**Returns**

- **grouped_sites** – The sites grouped together.

**Return type**

list of GroupedSite

---

**init_lattice** *(model_params)*

Initialize a lattice for the given model parameters.

This function reads out the model parameter *lattice*. This can be a full *Lattice* instance, in which case it is just returned without further action. Alternatively, the *lattice* parameter can be a string giving the name of one of the predefined lattices, which then gets initialized. Depending on the dimensionality of the lattice, this requires different model parameters.

**Parameters**

- **model_params** *(dict)* – The model parameters given to __init__.

**Returns**

- **lat** – An initialized lattice.

**Return type**

*Lattice*

---

**Options**

**option**

`CouplingMPOModel.lattice: str | Lattice`

The name of a lattice pre-defined in TeNPy to be initialized. Alternatively, a (possibly self-defined) Lattice instance. In the latter case, no further parameters are read out.

**option**

`CouplingMPOModel.bc_MPS: str`

Boundary conditions for the MPS.

**option**

`CouplingMPOModel.order: str`

The order of sites within the lattice for non-trivial lattices, e.g., 'default', 'snake', see `ordering()`. Only used if *lattice* is a string.

**option**

`CouplingMPOModel.L: int`

The length in x-direction; only read out for 1D lattices. For an infinite system the length of the unit cell.

**option**

`CouplingMPOModel.Lx: int`

**option**

`CouplingMPOModel.Ly: int`

The length in x- and y-direction; only read out for 2D lattices. For "infinite" *bc_MPS*, the system is infinite in x-direction and *Lx* is the number of "rings" in the infinite MPS unit cell, while *Ly* gives the circumference around the cylinder or width of the rung for a ladder (depending on *bc_y*).

**option**

`CouplingMPOModel.bc_y: str`

"cylinder" | "ladder": only read out for 2D lattices. The boundary conditions in y-direction.

**option**

`CouplingMPOModel.bc_x: str`

"open" | "periodic". Can be used to force "periodic" boundaries for the lattice, i.e., for the couplings in the Hamiltonian, even if the MPS is finite. Defaults to "open" for *bc_MPS="finite" and "periodic" for *bc_MPS="infinite". If you are not aware of the consequences, you should probably not use "periodic" boundary conditions. (The MPS is still "open", so this will introduce long-range couplings between the first and last sites of the MPS!)

**save_hdf5** *(hdf5_saver, h5gr, subpath)*

Export *self* into a HDF5 file.
This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.
This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute `format`.

**Parameters**

- `hdf5_saver (Hdf5Saver)` – Instance of the saving engine.
- `h5gr (:class:`Group`)` – HDF5 group which is supposed to represent `self`.
- `subpath (str)` – The name of `h5gr` with a `/` in the end.

**test_sanity()**
Sanity check, raises ValueErrors, if something is wrong.

**trivial_like_NNModel()**
Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

**Module description**

Prototypical example of a 1D quantum model: the spin-1/2 XXZ chain.
The XXZ chain is contained in the more general `SpinChain`; the idea of this module is more to serve as a pedagogical example for a model.

### 7.11.5 spins

- full name: tenpy.models.spins
- parent module: `tenpy.models`
- type: module
Classes

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpinChain</td>
<td>The SpinModel on a Chain, suitable for TEBD.</td>
</tr>
<tr>
<td>SpinModel</td>
<td>Spin-S sites coupled by nearest neighbour interactions.</td>
</tr>
</tbody>
</table>

**SpinChain**

- full name: `tenpy.models.spins.SpinChain`
- parent module: `tenpy.models.spins`
- type: class
Inheritance Diagram

```
Inheritance Diagram

```

Methods

```
<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpinChain.<strong>init</strong>(model_params)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>SpinChain.add_coupling(strength, u1, op1, ...)</td>
<td>Add two-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>SpinChain.add_coupling_term(strength, i, j, ...)</td>
<td>Add a two-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>SpinChain.add_exponentially_decaying_coupling</td>
<td>Add an exponentially decaying long-range coupling.</td>
</tr>
<tr>
<td>SpinChain.add_local_term(strength, term[, ...])</td>
<td>Add a single term to self.</td>
</tr>
<tr>
<td>SpinChain.add_multi_coupling(strength, ops)</td>
<td>Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>SpinChain.add_multi_coupling_term(strength, ops)</td>
<td>Add a general M-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>SpinChain.add_onsite(strength, u, opname[, ...])</td>
<td>Add on-site terms to on-site_terms.</td>
</tr>
</tbody>
</table>
```

continues on next page
Table 109 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpinChain.add_onsite_term(strength, i, op[, ...])</td>
<td>Add an onsite term on a given MPS site.</td>
</tr>
<tr>
<td>SpinChain.all_coupling_terms()</td>
<td>Sum of all coupling terms.</td>
</tr>
<tr>
<td>SpinChain.all_onsite_terms()</td>
<td>Sum of all onsite terms.</td>
</tr>
<tr>
<td>SpinChain.bond_energies(psi)</td>
<td>Calculate bond energies $\langle psi</td>
</tr>
<tr>
<td>SpinChain.calc_H_MPO([tol_zero])</td>
<td>Calculate MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td>SpinChain.calc_H_MPO_from_bond([tol_zero])</td>
<td>Calculate the MPO Hamiltonian from the bond Hamiltonian.</td>
</tr>
<tr>
<td>SpinChain.calc_H_bond([tol_zero])</td>
<td>Calculate $H_{bond}$ from coupling_terms and onsite_terms.</td>
</tr>
<tr>
<td>SpinChain.calc_H_bond_from_MPO([tol_zero])</td>
<td>Calculate the bond Hamiltonian from the MPO Hamiltonian.</td>
</tr>
<tr>
<td>SpinChain.coupling_strength_add_ext_flux([tol_zero])</td>
<td>Add an external flux to the coupling strength.</td>
</tr>
<tr>
<td>SpinChain.enlarge_mps_unit_cell([factor])</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>SpinChain.from_MPOModel(mpo_model)</td>
<td>Initialize a NearestNeighborModel from a model class defining an MPO.</td>
</tr>
<tr>
<td>SpinChain.from_hdf5(hdf5_loader, h5gr, subpath)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>SpinChain.group_sites([n, grouped_sites])</td>
<td>Modify self in place to group sites.</td>
</tr>
<tr>
<td>SpinChain.init_lattice(model_params)</td>
<td>Initialize a lattice for the given model parameters.</td>
</tr>
<tr>
<td>SpinChain.init_sites(model_params)</td>
<td>Define the local Hilbert space and operators; needs to be implemented in subclasses.</td>
</tr>
<tr>
<td>SpinChain.init_terms(model_params)</td>
<td>Add the onsite and coupling terms to the model; subclasses should implement this.</td>
</tr>
<tr>
<td>SpinChain.save_hdf5(hdf5_saver, h5gr, subpath)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>SpinChain.test_sanity()</td>
<td>Sanity check, raises ValueError, if something is wrong.</td>
</tr>
<tr>
<td>SpinChain.trivial_like_NNModel()</td>
<td>Return a NearestNeighborModel with same lattice, but trivial ($H=0$) bonds.</td>
</tr>
</tbody>
</table>

class tenpy.models.spins.SpinChain(model_params)

The SpinModel on a Chain, suitable for TEBD.

See the SpinModel for the documentation of parameters.

add_coupling(strength, u1, op1, u2, op2, dx, op_string=None, str_on_first=True, raise_op2_left=False, category=None, plus_hc=False)

Add two site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form $\sum_{x_0,\ldots\hat{x}_{dim-1}} strength[shift(\hat{x})] \cdot OP0 \cdot OP1$, where $OP0 := lat.unit_cell[u0].get_op(op0)$ acts on the site $(x_0, \ldots, x_{dim-1}, u1)$, and $OP1 := lat.unit_cell[u1].get_op(op1)$ acts on the site $(x_0+dx[0], \ldots, x_{-(dim-1)}+dx[dim-1], u1)$. Possible combinations $x_0, \ldots, x_{-(dim-1)}$ are determined from the boundary conditions in possible_couplings().

The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_couplings() and depends on the boundary conditions. The shift(...) depends on dx, and is chosen such that the first entry strength[0, 0, ...] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.
The necessary terms are just added to `coupling_terms`; this function does not rebuild the MPO.

Deprecated since version 0.4.0: The arguments `str_on_first` and `raise_op2_left` will be removed in version 1.0.0.

**Parameters**

- **strength** *(scalar|array)* – Prefactor of the coupling. May vary spatially (see above). If an array of smaller size is provided, it gets tiled to the required shape.
- **u1** *(int)* – Picks the site `lat.unit_cell[u1]` for OP1.
- **op1** *(str)* – Valid operator name of an onsite operator in `lat.unit_cell[u1]` for OP1.
- **u2** *(int)* – Picks the site `lat.unit_cell[u2]` for OP2.
- **op2** *(str)* – Valid operator name of an onsite operator in `lat.unit_cell[u2]` for OP2.
- **dx** *(iterable of int)* – Translation vector (of the unit cell) between OP1 and OP2. For a 1D lattice, a single int is also fine.
- **op_string** *(str|None)* – Name of an operator to be used between the OP1 and OP2 sites. Typical use case is the phase for a Jordan-Wigner transformation. The operator should be defined on all sites in the unit cell. If `None`, auto-determine whether a Jordan-Wigner string is needed, using `op_needs_JW()`.
- **str_on_first** *(bool)* – Whether the provided `op_string` should also act on the first site. This option should be chosen as `True` for Jordan-Wigner strings. When handling Jordan-Wigner strings we need to extend the `op_string` to also act on the ‘left’, first site (in the sense of the MPS ordering of the sites given by the lattice). In this case, there is a well-defined ordering of the operators in the physical sense (i.e. which of `op1` or `op2` acts first on a given state). We follow the convention that `op2` acts first (in the physical sense), independent of the MPS ordering. Deprecated.
- **raise_op2_left** *(bool)* – Raise an error when `op2` appears left of `op1` (in the sense of the MPS ordering given by the lattice). Deprecated.
- **category** *(str)* – Descriptive name used as key for `coupling_terms`. Defaults to a string of the form "{op1}_i {op2}_j".
- **plus_hc** *(bool)* – If `True`, the hermitian conjugate of the terms is added automatically.

**Examples**

When initializing a model, you can add a term \( J \sum_{<i,j>} S_i^z S_j^z \) on all nearest-neighbor bonds of the lattice like this:

```python
>>> J = 1.  # the strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(J, u1, 'Sz', u2, 'Sz', dx)
```

The strength can be an array, which gets tiled to the correct shape. For example, in a 1D `Chain` with an even number of sites and periodic (or infinite) boundary conditions, you can add alternating strong and weak couplings with a line like:

```python
>>> self.add_coupling([1.5, 1.], u1, 'Sz', u2, 'Sz', dx)
```

Make sure to use the `plus_hc` argument if necessary, e.g. for hoppings:
t = 1.  # hopping strength

>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx, plus_hc=True)

Alternatively, you can add the hermitian conjugate terms explicitly. The correct way is to complex conjugate the strength, take the hermitian conjugate of the operators and swap the order (including a swap $u1 \leftrightarrow u2$), and use the opposite direction $-dx$, i.e. the h.c. of $\text{add_coupling}(t, u1, 'A', u2, 'B', dx)$ is $\text{add_coupling}(\text{np.conj}(t), u2, \text{hc('B')}, u1, \text{hc('A')}, -dx)$, where $hc$ takes the hermitian conjugate of the operator names, see $\text{get_hc_op_name()}$. For spin-less fermions ($\text{FermionSite}$), this would be

>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(np.conj(t), u2, 'Cd', u1, 'C', -dx)  # h.c.

With spin-full fermions ($\text{SpinHalfFermions}$), it could be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cdu', u2, 'Cd', dx)  # Cdagger_up C_down
...     self.add_coupling(np.conj(t), u2, 'Cdd', u1, 'Cu', -dx)  # h.c.
```

Note that the Jordan-Wigner strings for the fermions are added automatically!

See also:

- **add_onsite** Add terms acting on one site only.
- **add_multi_coupling_term** for terms on more than two sites.
- **add_coupling_term** Add a single term without summing over $\text{vec}_x$

```python
add_coupling_term(strength, i, j, op1, op2, op_string='Id', category=None, plus_hc=False)
```

Add a two-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_coupling_term(...)`. 

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use $\text{add_local_term()}$ instead.

**Parameters**

- **strength** *(float)* – The strength of the coupling term.
- **i** *(int)* – The MPS indices of the two sites on which the operator acts. We require $0 \leq i < N_{\text{sites}}$ and $i < j$, i.e., $op_1$ acts “left” of $op_2$. If $j \geq N_{\text{sites}}$, it indicates couplings between unit cells of an infinite MPS.
- **j** *(int)* – The MPS indices of the two sites on which the operator acts. We require $0 \leq i < N_{\text{sites}}$ and $i < j$, i.e., $op_1$ acts “left” of $op_2$. If $j \geq N_{\text{sites}}$, it indicates couplings between unit cells of an infinite MPS.
- **op1** *(str)* – Names of the involved operators.
- **op2** *(str)* – Names of the involved operators.
- **op_string** *(str)* – The operator to be inserted between $i$ and $j$. 

---

462 Chapter 7. License
• **category** (*str*) – Descriptive name used as key for `coupling_terms`. Defaults to a string of the form "(op1)_i (op2)_j".

• **plus_hc** (*bool*) – If `True`, the hermitian conjugate of the term is added automatically.

### `add_exponentially_decaying_coupling` *(strength, lambda_, op_i, op_j, subsites=None, op_string=None, plus_hc=False)*

Add an exponentially decaying long-range coupling.

\[
\text{strength} \sum_{i<j} \lambda^{-|i-j|} A_{\text{subsites}[i]} B_{\text{subsites}[j]}
\]

Where the operator `A` is given by `op_i`, and `B` is given by `op_j`. Note that the sum over `i,j` is long-range, for infinite systems going beyond the MPS unit cell. Moreover, note that the distance in the exponent is the distance within `subsites`.

**Parameters**

• **strength** (*float*) – Overall prefactor.

• **lambda** (*float*) – Decay-rate

• **op_i** (*string*) – Names for the operators.

• **op_j** (*string*) – Names for the operators.

• **subsites** (*None | 1D array*) – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. `None` selects all sites.

• **op_string** (*None | str*) – The operator to be inserted between `A` and `B`; If `None`, this function checks whether a fermionic "JW" string is needed for the given operators; in this case the right `op_j` acts first.

• **plus_hc** (*bool*) – If `True`, the hermitian conjugate of the term is added automatically.

### Examples

At least for simple enough 1D chains (or ladders), you can use `fit_with_sum_of_exp()` to approximate a long-range function with a few sum of exponentials and then add them with this function.

```python
>>> def decay(x):
...     return np.exp(-0.1*x) / x**2
>>> from tenpy.tools.fit import fit_with_sum_of_exp, sum_of_exp
>>> n_exp = 5
>>> fit_range = 50
>>> lam, pref = fit_with_sum_of_exp(decay, n_exp, fit_range)
>>> x = np.arange(1, fit_range + 1)
>>> print('error in fit: {0:.3e}'.format(np.sum(np.abs(decay(x) - sum_of_exp(lam, pref, x)))))
error in fit: 1.073e-04
>>> for pr, la in zip(pref, lam):
...     self.add_exponentially_decaying_coupling(pr, la, 'N', 'N')
```

### `add_local_term` *(strength, term, category=None, plus_hc=False)*

Add a single term to `self`.

The represented term is `strength` times the product of the operators given in `terms`. Each operator is specified by the name and the site it acts on; the latter given by a lattice index, see `Lattice`.

Depending on the length of `term`, it can add an onsite term or a coupling term to `onsite_terms` or `coupling_terms`, respectively.
Parameters

- **strength** (float/complex) – The prefactor of the term.

- **term** (list of (str, array_like)) – List of tuples (opname, lat_idx) where opname is a string describing the operator acting on the site given by the lattice index lat_idx. Here, lat_idx is for example [x, y, u] for a 2D lattice, with u being the index within the unit cell.

- **category** – Descriptive name used as key for onsite_terms or coupling_terms.

- **plus_hc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

**add_multi_coupling**(strength, ops, _deprecate_1='DEPRECATED', _deprecate_2='DEPRECATED', op_string=None, category=None, plus_hc=False)

Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \( \sum x \) strength[\( shift(x) \)] \( \times \) \( OP_0 \times OP_1 \times \ldots \times OP_{M-1} \), involving \( M \) operators. Here, \( OP_m \) stands for the operator defined by the \( m \)-th tuple (opname, dx, u) given in the argument ops, which determines the position \( \vec{x} + \vec{dx} \) and unit-cell index \( u \) of the site it acts on; the actual operator is given by self.lat.unit_cell[\( u \)].get_op(opname).

The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_multi_couplings() and depends on the boundary conditions. The \( \text{shift}(...) \) depends on the dx entries of ops and is chosen such that the first entry strength[\( 0, 0, \ldots \)] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to coupling_terms; this function does not rebuild the MPO.

Deprecated since version 0.6.0: We switched from the three arguments \( u_0, op_0 \) and other_op with other_ops=[(u1, op1, dx1), (op2, u2, dx2), \ldots] to a single, equivalent argument ops which should now read ops=[(op0, dx0, u0), (op1, dx1, u1), (op2, dx2, u2), \ldots], where dx0 = [0]*self.lat.dim. Note the changed order inside the tuples!

Parameters

- **strength** (scalar | array) – Prefactor of the coupling. May vary spatially, and is tiled to the required shape.

- **ops** (list of (opname, dx, u)) – Each tuple determines one operator of the coupling, see the description above. opname (str) is the name of the operator, dx (list of length lat.dim) is a translation vector, and u (int) is the index of lat.unit_cell on which the operator acts. The first entry of ops corresponds to \( OP_0 \) and acts last in the physical sense.

- **op_string** (str | None) – If a string is given, we use this as the name of an operator to be used inbetween the operators, excluding the sites on which any operators act. This operator should be defined on all sites in the unit cell.

If None, auto-determine whether a Jordan-Wigner string is needed (using op_needs_JW()) for each of the segments inbetween the operators and also on the sites of the left operators.

- **category** (str) – Descriptive name used as key for coupling_terms. Defaults to a string of the form "\( op_0 \_i \) (\( other\_ops[0] \)) \_j (\( other\_ops[1] \)) \_k \ldots".

- **plus_hc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

Examples
A call to `add_coupling()` with arguments `add_coupling(strength, u1, 'A', u2, 'B', dx)` is equivalent to the following:

```python
>>> dx_0 = [0] * self.lat.dim  # = [0] for a 1D lattice, [0, 0] in 2D
>>> self.add_multi_coupling(strength, [('A', dx_0, u1), ('B', dx, u2)])
```

To explicitly add the hermitian conjugate (instead of simply using `plus_hc = True`), you need to take the complex conjugate of the `strength`, reverse the order of the operators and take the hermitian conjugates of the individual operator names (indicated by the `hc(...), see `get_hc_op_name()`):

```python
>>> self.add_multi_coupling(np.conj(strength), [(hc('B'), dx, u2), (hc('A'),
˓→dx_0, u1)])
```

See also:

- `add_onsite` Add terms acting on one site only.
- `add_coupling` Add terms acting on two sites.
- `add_multi_coupling_term` Add a single term, not summing over the possible $\vec{x}$.

`add_multi_coupling_term(strength, ijk, ops_ijkl, op_string=None, category=None, plus_hc=False)`

Add a general M-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_multi_coupling_term(...)`.

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use `add_local_term()` instead.

**Parameters**

- `strength` (`float`) – The strength of the coupling term.
- `ijkl` (`list of int`) – The MPS indices of the sites on which the operators acts. With $i, j, k, ... = ijk$, we require that they are ordered ascending, $i < j < k < ...$ and that $0 <= i < N\_sites$. Indices $>= N\_sites$ indicate couplings between different unit cells of an infinite MPS.
- `ops_ijkl` (`list of str`) – Names of the involved operators on sites $i, j, k, ...$.
- `op_string` (`list of str`) – Names of the operator to be inserted between the operators, e.g., `op_string[0]` is inserted between $i$ and $j$.
- `category` (`str`) – Descriptive name used as key for `coupling_terms`. Defaults to a string of the form "\(\text{op0}_i \text{op1}_j \text{op2}_k \ldots\)".
- `plus_hc` (`bool`) – If `True`, the hermitian conjugate of the term is added automatically.

`add_onsite(strength, u, opname, category=None, plus_hc=False)`

Add onsite terms to `onsite_terms`.

Adds $\sum_{\vec{x}} strength[\vec{x}] \cdot OP$ to the represented Hamiltonian, where the operator $OP=\text{lat. unit\_cell'][u].\text{get\_op}(\text{opname})$ acts on the site given by a lattice index $(x_0, \ldots, x_{(\text{dim}-1)}, u)$.

The necessary terms are just added to `onsite_terms`; doesn’t rebuild the MPO.

**Parameters**
• **strength** *(scalar | array)* – Prefactor of the onsite term. May vary spatially. If an array of smaller size is provided, it gets tiled to the required shape.

• **u** *(int)* – Picks a **Site** `lat.unit_cell[u]` out of the unit cell.

• **opname** *(str)* – Valid operator name of an onsite operator in `lat.unit_cell[u]`.

• **category** *(str)* – Descriptive name used as key for `onsite_terms`. Defaults to `opname`.

• **plus_hc** *(bool)* – If `True`, the hermitian conjugate of the terms is added automatically.

See also:

*add_coupling* Add a terms acting on two sites.

*add_onsite_term* Add a single term without summing over `vecx`.

**add_onsite_term** *(strength, i, op, category=None, plus_hc=False)*

Add an onsite term on a given MPS site.

Wrapper for `self.onsite_terms[category].add_onsite_term(...)`.

**Parameters**

• **strength** *(float)* – The strength of the term.

• **i** *(int)* – The MPS index of the site on which the operator acts. We require `0 <= i < L`.

• **op** *(str)* – Name of the involved operator.

• **category** *(str)* – Descriptive name used as key for `onsite_terms`. Defaults to `op`.

• **plus_hc** *(bool)* – If `True`, the hermitian conjugate of the term is added automatically.

**all_coupling_terms** ()

Sum of all `coupling_terms`.

**all_onsite_terms** ()

Sum of all `onsite_terms`.

**bond_energies** *(psi)*

Calculate bond energies `<psi|H_bond|psi>`.

**Parameters** psi *(MPS)* – The MPS for which the bond energies should be calculated.

**Returns** E_bond – List of bond energies: for finite bc, `E_bond[i]` is the energy of bond `i, i+1` (i.e. we omit bond `0` between sites `L-1` and `0`); for infinite bc `E_bond[i]` is the energy of bond `i-1, i`.

**Return type** 1D ndarray

**calc_H_MPO** *(tol_zero=1e-15)*

Calculate MPO representation of the Hamiltonian.

Uses `onsite_terms` and `coupling_terms` to build an MPOGraph (and then an MPO).

**Parameters** tol_zero *(float)* – Prefactors with `abs(strength) < tol_zero` are considered to be zero.

**Returns** H_MPO – MPO representation of the Hamiltonian.

**Return type** MPO
calc_H_MPO_from_bond(tol_zero=1e-15)
Calculate the MPO Hamiltonian from the bond Hamiltonian.

Parameters tol_zero (float) – Arrays with norm < tol_zero are considered to be zero.

Returns H_MPO – MPO representation of the Hamiltonian.

Return type MPO

calc_H_bond(tol_zero=1e-15)
calculate H_bond from coupling_terms and onsite_terms.

Parameters tol_zero (float) – prefactors with abs(strength) < tol_zero are considered to be zero.

Returns H_bond – Bond terms as required by the constructor of NearestNeighborModel.
Legs are ['p0', 'p0*', 'p1', 'p1*']

Return type list of Array
:raises ValueError : if the Hamiltonian contains longer-range terms.

calc_H_bond_from_MPO(tol_zero=1e-15)
Calculate the bond Hamiltonian from the MPO Hamiltonian.

Parameters tol_zero (float) – Arrays with norm < tol_zero are considered to be zero.

Returns H_bond – Bond terms as required by the constructor of NearestNeighborModel.
Legs are ['p0', 'p0*', 'p1', 'p1*']

Return type list of Array
:raises ValueError : if the Hamiltonian contains longer-range terms.

calc_H_onsite(tol_zero=1e-15)
Calculate H_onsite from self.onsite_terms.

Deprecated since version 0.4.0: This function will be removed in 1.0.0. Replace calls to this
function by self.all_onsite_terms().remove_zeros(tol_zero).to_Arrays(self.lat.mps_sites()). You might also want to take explicit_plus_hc into account.

Parameters tol_zero (float) – prefactors with abs(strength) < tol_zero are considered to be zero.

Returns
• H_onsite (list of npc.Array)
  onsite terms of the Hamiltonian. If explicit_plus_hc is True, – Hermitian conjugates of the onsite terms will be included.

coupling_strength_add_ext_flux(strength, dx, phase)
Add an external flux to the coupling strength.

When performing DMRG on a “cylinder” geometry, it might be useful to put an “external flux” through the cylinder. This means that a particle hopping around the cylinder should pick up a phase given by the external flux [resta1998]. This is also called “twisted boundary conditions” in literature. This function adds a complex phase to the strength array on some bonds, such that particles hopping in positive direction around the cylinder pick up $exp(+i \text{phase})$.

**Warning:** For the sign of phase it is important that you consistently use the creation operator as op1 and the annihilation operator as op2 in add_coupling().

7.11. models
Parameters

- **strength** *(scalar / array)* – The strength to be used in `add_coupling()`, when no external flux would be present.
- **dx** *(iterable of int)* – Translation vector (of the unit cell) between `op1` and `op2` in `add_coupling()`.
- **phase** *(iterable of float)* – The phase of the external flux for hopping in each direction of the lattice. E.g., if you want flux through the cylinder on which you have an infinite MPS, you should give `phase=[0, phi]` such that particles pick up a phase `phi` when hopping around the cylinder.

Returns **strength** – The strength array to be used as `strength` in `add_coupling()` with the given `dx`.

Return type **complex array**

Examples

Let’s say you have an infinite MPS on a cylinder, and want to add nearest-neighbor hopping of fermions with the `FermionSite`. The cylinder axis is the x-direction of the lattice, so to put a flux through the cylinder, you want particles hopping around the cylinder to pick up a phase `phi` given by the external flux.

```python
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0, phi])
...    self.add_coupling(strength_with_flux, u1, 'Cd', u2, 'C', dx)
...    self.add_coupling(np.conj(strength_with_flux), u2, 'Cd', u1, 'C', -dx)
```

`enlarge_mps_unit_cell(factor=2)`

Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and cannot be reverted.

Parameters **factor** *(int)* – The new number of sites in the MPS unit cell will be increased from `N_sites` to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from 

(Lx, Ly, ..., Lu) to (Lx*factor, Ly, ..., Lu).

**classmethod from_MPOModel(mpo_model)**

Initialize a NearestNeighborModel from a model class defining an MPO.

This is especially usefull in combination with `MPOModel.group_sites()`.

Parameters **mpo_model** *(MPOModel)* – A model instance implementing the MPO. Does not need to be a `NearestNeighborModel`, but should only have nearest-neighbor couplings.

Examples

The `SpinChainNNN2` has next-nearest-neighbor couplings and thus only implements an MPO:

```python
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20, 'verbose': 0})
>>> print(isinstance(nnn_chain, NearestNeighborModel))
False
```
By grouping each two neighboring sites, we can bring it down to nearest neighbors.

>>> grouped_sites = nnn_chain.group_sites(2)
>>> print("range after grouping:", nnn_chain.H_MPO.max_range)
range after grouping: 1

Yet, TEBD will not yet work, as the model doesn’t define $H_{\text{bond}}$. However, we can initialize a Nearest-NeighborModel from the MPO:

>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
>>> isinstance(nnn_chain_for_tebd, NearestNeighborModel)
True

**class method** from_hdf5(hdf5_loader, h5gr, subpath)

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

**Parameters**

- **hdf5_loader** (Hdf5Loader) – Instance of the loading engine.
- **h5gr** (Group) – HDF5 group which is represent the object to be constructed.
- **subpath** (str) – The name of `h5gr` with a ‘/’ in the end.

**Returns** obj – Newly generated class instance containing the required data.

**Return type** cls

**group_sites**(n=2, grouped_sites=None)

Modify `self` in place to group sites.

Group each $n$ sites together using the `GroupedSite`. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and can not be reverted.

**Parameters**

- **n** (int) – Number of sites to be grouped together.
- **grouped_sites** (None | list of `GroupedSite`) – The sites grouped together.

**Returns** grouped_sites – The sites grouped together.

**Return type** list of `GroupedSite`

**init_lattice**(model_params)

Initialize a lattice for the given model parameters.

This function reads out the model parameter `lattice`. This can be a full `Lattice` instance, in which case it is just returned without further action. Alternatively, the `lattice` parameter can be a string giving the name of one of the predefined lattices, which then gets initialized. Depending on the dimensionality of the lattice, this requires different model parameters.

**Parameters** model_params (dict) – The model parameters given to `__init__`.

**Returns** lat – An initialized lattice.
Return type \textit{Lattice}

\textbf{Options}

\textbf{option} CouplingMPOModel.\texttt{lattice: str \mid Lattice}

The name of a lattice pre-defined in TeNPy to be initialized. Alternatively, a (possibly self-defined) Lattice instance. In the latter case, no further parameters are read out.

\textbf{option} CouplingMPOModel.\texttt{bc\_MPS: str}

Boundary conditions for the MPS.

\textbf{option} CouplingMPOModel.\texttt{order: str}

The order of sites within the lattice for non-trivial lattices, e.g., \texttt{default}, \texttt{snake}, see \texttt{ordering()}. Only used if \texttt{lattice} is a string.

\textbf{option} CouplingMPOModel.\texttt{L: int}

The length in x-direction; only read out for 1D lattices. For an infinite system the length of the unit cell.

\textbf{option} CouplingMPOModel.\texttt{Lx: int}

\textbf{option} CouplingMPOModel.\texttt{Ly: int}

The length in x- and y-direction; only read out for 2D lattices. For \texttt{"infinite" bc\_MPS}, the system is infinite in x-direction and \texttt{Lx} is the number of “rings” in the infinite MPS unit cell, while \texttt{Ly} gives the circumference around the cylinder or width of the rung for a ladder (depending on bc\_y).

\textbf{option} CouplingMPOModel.\texttt{bc\_y: str}

\texttt{"cylinder" \mid "ladder"}; only read out for 2D lattices. The boundary conditions in y-direction.

\textbf{option} CouplingMPOModel.\texttt{bc\_x: str}

\texttt{"open" \mid "periodic"}. Can be used to force “periodic” boundaries for the lattice, i.e., for the couplings in the Hamiltonian, even if the MPS is finite. Defaults to \texttt{"open"} for \texttt{bc\_MPS=\&quot;finite\&quot;} and \texttt{"periodic"} for \texttt{bc\_MPS=\&quot;infinite\&quot;}. If you are not aware of the consequences, you should probably not use “periodic” boundary conditions. (The MPS is still “open”, so this will introduce long-range couplings between the first and last sites of the MPS!)

\textbf{init\_sites} (\texttt{model\_params})

Define the local Hilbert space and operators; needs to be implemented in subclasses.

This function gets called by \texttt{init\_lattice()} to get the \textit{Site} for the lattice unit cell.

\textbf{Note:} Initializing the sites requires to define the conserved quantum numbers. All pre-defined sites accept \texttt{conserve=None} to disable using quantum numbers. Many models in TeNPy read out the \texttt{conserve} model parameter, which can be set to \texttt{"best"} to indicate the optimal parameters.

If you need to initialize more than one site, the function \texttt{tenpy.networks.site.set\_common\_charges()} should be helpful.

Parameters \texttt{model\_params} (\texttt{dict}) – The model parameters given to \texttt{\_\_init\_\_}.

Returns \texttt{sites} – The local sites of the lattice, defining the local basis states and operators.

Return type \texttt{(tuple of) Site}

\textbf{init\_terms} (\texttt{model\_params})

Add the onsite and coupling terms to the model; subclasses should implement this.

\textbf{save\_hdf5} (\texttt{hdf5\_saver, h5gr, subpath})

Export \texttt{self} into a HDF5 file.
This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.
This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute `'format'`.

Parameters

- `hdf5_saver (Hdf5Saver)` – Instance of the saving engine.
- `h5gr (:class:`Group`)` – HDF5 group which is supposed to represent `self`.
- `subpath (str)` – The name of `h5gr` with a `'/'` in the end.

`test_sanity()`
Sanity check, raises ValueErrors, if something is wrong.

`trivial_like_NNModel()`
Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

Module description

Nearest-neighbour spin-S models.
Uniform lattice of spin-S sites, coupled by nearest-neighbour interactions.

7.11.6 `spins_nnn`

- full name: `tenpy.models.spins_nnn`
- parent module: `tenpy.models`
- type: module
Classes

Module description

Next-Nearest-neighbour spin-S models.

Uniform lattice of spin-S sites, coupled by next-nearest-neighbour interactions. We have two variants implementing the same hamiltonian. The SpinChainNNN uses the GroupedSite to keep it a NearestNeighborModel suitable for TEBD, while the SpinChainNNN2 just involves longer-range couplings in the MPO. The latter is preferable for pure DMRG calculations and avoids having to add each of the short range couplings twice for the grouped sites.

Note that you can also get a NearestNeighborModel for TEBD from the latter by using group_sites() and from_MPOModel(). An example for such a case is given in the file examples/c_tebd.py.
7.11.7 fermions_spinless

- full name: tenpy.models.fermions_spinless
- parent module: tenpy.models
- type: module

Classes

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FermionChain</td>
<td>The FermionModel on a Chain, suitable for TEBD.</td>
</tr>
<tr>
<td>FermionModel</td>
<td>Spinless fermions with particle number conservation.</td>
</tr>
</tbody>
</table>
FermionChain

- full name: tenpy.models.fermions_spinless.FermionChain
- parent module: tenpy.models.fermions_spinless
- type: class

Inheritance Diagram

![Inheritance Diagram]

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FermionChain.<strong>init</strong>(model_params)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>FermionChain.add_coupling(strength, u1, op1,...)</td>
<td>Add two-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>FermionChain.add_coupling_term(strength, i,...)</td>
<td>Add a two-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>FermionChain.add_exponentially_decaying_coupling(...)</td>
<td>Add an exponentially decaying long-range coupling.</td>
</tr>
</tbody>
</table>

continues on next page
Table 112 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FermionChain.add_local_term(strength, term)</td>
<td>Add a single term to self.</td>
</tr>
<tr>
<td>FermionChain.add_multi_coupling(strength, ops)</td>
<td>Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>FermionChain.add_multi_coupling_term(...[, ...])</td>
<td>Add a general M-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>FermionChain.add_onsite(strength, u, opname)</td>
<td>Add onsite terms to onsite_terms.</td>
</tr>
<tr>
<td>FermionChain.add_onsite_term(strength, i, op)</td>
<td>Add an onsite term on a given MPS site.</td>
</tr>
<tr>
<td>FermionChain.all_coupling_terms()</td>
<td>Sum of all coupling_terms.</td>
</tr>
<tr>
<td>FermionChain.all_onsite_terms()</td>
<td>Sum of all onsite_terms.</td>
</tr>
<tr>
<td>FermionChain.bond_energies(psi)</td>
<td>Calculate bond energies &lt;psi</td>
</tr>
<tr>
<td>FermionChain.calc_H_MPO([tol_zero])</td>
<td>Calculate MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td>FermionChain.calc_H_MPO_from_bond([tol_zero])</td>
<td>Calculate the MPO Hamiltonian from the bond Hamiltonian.</td>
</tr>
<tr>
<td>FermionChain.calc_H_bond([tol_zero])</td>
<td>Calculate H_bond from coupling_terms and onsite_terms.</td>
</tr>
<tr>
<td>FermionChain.calc_H_bond_from_MPO([tol_zero])</td>
<td>Calculate the bond Hamiltonian from the MPO Hamiltonian.</td>
</tr>
<tr>
<td>FermionChain.calc_H_onsite([tol_zero])</td>
<td>Calculate H_onsite from self.onsite_terms.</td>
</tr>
<tr>
<td>FermionChain.coupling_strength_add_ext_flux([,...])</td>
<td>Add an external flux to the coupling strength.</td>
</tr>
<tr>
<td>FermionChain.enlarge_mps_unit_cell([factor])</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>FermionChain.from_MPOModel(mpo_model)</td>
<td>Initialize a NearestNeighborModel from a model class defining an MPO.</td>
</tr>
<tr>
<td>FermionChain.from_hdf5(hdf5 Loader, h5gr, ...)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>FermionChain.group_sites([n, grouped_sites])</td>
<td>Modify self in place to group sites.</td>
</tr>
<tr>
<td>FermionChain.init_lattice(model_params)</td>
<td>Initialize a lattice for the given model parameters.</td>
</tr>
<tr>
<td>FermionChain.init_sites(model_params)</td>
<td>Define the local Hilbert space and operators; needs to be implemented in subclasses.</td>
</tr>
<tr>
<td>FermionChain.init_terms(model_params)</td>
<td>Add the onsite and coupling terms to the model; subclasses should implement this.</td>
</tr>
<tr>
<td>FermionChain.save_hdf5(hdf5_saver, h5gr, subpath)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>FermionChain.test_sanity()</td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td>FermionChain.trivial_like_NNModel()</td>
<td>Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.</td>
</tr>
</tbody>
</table>

class tenpy.models.fermions_spinless.FermionChain(model_params)

The FermionModel on a Chain, suitable for TEBD.

See the FermionModel for the documentation of parameters.

add_coupling(strength, u1, op1, u2, op2, dx, op_string=None, str_on_first=True, raise_op2_left=False, category=None, plus_hc=False)

Add two-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \( \sum_{\bar{x}} \text{strength}(\text{shift}(\bar{x})) \cdot OP0 \cdot OP1 \), where \( OP0 \)}
The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_couplings() and depends on the boundary conditions. The shift(...) depends on dx, and is chosen such that the first entry strength[0, 0, ...] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to coupling_terms; this function does not rebuild the MPO.

Deprecated since version 0.4.0: The arguments str_on_first and raise_op2_left will be removed in version 1.0.0.

Parameters

- **strength** (scalar / array) – Prefactor of the coupling. May vary spatially (see above). If an array of smaller size is provided, it gets tiled to the required shape.
- **u1** (int) – Picks the site lat.unit_cell[u1] for OP1.
- **op1** (str) – Valid operator name of an onsite operator in lat.unit_cell[u1] for OP1.
- **u2** (int) – Picks the site lat.unit_cell[u2] for OP2.
- **op2** (str) – Valid operator name of an onsite operator in lat.unit_cell[u2] for OP2.
- **dx** (iterable of int) – Translation vector (of the unit cell) between OP1 and OP2. For a 1D lattice, a single int is also fine.
- **op_string** (str | None) – Name of an operator to be used between the OP1 and OP2 sites. Typical use case is the phase for a Jordan-Wigner transformation. The operator should be defined on all sites in the unit cell. If None, auto-determine whether a Jordan-Wigner string is needed, using op_needs_JW().
- **str_on_first** (bool) – Whether the provided op_string should also act on the first site. This option should be chosen as True for Jordan-Wigner strings. When handling Jordan-Wigner strings we need to extend the op_string to also act on the ‘left’, first site (in the sense of the MPS ordering of the sites given by the lattice). In this case, there is a well-defined ordering of the operators in the physical sense (i.e. which of op1 or op2 acts first on a given state). We follow the convention that op2 acts first (in the physical sense), independent of the MPS ordering. Deprecated.
- **raise_op2_left** (bool) – Raise an error when op2 appears left of op1 (in the sense of the MPS ordering given by the lattice). Deprecated.
- **category** (str) – Descriptive name used as key for coupling_terms. Defaults to a string of the form "{op1}_i {op2}_j".
- **plus_hc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

Examples

When initializing a model, you can add a term \( J \sum_{<i,j>} S_i^z S_j^z \) on all nearest-neighbor bonds of the lattice like this:

```python
:= lat.unit_cell[u0].get_op(op0) acts on the site \((x_0, ..., x_{(dim-1)}, u0)\), and OP1 := lat.unit_cell[u1].get_op(op1) acts on the site \((x_0+dx[0], ..., x_{(dim-1)}+dx[\text{dim-1}], u1)\). Possible combinations \(x_0,...,x_{\text{dim-1}}\) are determined from the boundary conditions in possible_couplings().
```
The strength can be an array, which gets tiled to the correct shape. For example, in a 1D Chain with an even number of sites and periodic (or infinite) boundary conditions, you can add alternating strong and weak couplings with a line like:

```python
>>> self.add_coupling([1.5, 1.], u1, 'Sz', u2, 'Sz', dx)
```

Make sure to use the `plus_hc` argument if necessary, e.g. for hoppings:

```python
>>> t = 1.  # hopping strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```

Alternatively, you can add the hermitian conjugate terms explicitly. The correct way is to complex conjugate the strength, take the hermitian conjugate of the operators and swap the order (including a swap `u1 <-> u2`), and use the opposite direction `-dx`, i.e. the `h.c.` of `add_coupling(t, u1, 'A', u2, 'B', dx)` is `add_coupling(np.conj(t), u2, hc('B'), u1, hc('A'), -dx)`, where `hc` takes the hermitian conjugate of the operator names, see `get_hc_op_name()`. For spin-less fermions (`FermionSite`), this would be

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx)
...     self.add_coupling(np.conj(t), u2, 'Cd', u1, 'C', -dx)  # h.c.
```

With spin-full fermions (`SpinHalfFermions`), it could be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cdu', u2, 'Cd', dx)  # Cdagger_up C_down
...     self.add_coupling(np.conj(t), u2, 'Cdd', u1, 'Cu', -dx)  # h.c.
```

Note that the Jordan-Wigner strings for the fermions are added automatically!

See also:

- `add_onsite` Add terms acting on one site only.
- `add_multi_coupling_term` for terms on more than two sites.
- `add_coupling_term` Add a single term without summing over `veccx`.

`add_coupling_term` *(strength, i, j, op_i, op_j, op_string='Id', category=None, plus_hc=False)*

Add a two-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_coupling_term(...)`.

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use `add_local_term()` instead.

**Parameters**

- `strength` *(float)* – The strength of the coupling term.
i (int) – The MPS indices of the two sites on which the operator acts. We require 0 <= i < N_sites and i < j, i.e., op\_i acts “left” of op\_j. If j >= N_sites, it indicates couplings between unit cells of an infinite MPS.

j (int) – The MPS indices of the two sites on which the operator acts. We require 0 <= i < N_sites and i < j, i.e., op\_i acts “left” of op\_j. If j >= N_sites, it indicates couplings between unit cells of an infinite MPS.

op1 (str) – Names of the involved operators.

op2 (str) – Names of the involved operators.

op\_string (str) – The operator to be inserted between i and j.

category (str) – Descriptive name used as key for coupling\_terms. Defaults to a string of the form "{op1}\_i {op2}\_j".

plus\_hc (bool) – If True, the hermitian conjugate of the term is added automatically.

add\_exponentially\_decaying\_coupling (strength, lambda\_, op\_i, op\_j, subsites=None, op\_string=None, plus\_hc=False)
Add an exponentially decaying long-range coupling.

\[
\text{strength} \sum_{i<j} \lambda^{i-j} A_{\text{subsites}[i]} B_{\text{subsites}[j]}
\]

Where the operator A is given by op\_i, and B is given by op\_j. Note that the sum over i,j is long-range, for infinite systems going beyond the MPS unit cell. Moreover, note that the distance in the exponent is the distance within subsites.

Parameters

- strength (float) – Overall prefactor.
- lambda (float) – Decay-rate
- op\_i (string) – Names for the operators.
- op\_j (string) – Names for the operators.
- subsites (None / 1D array) – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. None selects all sites.
- op\_string (None / str) – The operator to be inserted between A and B: If None, this function checks whether a fermionic "JW" string is needed for the given operators; in this case the right op\_j acts first.
- plus\_hc (bool) – If True, the hermitian conjugate of the term is added automatically.

Examples

At least for simple enough 1D chains (or ladders), you can use fit\_with\_sum\_of\_exp() to approximate a long-range function with a few sum of exponentials and then add them with this function.

```python
>>> def decay(x):
...     return np.exp(-0.1*x) / x**2

>>> from tenpy.tools.fit import fit_with_sum_of_exp, sum_of_exp

>>> n_exp = 5
>>> fit_range = 50
>>> lam, pref = fit_with_sum_of_exp(decay, n_exp, fit_range)
>>> x = np.arange(1, fit_range + 1)

>>> print('error in fit: {0:.3e}'.format(np.sum(np.abs(decay(x) - sum_of_exp(lam, pref, x))))))
```
add_local_term(strength, term, category=None, plus hc=False)

Add a single term to self.

The represented term is strength times the product of the operators given in term. Each operator is specified by the name and the site it acts on; the latter given by a lattice index, see Lattice.

Depending on the length of term, it can add an onsite term or a coupling term to onsite_terms or coupling_terms, respectively.

Parameters

- **strength** (float/complex) – The prefactor of the term.
- **term** (list of (str, array_like)) – List of tuples (opname, lat_idx) where opname is a string describing the operator acting on the site given by the lattice index lat_idx. Here, lat_idx is for example [x, y, u] for a 2D lattice, with u being the index within the unit cell.
- **category** – Descriptive name used as key for onsite_terms or coupling_terms.
- **plus hc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

add_multi_coupling(strength, ops, _deprecate_1='DEPRECATED', _deprecate_2='DEPRECATED', op_string=None, category=None, plus hc=False)

Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \( \sum \_{\vec{x}} strength[\text{shift}(\vec{x})] \ast OP_0 \ast OP_1 \ast \ldots \ast OP_{M-1} \), involving \( M \) operators. Here, \( OP_m \) stands for the operator defined by the \( m \)-th tuple (opname, dx, u) given in the argument ops, which determines the position \( \vec{x} + \vec{dx} \) and unit-cell index \( u \) of the site it acts on; the actual operator is given by self.lat.unit_cell[u].get_op(opname).

The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_multi_couplings() and depends on the boundary conditions. The shift(...) depends on the dx entries of ops and is chosen such that the first entry strength[0, 0, 0, ...] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to coupling_terms; this function does not rebuild the MPO.

Deprecated since version 0.6.0: We switched from the three arguments \( u_0, op_0 \) and other_op with
other_ops=[(u1, op1, dx1), (op2, u2, dx2), ...] to a single, equivalent argument ops which should now read ops=[(op0, dx0, u0), (op1, dx1, u1), (op2, dx2, u2), ...], where dx0 = [0]*self.lat.dim. Note the changed order inside the tuples!

Parameters

- **strength** (scalar | array) – Prefactor of the coupling. May vary spatially, and is tiled to the required shape.
- **ops** (list of (opname, dx, u)) – Each tuple determines one operator of the coupling, see the description above. opname (str) is the name of the operator, dx (list of length lat.dim) is a translation vector, and u (int) is the index of lat.unit_cell on which the operator acts. The first entry of ops corresponds to \( OP_0 \) and acts last in the physical sense.
• **op_string** *(str | None)* – If a string is given, we use this as the name of an operator to be used inbetween the operators, excluding the sites on which any operators act. This operator should be defined on all sites in the unit cell.

If `None`, auto-determine whether a Jordan-Wigner string is needed (using `op_needs_JW()` for each of the segments inbetween the operators and also on the sites of the left operators.

• **category** *(str)* – Descriptive name used as key for `coupling_terms`. Defaults to a string of the form "{op0}_i {other_ops[0]}_j {other_ops[1]}_k ...".

• **plus_hc** *(bool)* – If `True`, the hermitian conjugate of the terms is added automatically.

### Examples

A call to `add_coupling()` with arguments `add_coupling(strength, u1, 'A', u2, 'B', dx)` is equivalent to the following:

```python
>>> dx_0 = [0] * self.lat.dim  # = [0] for a 1D lattice, [0, 0] in 2D
>>> self.add_multi_coupling(strength, [('A', dx_0, u1), ('B', dx, u2)])
```

To explicitly add the hermitian conjugate (instead of simply using `plus_hc = True`), you need to take the complex conjugate of the `strength`, reverse the order of the operators and take the hermitian conjugates of the individual operator names (indicated by the `hc(...)`), see `get_hc_op_name()`:

```python
>>> self.add_multi_coupling(np.conj(strength), [(hc('B'), dx, u2), (hc('A'), ...
     ←dx_0, u1)])
```

See also:

* **add_onsite** Add terms acting on one site only.
* **add_coupling** Add terms acting on two sites.
* **add_multi_coupling_term** Add a single term, not summing over the possible \( \vec{x} \).

**add_multi_coupling_term**(strength, ijk, ops_ijkl, op_string=None, category=None, plus_hc=False)

Add a general M-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_multi_coupling_term(...)`.

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use `add_local_term()` instead.

### Parameters

• **strength** *(float)* – The strength of the coupling term.

• **ijk** *(list of int)* – The MPS indices of the sites on which the operators acts. With \( i, j, k, \ldots = ijk \), we require that they are ordered ascending, \( i < j < k < \ldots \) and that \( 0 \leq i < N_{\text{sites}} \). Indices \( \geq N_{\text{sites}} \) indicate couplings between different unit cells of an infinite MPS.

• **ops_ijkl** *(list of str)* – Names of the involved operators on sites \( i, j, k, \ldots \).

• **op_string** *(list of str)* – Names of the operator to be inserted between the operators, e.g., `op_string[0]` is inserted between `i` and `j`.  

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480 Chapter 7. License

TeNPy, Release 0.7.2.dev55+68eae2c
• **category** (*str*) – Descriptive name used as key for `coupling_terms`. Defaults to a string of the form "\( (op0)_i \ (op1)_j \ (op2)_k \ ... \)".

• **plus_hc** (*bool*) – If True, the hermitian conjugate of the term is added automatically.

### `add_onsite(strength, u, opname, category=None, plus_hc=False)`

Add onsite terms to `onsite_terms`.

Adds \( \sum_x strength[x] \times OP \) to the represented Hamiltonian, where the operator \( OP=lat.\) unit_cell[u].get_op(opname) acts on the site given by a lattice index \((x_0, \ldots, x_{(dim-1)}, u)\).

The necessary terms are just added to `onsite_terms`; doesn’t rebuild the MPO.

**Parameters**

- **strength** (*scalar | array*) – Prefactor of the onsite term. May vary spatially. If an array of smaller size is provided, it gets tiled to the required shape.
- **u** (*int*) – Picks a site `lat.unit_cell[u]` out of the unit cell.
- **opname** (*str*) – valid operator name of an onsite operator in `lat.unit_cell[u]`.
- **category** (*str*) – Descriptive name used as key for `onsite_terms`. Defaults to `opname`.
- **plus_hc** (*bool*) – If True, the hermitian conjugate of the term is added automatically.

See also:

- **add_coupling** Add a terms acting on two sites.
- **add_onsite_term** Add a single term without summing over vecx.

### `add_onsite_term(strength, i, op, category=None, plus_hc=False)`

Add an onsite term on a given MPS site.

Wrapper for `self.onsite_terms[category].add_onsite_term(...)`.

**Parameters**

- **strength** (*float*) – The strength of the term.
- **i** (*int*) – The MPS index of the site on which the operator acts. We require 0 <= i < L.
- **op** (*str*) – Name of the involved operator.
- **category** (*str*) – Descriptive name used as key for `onsite_terms`. Defaults to `op`.
- **plus_hc** (*bool*) – If True, the hermitian conjugate of the term is added automatically.

### `all_coupling_terms()`

Sum of all `coupling_terms`.

### `all_onsite_terms()`

Sum of all `onsite_terms`.

### `bond_energies(psi)`

Calculate bond energies \(<\psi|H_{\text{bond}}|\psi>\).

**Parameters** `psi` (*MPS*) – The MPS for which the bond energies should be calculated.
Returns `E_bond` – List of bond energies: for finite bc, `E_Bond[i]` is the energy of bond \( i, i+1 \) (i.e. we omit bond 0 between sites L-1 and 0); for infinite bc `E_bond[i]` is the energy of bond \( i-1, i \).

Return type 1D ndarray

calc_H_MPO (tol_zero=1e-15)
Calculate MPO representation of the Hamiltonian.

   Uses onsite_terms and coupling_terms to build an MPOGraph (and then an MPO).

Parameters `tol_zero (float)` – Prefactors with abs(strength) < tol_zero are considered to be zero.

Returns `H_MPO` – MPO representation of the Hamiltonian.

Return type MPO

calc_H_MPO_from_bond (tol_zero=1e-15)
Calculate the MPO Hamiltonian from the bond Hamiltonian.

Parameters `tol_zero (float)` – Arrays with norm < tol_zero are considered to be zero.

Returns `H_MPO` – MPO representation of the Hamiltonian.

Return type MPO

calc_H_bond (tol_zero=1e-15)
calculate \( H_{bond} \) from coupling_terms and onsite_terms.

Parameters `tol_zero (float)` – prefactors with abs(strength) < tol_zero are considered to be zero.

Returns `H_bond` – Bond terms as required by the constructor of NearestNeighborModel.
Legs are \[ 'p0', 'p0*', 'p1', 'p1*']

Return type list of Array

:raises ValueError : if the Hamiltonian contains longer-range terms.

calc_H_bond_from_MPO (tol_zero=1e-15)
Calculate the bond Hamiltonian from the MPO Hamiltonian.

Parameters `tol_zero (float)` – Arrays with norm < tol_zero are considered to be zero.

Returns `H_bond` – Bond terms as required by the constructor of NearestNeighborModel.
Legs are \[ 'p0', 'p0*', 'p1', 'p1*']

Return type list of Array

:raises ValueError : if the Hamiltonian contains longer-range terms.

calc_H_onsite (tol_zero=1e-15)
Calculate \( H_{onsite} \) from self.onsite_terms.

Deprecated since version 0.4.0: This function will be removed in 1.0.0. Replace calls to this function by \[ self.all_onsite_terms().remove_zeros(tol_zero).to_Arrays(self.lat.mps_sites()) \]. You might also want to take explicit_plus_hc into account.

Parameters `tol_zero (float)` – prefactors with abs(strength) < tol_zero are considered to be zero.

Returns

• `H_onsite (list of npc.Array)`
• onsite terms of the Hamiltonian. If `explicit_plus_hc` is True, – Hermitian conjugates of the onsite terms will be included.

`coupling_strength_add_ext_flux(strength, dx, phase)`

Add an external flux to the coupling strength.

When performing DMRG on a “cylinder” geometry, it might be useful to put an “external flux” through the cylinder. This means that a particle hopping around the cylinder should pick up a phase given by the external flux `[resta1998]`. This is also called “twisted boundary conditions” in literature. This function adds a complex phase to the `strength` array on some bonds, such that particles hopping in positive direction around the cylinder pick up `exp(+i phase)`.

**Warning:** For the sign of `phase` it is important that you consistently use the creation operator as `op1` and the annihilation operator as `op2` in `add_coupling()`.

**Parameters**

- `strength` *(scalar / array)* – The strength to be used in `add_coupling()`, when no external flux would be present.
- `dx` *(iterable of int)* – Translation vector (of the unit cell) between `op1` and `op2` in `add_coupling()`.
- `phase` *(iterable of float)* – The phase of the external flux for hopping in each direction of the lattice. E.g., if you want flux through the cylinder on which you have an infinite MPS, you should give `phase=[0, phi]` such that particles pick up a phase `phi` when hopping around the cylinder.

**Returns** `strength` – The strength array to be used as `strength` in `add_coupling()` with the given `dx`.

**Return type** complex array

**Examples**

Let’s say you have an infinite MPS on a cylinder, and want to add nearest-neighbor hopping of fermions with the `FermionSite`. The cylinder axis is the x-direction of the lattice, so to put a flux through the cylinder, you want particles hopping around the cylinder to pick up a phase `phi` given by the external flux.

```python
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> for ul, u2, dx in self.lat.pairs['nearest_neighbors']:
...     strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0, phi])
...     self.add_coupling(strength_with_flux, ul, 'Cd', u2, 'C', dx)
...     self.add_coupling(np.conj(strength_with_flux), u2, 'Cd', ul, 'C', -dx)
```

`enlarge_mps_unit_cell(factor=2)`

Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and can not be reverted.

**Parameters** `factor` *(int)* – The new number of sites in the MPS unit cell will be increased from `N_sites` to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.
classmethod from_MPOModel (mpo_model)
Initialize a NearestNeighborModel from a model class defining an MPO.

This is especially useful in combination with MPOModel.group_sites().

Parameters mpo_model (MPOModel) – A model instance implementing the MPO. Does not need to be a NearestNeighborModel, but should only have nearest-neighbor couplings.

Examples
The SpinChainNNN2 has next-nearest-neighbor couplings and thus only implements an MPO:

```python
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20, 'verbose': 0})
>>> print(isinstance(nnn_chain, NearestNeighborModel))
False
>>> print("range before grouping:", nnn_chain.H_MPO.max_range)
range before grouping: 2
```

By grouping each two neighboring sites, we can bring it down to nearest neighbors.

```python
>>> grouped_sites = nnn_chain.group_sites(2)
>>> print("range after grouping:", nnn_chain.H_MPO.max_range)
range after grouping: 1
```

Yet, TEBD will not yet work, as the model doesn’t define $H_{bond}$. However, we can initialize a NearestNeighborModel from the MPO:

```python
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
>>> isinstance(nnn_chain_for_tebd, NearestNeighborModel)
True
```

classmethod from_hdf5 (hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

Parameters
- hdf5_loader (Hdf5Loader) – Instance of the loading engine.
- h5gr (Group) – HDF5 group which is represent the object to be constructed.
- subpath (str) – The name of h5gr with a '/' in the end.

Returns obj – Newly generated class instance containing the required data.

Return type cls
group_sites (n=2, grouped_sites=None)
Modify self in place to group sites.

Group each $n$ sites together using the GroupedSite. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and can not be reverted.

Parameters
- n (int) – Number of sites to be grouped together.
- grouped_sites (None | list of GroupedSite) – The sites grouped together.
Returns grouped_sites – The sites grouped together.

Return type list of GroupedSite

init_lattice(model_params)
Initialize a lattice for the given model parameters.

This function reads out the model parameter lattice. This can be a full Lattice instance, in which case it is just returned without further action. Alternatively, the lattice parameter can be a string giving the name of one of the predefined lattices, which then gets initialized. Depending on the dimensionality of the lattice, this requires different model parameters.

Parameters model_params (dict) – The model parameters given to __init__.

Returns lat – An initialized lattice.

Return type Lattice

Options

option CouplingMPOModel.lattice: str | Lattice
  The name of a lattice pre-defined in TeNPy to be initialized. Alternatively, a (possibly self-defined) Lattice instance. In the latter case, no further parameters are read out.

option CouplingMPOModel.bc_MPS: str
  Boundary conditions for the MPS.

option CouplingMPOModel.order: str
  The order of sites within the lattice for non-trivial lattices, e.g. 'default', 'snake', see ordering(). Only used if lattice is a string.

option CouplingMPOModel.L: int
  The length in x-direction; only read out for 1D lattices. For an infinite system the length of the unit cell.

option CouplingMPOModel.Lx: int
option CouplingMPOModel.Ly: int
  The length in x- and y-direction; only read out for 2D lattices. For "infinite" bc_MPS, the system is infinite in x-direction and Lx is the number of “rings” in the infinite MPS unit cell, while Ly gives the circumference around the cylinder or width of the rung for a ladder (depending on bc_y).

option CouplingMPOModel.bc_y: str
  "cylinder" | "ladder"; only read out for 2D lattices. The boundary conditions in y-direction.

option CouplingMPOModel.bc_x: str
  "open" | "periodic". Can be used to force “periodic” boundaries for the lattice, i.e., for the couplings in the Hamiltonian, even if the MPS is finite. Defaults to "open" for bc_MPS="finite" and "periodic" for bc_MPS="infinite. If you are not aware of the consequences, you should probably not use “periodic” boundary conditions. (The MPS is still “open”, so this will introduce long-range couplings between the first and last sites of the MPS!)

init_sites(model_params)
Define the local Hilbert space and operators; needs to be implemented in subclasses.

This function gets called by init_lattice() to get the Site for the lattice unit cell.

Note: Initializing the sites requires to define the conserved quantum numbers. All pre-defined sites accept conserve=None to disable using quantum numbers. Many models in TeNPy read out the conserve model parameter, which can be set to "best" to indicate the optimal parameters.
If you need to initialize more than one site, the function `tenpy.networks.site.set_common_charges()` should be helpful.

**Parameters**

- `model_params` (*dict*) – The model parameters given to `__init__`.

**Returns**

- `sites` – The local sites of the lattice, defining the local basis states and operators.

**Return type**

- (tuple of) `Site`

`init_terms(model_params)`

Add the onsite and coupling terms to the model; subclasses should implement this.

`save_hdf5(hdf5_saver, h5gr, subpath)`

Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute `format`.

**Parameters**

- `hdf5_saver` (*Hdf5Saver*) – Instance of the saving engine.
- `h5gr` (:class:`Group`) – HDF5 group which is supposed to represent `self`.
- `subpath` (*str*) – The name of `h5gr` with a `/` in the end.

`test_sanity()`

Sanity check, raises ValueErrors, if something is wrong.

`trivial_like_NNModel()`

Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

**Module description**

Spinless fermions with hopping and interaction.

**Todo:** add further terms (e.g. c^dagger c^dagger + h.c.) to the Hamiltonian.

### 7.11.8 hubbard

- full name: `tenpy.models.hubbard`
- parent module: `tenpy.models`
- type: module
Classes

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BoseHubbardChain</td>
<td>The BoseHubbardModel on a Chain, suitable for TEBD.</td>
</tr>
<tr>
<td>BoseHubbardModel</td>
<td>Spinless Bose-Hubbard model.</td>
</tr>
<tr>
<td>FermiHubbardChain</td>
<td>The FermiHubbardModel on a Chain, suitable for TEBD.</td>
</tr>
<tr>
<td>FermiHubbardModel</td>
<td>Spin-1/2 Fermi-Hubbard model.</td>
</tr>
</tbody>
</table>

BoseHubbardModel (model_params)

FermiHubbardModel (model_params)
BoseHubbardChain

- full name: tenpy.models.hubbard.BoseHubbardChain
- parent module: tenpy.models.hubbard
- type: class

Inheritance Diagram

![Inheritance Diagram](image)

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BoseHubbardChain.<strong>init</strong>(model_params)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>BoseHubbardChain.add_coupling(strength, u1,...)</td>
<td>Add two-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>BoseHubbardChain.add_coupling_term(strength,...)</td>
<td>Add a two-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>BoseHubbardChain.add_exponentially_decaying_coupling(...)</td>
<td>Add an exponentially decaying long-range coupling.</td>
</tr>
</tbody>
</table>

continues on next page
Table 114 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BoseHubbardChain.add_local_term</td>
<td>Add a single term to self.</td>
</tr>
<tr>
<td>BoseHubbardChain.add_multi_coupling</td>
<td>Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>BoseHubbardChain.add_multi_coupling_term</td>
<td>Add a general M-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>BoseHubbardChain.add_onsite</td>
<td>Add onsite terms to onsite_terms.</td>
</tr>
<tr>
<td>BoseHubbardChain.add_onsite_term</td>
<td>Add an onsite term on a given MPS site.</td>
</tr>
<tr>
<td>BoseHubbardChain.all_coupling_terms</td>
<td>Sum of all coupling_terms.</td>
</tr>
<tr>
<td>BoseHubbardChain.all_onsite_terms</td>
<td>Sum of all onsite_terms.</td>
</tr>
<tr>
<td>BoseHubbardChain.calc_H_MPO</td>
<td>Calculate MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td>BoseHubbardChain.calc_H_MPO_from_bond</td>
<td>Calculate the MPO Hamiltonian from the bond Hamiltonian.</td>
</tr>
<tr>
<td>BoseHubbardChain.calc_H_bond</td>
<td>Calculate the bond Hamiltonian from the MPO Hamiltonian.</td>
</tr>
<tr>
<td>BoseHubbardChain.calc_H_onsite</td>
<td>Calculate ( H_{\text{onsite}} ) from self.onsite_terms.</td>
</tr>
<tr>
<td>BoseHubbardChain.coupling_strength_add_ext_flux</td>
<td>Add an external flux to the coupling strength.</td>
</tr>
<tr>
<td>BoseHubbardChain.enlarge_mps_unit_cell</td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td>BoseHubbardChain.from_MPOModel</td>
<td>Initialize a NearestNeighborModel from a model class defining an MPO.</td>
</tr>
<tr>
<td>BoseHubbardChain.from_hdf5</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>BoseHubbardChain.group_sites</td>
<td>Modify self in place to group sites.</td>
</tr>
<tr>
<td>BoseHubbardChain.init_lattice</td>
<td>Initialize a lattice for the given model parameters.</td>
</tr>
<tr>
<td>BoseHubbardChain.init_sites</td>
<td>Define the local Hilbert space and operators; needs to be implemented in subclasses.</td>
</tr>
<tr>
<td>BoseHubbardChain.init_terms</td>
<td>Add the onsite and coupling terms to the model; subclasses should implement this.</td>
</tr>
<tr>
<td>BoseHubbardChain.save_hdf5</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>BoseHubbardChain.test_sanity</td>
<td>Sanity check, raises ValueError, if something is wrong.</td>
</tr>
<tr>
<td>BoseHubbardChain.trivial_like_NNModel</td>
<td>Return a NearestNeighborModel with same lattice, but trivial (( H=0 )) bonds.</td>
</tr>
</tbody>
</table>

class tenpy.models.hubbard.BoseHubbardChain(model_params)


The BoseHubbardModel on a Chain, suitable for TEBD.

See the BoseHubbardModel for the documentation of parameters.

add_coupling(strength, u1, op1, u2, op2, dx, op_string=None, str_on_first=True, raise_op2_left=False, category=None, plus_he=False)
Add two site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \( \sum_{x_0, \ldots, x_{\text{dim}-1}} \text{strength}[\text{shift}(\vec{x})] \ast \text{OP0} \ast \text{OP1} \), where \( \text{OP0} := \text{lat.unit_cell}[u0].\text{get_op}(\text{op0}) \) acts on the site \((x_0, \ldots, x_{\text{dim}-1}, u1)\), and \( \text{OP1} := \text{lat.unit_cell}[u1].\text{get_op}(\text{op1}) \) acts on the site \((x_0+dx[0], \ldots, x_{\text{dim}-1}+dx[\text{dim}-1], u1)\). Possible combinations \( x_0, \ldots, x_{\text{dim}-1} \) are determined from the boundary conditions in \text{possible_couplings}().

The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by \text{tenpy.models.lattice.possible_couplings}() and depends on the boundary conditions. The shift(...) depends on \( dx \), and is chosen such that the first entry strength[0, 0, \ldots] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to \text{coupling_terms}; this function does not rebuild the MPO.

Deprecated since version 0.4.0: The arguments \text{str_on_first} and \text{raise_op2_left} will be removed in version 1.0.0.

Parameters

- \text{strength} (scalar / array) – Prefactor of the coupling. May vary spatially (see above). If an array of smaller size is provided, it gets tiled to the required shape.
- \text{u1} (int) – Picks the site \text{lat.unit_cell}[u1] for OP1.
- \text{op1} (str) – Valid operator name of an onsite operator in \text{lat.unit_cell}[u1] for OP1.
- \text{u2} (int) – Picks the site \text{lat.unit_cell}[u2] for OP2.
- \text{op2} (str) – Valid operator name of an onsite operator in \text{lat.unit_cell}[u2] for OP2.
- \text{dx} (iterable of int) – Translation vector (of the unit cell) between OP1 and OP2. For a 1D lattice, a single int is also fine.
- \text{op_string} (str / None) – Name of an operator to be used between the OP1 and OP2 sites. Typical use case is the phase for a Jordan-Wigner transformation. The operator should be defined on all sites in the unit cell. If None, auto-determine whether a Jordan-Wigner string is needed, using \text{op_needs_JW}().
- \text{str_on_first} (bool) – Whether the provided \text{op_string} should also act on the first site. This option should be chosen as True for Jordan-Wigner strings. When handling Jordan-Wigner strings we need to extend the \text{op_string} to also act on the ‘left’, first site (in the sense of the MPS ordering of the sites given by the lattice). In this case, there is a well-defined ordering of the operators in the physical sense (i.e. which of \text{op1} or \text{op2} acts first on a given state). We follow the convention that \text{op2} acts first (in the physical sense), independent of the MPS ordering. Deprecated.
- \text{raise_op2_left} (bool) – Raise an error when \text{op2} appears left of \text{op1} (in the sense of the MPS ordering given by the lattice). Deprecated.
- \text{category} (str) – Descriptive name used as key for \text{coupling_terms}. Defaults to a string of the form "\{(\text{op1} \_i \_ \text{op2} \_j\}\}".
- \text{plus_hc} (bool) – If True, the hermitian conjugate of the terms is added automatically.

Examples

When initializing a model, you can add a term \( J \sum_{<i,j>} S_i^z S_j^z \) on all nearest-neighbor bonds of the lattice like this:
The strength can be an array, which gets tiled to the correct shape. For example, in a 1D Chain with an even number of sites and periodic (or infinite) boundary conditions, you can add alternating strong and weak couplings with a line like:

```python
>>> self.add_coupling([1.5, 1.], u1, 'Sz', u2, 'Sz', dx)
```

Make sure to use the `plus_hc` argument if necessary, e.g. for hoppings:

```python
>>> t = 1. # hopping strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(t, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```

Alternatively, you can add the hermitian conjugate terms explicitly. The correct way is to complex conjugate the strength, take the hermitian conjugate of the operators and swap the order (including a swap `u1 <-> u2`), and use the opposite direction `-dx`, i.e. the h.c. of `add_coupling(t, u1, 'A', u2, 'B', dx)` is `add_coupling(np.conj(t), u2, hc('B'), u1, hc('A'), -dx)`, where `hc` takes the hermitian conjugate of the operator names, see `get_hc_op_name()`. For spin-less fermions (FermionSite), this would be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(t, u1, 'Cd', u2, 'C', dx)
...    self.add_coupling(np.conj(t), u2, 'Cd', u1, 'C', -dx) # h.c.
```

With spin-full fermions (SpinHalfFermions), it could be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...    self.add_coupling(t, u1, 'Cdu', u2, 'Cd', dx) # Cdagger_up C_down
...    self.add_coupling(np.conj(t), u2, 'Cdd', u1, 'Cu', -dx) # h.c.
```

Note that the Jordan-Wigner strings for the fermions are added automatically!

See also:

- `add_onsite` Add terms acting on one site only.
- `add_multi_coupling_term` for terms on more than two sites.
- `add_coupling_term` Add a single term without summing over `vecx`.

### add_coupling_term

```python
add_coupling_term(strength, i, j, op_i, op_j, op_string='Id', category=None, plus_hc=False)
```

Add a two-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_coupling_term(...)`.

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use `add_local_term()` instead.

**Parameters**

- `strength` *(float)* – The strength of the coupling term.
• **i (int)** – The MPS indices of the two sites on which the operator acts. We require $0 \leq i < N\_sites$ and $i < j$, i.e., $op\_i$ acts “left” of $op\_j$. If $j \geq N\_sites$, it indicates couplings between unit cells of an infinite MPS.

• **j (int)** – The MPS indices of the two sites on which the operator acts. We require $0 \leq i < N\_sites$ and $i < j$, i.e., $op\_i$ acts “left” of $op\_j$. If $j \geq N\_sites$, it indicates couplings between unit cells of an infinite MPS.

• **op1 (str)** – Names of the involved operators.

• **op2 (str)** – Names of the involved operators.

• **op\_string (str)** – The operator to be inserted between $i$ and $j$.

• **category (str)** – Descriptive name used as key for coupling\_terms. Defaults to a string of the form "\{op1\}_i \{op2\}_j".

• **plus\_hc (bool)** – If True, the hermitian conjugate of the term is added automatically.

```python
add\_exponentially\_decaying\_coupling(strength, lambda\_\_, op\_i, op\_j, subsites=None, op\_string=None, plus\_hc=False)
```

Add an exponentially decaying long-range coupling.

$$
strength \sum_{i < j} \lambda^{i-j} A_{\text{subsites}[i]} B_{\text{subsites}[j]}
$$

Where the operator $A$ is given by $op\_i$, and $B$ is given by $op\_j$. Note that the sum over $ij$ is long-range, for infinite systems going beyond the MPS unit cell. Moreover, note that the distance in the exponent is the distance within subsites.

**Parameters**

• **strength (float)** – Overall prefactor.

• **lambda\_ (float)** – Decay-rate

• **op\_i (string)** – Names for the operators.

• **op\_j (string)** – Names for the operators.

• **subsites (None | 1D array)** – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. None selects all sites.

• **op\_string (None | str)** – The operator to be inserted between $A$ and $B$. If None, this function checks whether a fermionic "JW" string is needed for the given operators; in this case the right $op\_j$ acts first.

• **plus\_hc (bool)** – If True, the hermitian conjugate of the term is added automatically.

**Examples**

At least for simple enough 1D chains (or ladders), you can use `fit\_with\_sum\_of\_exp()` to approximate a long-range function with a few sum of exponentials and then add them with this function.

```python
>>> def decay(x):
...     return np.exp(-0.1*x) / x**2
>>> from tenpy\_tools\_fit import fit\_with\_sum\_of\_exp, sum\_of\_exp
>>> n\_exp = 5
>>> fit\_range = 50
>>> lam, pref = fit\_with\_sum\_of\_exp(decay, n\_exp, fit\_range)
>>> x = np.arange(1, fit\_range + 1)
>>> print('error in fit: {:.3e}'.format(np.sum(np.abs(decay(x) - sum\_of\_exp(lam, pref, x)))))
```

(continues on next page)
error in fit: 1.073e-04
>>> for pr, la in zip(pref, lam):
...     self.add_exponentially_decaying_coupling(pr, la, 'N', 'N')

add_local_term(strength, term, category=None, plus_hc=False)
Add a single term to self.

The represented term is strength times the product of the operators given in terms. Each operator is specified by the name and the site it acts on; the latter given by a lattice index, see Lattice.

Depending on the length of term, it can add an onsite term or a coupling term to onsite_terms or coupling_terms, respectively.

Parameters

- **strength** (float/complex) – The prefactor of the term.
- **term** (list of (str, array_like)) – List of tuples (opname, lat_idx) where opname is a string describing the operator acting on the site given by the lattice index lat_idx. Here, lat_idx is for example [x, y, u] for a 2D lattice, with u being the index within the unit cell.
- **category** – Descriptive name used as key for onsite_terms or coupling_terms.
- **plus_hc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

add_multi_coupling(strength, ops, _deprecate_1='DEPRECATED', _deprecate_2='DEPRECATED', op_string=None, category=None, plus_hc=False)
Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form \( \sum \delta x \text{strength}[\text{shift}(\vec{x})] \cdot O_{P_0} \cdot O_{P_1} \cdots \cdot O_{P_{M-1}} \), involving \( M \) operators. Here, \( O_{P_m} \) stands for the operator defined by the \( m \)-th tuple (opname, dx, u) given in the argument ops, which determines the position \( \vec{x} + \delta x \) and unit-cell index u of the site it acts on; the actual operator is given by self.latunit_cell[u].get_op(opname).

The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_multi_couplings() and depends on the boundary conditions. The \( \text{shift}(\ldots) \) depends on the \( dx \) entries of \( ops \) and is chosen such that the first entry \( \text{strength}[0, 0, \ldots] \) of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to coupling_terms; this function does not rebuild the MPO.

Deprecated since version 0.6.0: We switched from the three arguments \( u0, op0 \) and \( \text{other}_\text{op} \) with \( \text{other}_\text{ops}=[(u1, op1, dx1), (op2, u2, dx2), \ldots] \) to a single, equivalent argument \( ops \) which should now read \( ops=[(op0, dx0, u0), (op1, dx1, u1), (op2, dx2, u2), \ldots] \), where \( dx0 = [0]*self.lat.dim \). Note the changed order inside the tuples!

Parameters

- **strength** (scalar | array) – Prefactor of the coupling. May vary spatially, and is tiled to the required shape.
- **ops** (list of (opname, dx, u)) – Each tuple determines one operator of the coupling, see the description above. opname (str) is the name of the operator, dx (list of length lat.dim) is a translation vector, and u (int) is the index of lat.unit_cell on which the operator acts. The first entry of \( ops \) corresponds to \( O_{P_0} \) and acts last in the physical sense.
• **op_string**(str / None) – If a string is given, we use this as the name of an operator to be used inbetween the operators, excluding the sites on which any operators act. This operator should be defined on all sites in the unit cell.

If None, auto-determine whether a Jordan-Wigner string is needed (using \texttt{op\_needs\_JW()}) for each of the segments inbetween the operators and also on the sites of the left operators.

• **category**(str) – Descriptive name used as key for \texttt{coupling\_terms}. Defaults to a string of the form "\{op0\}_i \{other\_ops[0]\}_j \{other\_ops[1]\}_k ...".

• **plus hc**(bool) – If True, the hermitian conjugate of the terms is added automatically.

**Examples**

A call to \texttt{add\_coupling()} with arguments
\begin{verbatim}add_coupling(strength, u1, 'A', u2, 'B', dx)\end{verbatim}
is equivalent to the following:

\begin{verbatim}
>>> dx_0 = [0] * self.lat.dim  # = [0] for a 1D lattice, [0, 0] in 2D
>>> self.add_multi_coupling(strength, [('A', dx_0, u1), ('B', dx, u2)])
\end{verbatim}

To explicitly add the hermitian conjugate (instead of simply using \texttt{plus\_hc = True}), you need to take the complex conjugate of the strength, reverse the order of the operators and take the hermitian conjugates of the individual operator names (indicated by the \texttt{hc(...)}, see \texttt{get\_hc\_op\_name()}):

\begin{verbatim}
>>> self.add_multi_coupling(np.conj(strength), [(hc('B'), dx, u2), (hc('A'),
         -dx_0, u1)])
\end{verbatim}

See also:

- \texttt{add\_onsite} Add terms acting on one site only.
- \texttt{add\_coupling} Add terms acting on two sites.
- \texttt{add\_multi\_coupling\_term} Add a single term, not summing over the possible \( \vec{x} \).

\texttt{add\_multi\_coupling\_term}(strength, ijk, ops\_ijkl, op\_string=None, category=None, plus\_hc=False)

Add a general M-site coupling term on given MPS sites.

Wrapper for \texttt{self.coupling\_terms[category].add\_multi\_coupling\_term(...)}.

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use \texttt{add\_local\_term()} instead.

**Parameters**

• **strength**(float) – The strength of the coupling term.

• **ijk** (list of int) – The MPS indices of the sites on which the operators acts. With \( i, j, k, ... = ijk \), we require that they are ordered ascending, \( i < j < k < ... \) and that \( 0 <= i < N\_sites \). Indices >= N\_sites indicate couplings between different unit cells of an infinite MPS.

• **ops\_ijkl**(list of str) – Names of the involved operators on sites \( i, j, k, ... \).

• **op\_string**(list of str) – Names of the operator to be inserted between the operators, e.g., op\_string[0] is inserted between \( i \) and \( j \).
• **category** *(str)* – Descriptive name used as key for coupling_terms. Defaults to a string of the form "\( (\text{op0})_i (\text{op1})_j (\text{op2})_k \ldots \)".

• **plus hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.

### add_onsite *(strength, u, opname, category=None, plus hc=False)*

Add onsite terms to onsite_terms.

Add \( \sum_\mathbf{x} \text{strength}[\mathbf{x}] \times \text{OP} \) to the represented Hamiltonian, where the operator \( \text{OP}=\text{lat. unit_cell}[u].\text{get_op}(\text{opname}) \) acts on the site given by a lattice index \( (x_0, \ldots, x_{(\text{dim}-1)}, u) \).

The necessary terms are just added to onsite_terms; doesn’t rebuild the MPO.

**Parameters**

- **strength** *(scalar | array)* – Prefactor of the onsite term. May vary spatially. If an array of smaller size is provided, it gets tiled to the required shape.

- **u** *(int)* – Picks a Site `lat. unit_cell[u]` out of the unit cell.

- **opname** *(str)* – valid operator name of an onsite operator in `lat. unit_cell[u]`.

- **category** *(str)* – Descriptive name used as key for onsite_terms. Defaults to `opname`.

- **plus hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

See also:

- **add_coupling** Add a terms acting on two sites.

- **add_onsite_term** Add a single term without summing over \( \mathbf{vecx} \).

### add_onsite_term *(strength, i, op, category=None, plus hc=False)*

Add an onsite term on a given MPS site.

Wrapper for `self.onsite_terms[category].add_onsite_term(...)`.

**Parameters**

- **strength** *(float)* – The strength of the term.

- **i** *(int)* – The MPS index of the site on which the operator acts. We require \( 0 \leq i < L \).

- **op** *(str)* – Name of the involved operator.

- **category** *(str)* – Descriptive name used as key for onsite_terms. Defaults to `op`.

- **plus hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

### all_coupling_terms()

Sum of all coupling_terms.

### all_onsite_terms()

Sum of all onsite_terms.

### bond_energies *(psi)*

Calculate bond energies \(<\psi | H_{\text{bond}} | \psi>\).

**Parameters** `psi` *(MPS)* – The MPS for which the bond energies should be calculated.
Returns $E_{\text{bond}}$ – List of bond energies: for finite bc, $E_{\text{bond}}[i]$ is the energy of bond $i$, $i+1$. (i.e. we omit bond 0 between sites $L-1$ and 0); for infinite bc $E_{\text{bond}}[i]$ is the energy of bond $i-1$, $i$.

Return type 1D ndarray

calc_H_MPO (tol_zero=1e-15)
Calculate MPO representation of the Hamiltonian.

Uses onsite_terms and coupling_terms to build an MPOGraph (and then an MPO).

Parameters tol_zero (float) – Prefactors with abs(strength) < tol_zero are considered to be zero.

Returns H_MPO – MPO representation of the Hamiltonian.

Return type MPO

calc_H_MPO_from_bond (tol_zero=1e-15)
Calculate the MPO Hamiltonian from the bond Hamiltonian.

Parameters tol_zero (float) – Arrays with norm < tol_zero are considered to be zero.

Returns H_MPO – MPO representation of the Hamiltonian.

Return type MPO

calc_H_bond (tol_zero=1e-15)
calculate $H_{\text{bond}}$ from coupling_terms and onsite_terms.

Parameters tol_zero (float) – prefactors with abs(strength) < tol_zero are considered to be zero.

Returns H_bond – Bond terms as required by the constructor of NearestNeighborModel.
Legs are ['p0', 'p0*', 'p1', 'p1*']

Return type list of Array

:raises ValueError : if the Hamiltonian contains longer-range terms.

calc_H_bond_from_MPO (tol_zero=1e-15)
Calculate the bond Hamiltonian from the MPO Hamiltonian.

Parameters tol_zero (float) – Arrays with norm < tol_zero are considered to be zero.

Returns H_bond – Bond terms as required by the constructor of NearestNeighborModel.
Legs are ['p0', 'p0*', 'p1', 'p1*']

Return type list of Array

:raises ValueError : if the Hamiltonian contains longer-range terms.

calc_H_onsite (tol_zero=1e-15)
Calculate $H_{\text{onsite}}$ from self.onsite_terms.

Deprecated since version 0.4.0: This function will be removed in 1.0.0. Replace calls to this function by self.all_onsite_terms().remove_zeros(tol_zero).to_Arrays(self.lat.mps_sites()). You might also want to take explicit_plus_hc into account.

Parameters tol_zero (float) – prefactors with abs(strength) < tol_zero are considered to be zero.

Returns

* H_onsite (list of npc.Array)
- onsite terms of the Hamiltonian. If `explicit_plus_hc` is True, Hermitian conjugates of the onsite terms will be included.

`coupling_strength_add_ext_flux(strength, dx, phase)`

Add an external flux to the coupling strength.

When performing DMRG on a “cylinder” geometry, it might be useful to put an “external flux” through the cylinder. This means that a particle hopping around the cylinder should pick up a phase given by the external flux [resta1998]. This is also called “twisted boundary conditions” in literature. This function adds a complex phase to the `strength` array on some bonds, such that particles hopping in positive direction around the cylinder pick up $\exp(+i \text{phase})$.

**Warning:** For the sign of `phase` it is important that you consistently use the creation operator as `op1` and the annihilation operator as `op2` in `add_coupling()`.

**Parameters**

- `strength` *(scalar | array)* – The strength to be used in `add_coupling()`, when no external flux would be present.
- `dx` *(iterable of int)* – Translation vector (of the unit cell) between `op1` and `op2` in `add_coupling()`.
- `phase` *(iterable of float)* – The phase of the external flux for hopping in each direction of the lattice. E.g., if you want flux through the cylinder on which you have an infinite MPS, you should give `phase=[0, phi]` such that particles pick up a phase `phi` when hopping around the cylinder.

**Returns** `strength` – The strength array to be used as `strength` in `add_coupling()` with the given `dx`.

**Return type** complex array

**Examples**

Let’s say you have an infinite MPS on a cylinder, and want to add nearest-neighbor hopping of fermions with the `FermionSite`. The cylinder axis is the x-direction of the lattice, so to put a flux through the cylinder, you want particles hopping around the cylinder to pick up a phase `phi` given by the external flux.

```python
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> for ul, u2, dx in self.lat.pairs['nearest_neighbors']:
...     strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, ...
...     self.add_coupling(strength_with_flux, ul, 'Cd', u2, 'C', dx)
...     self.add_coupling(np.conj(strength_with_flux), u2, 'Cd', ul, 'C', -dx)
```

`enlarge_mps_unit_cell(factor=2)`

Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and can not be reverted.

**Parameters** `factor` *(int)* – The new number of sites in the MPS unit cell will be increased from $N_{sites}$ to $factor*N_{sites\_per\_ring}$. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from $(Lx, Ly, \ldots, Lu)$ to $(Lx*factor, Ly, \ldots, Lu)$. 

7.11. models
classmethod from_MPOModel (mpo_model)
Initialize a NearestNeighborModel from a model class defining an MPO.
This is especially useful in combination with MPOModel.group_sites().

Parameters

mpo_model (MPOModel) – A model instance implementing the MPO. Does not
need to be a NearestNeighborModel, but should only have nearest-neighbor couplings.

Examples

The SpinChainNNN2 has next-nearest-neighbor couplings and thus only implements an MPO:

```
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20, 'verbose': 0})
>>> print(isinstance(nnn_chain, NearestNeighborModel))
False
>>> print("range before grouping:", nnn_chain.H_MPO.max_range)
range before grouping: 2
```

By grouping each two neighboring sites, we can bring it down to nearest neighbors.

```
>>> grouped_sites = nnn_chain.group_sites(2)
>>> print("range after grouping:", nnn_chain.H_MPO.max_range)
range after grouping: 1
```

Yet, TEBD will not yet work, as the model doesn’t define H_bond. However, we can initialize a Nearest-
NeighborModel from the MPO:

```
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
>>> isinstance(nnn_chain_for_tebd, NearestNeighborModel)
True
```

classmethod from_hdf5 (hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.
This method reconstructs a class instance from the data saved with save_hdf5().

Parameters

• hdf5_loader (Hdf5Loader) – Instance of the loading engine.
• h5gr (Group) – HDF5 group which is represent the object to be constructed.
• subpath (str) – The name of h5gr with a '/' in the end.

Returns

obj – Newly generated class instance containing the required data.

Return type
cls
group_sites (n=2, grouped_sites=None)
Modify self in place to group sites.
Group each n sites together using the GroupedSite. This might allow to do TEBD with a Trotter
decomposition, or help the convergence of DMRG (in case of too long range interactions).
This has to be done after finishing initialization and can not be reverted.

Parameters

• n (int) – Number of sites to be grouped together.
• grouped_sites (None | list of GroupedSite) – The sites grouped together.
Returns grouped_sites – The sites grouped together.

Return type list of GroupedSite

init_lattice(model_params)

Initialize a lattice for the given model parameters.

This function reads out the model parameter lattice. This can be a full Lattice instance, in which case it is just returned without further action. Alternatively, the lattice parameter can be a string giving the name of one of the predefined lattices, which then gets initialized. Depending on the dimensionality of the lattice, this requires different model parameters.

Parameters model_params (dict) – The model parameters given to __init__.

Returns lat – An initialized lattice.

Return type Lattice

Options

option CouplingMPOModel.lattice: str | Lattice
The name of a lattice pre-defined in TeNPy to be initialized. Alternatively, a (possibly self-defined) Lattice instance. In the latter case, no further parameters are read out.

option CouplingMPOModel.bc_MPS: str
Boundary conditions for the MPS.

option CouplingMPOModel.order: str
The order of sites within the lattice for non-trivial lattices, e.g, 'default', 'snake', see ordering(). Only used if lattice is a string.

option CouplingMPOModel.L: int
The length in x-direction; only read out for 1D lattices. For an infinite system the length of the unit cell.

option CouplingMPOModel.Lx: int
option CouplingMPOModel.Ly: int
The length in x- and y-direction; only read out for 2D lattices. For "infinite" bc_MPS, the system is infinite in x-direction and Lx is the number of "rings" in the infinite MPS unit cell, while Ly gives the circumference around the cylinder or width of th the rung for a ladder (depending on bc_y).

option CouplingMPOModel.bc_y: str
"cylinder" | "ladder"; only read out for 2D lattices. The boundary conditions in y-direction.

option CouplingMPOModel.bc_x: str
"open" | "periodic". Can be used to force "periodic" boundaries for the lattice, i.e., for the couplings in the Hamiltonian, even if the MPS is finite. Defaults to "open" for bc_MPS="finite" and "periodic" for bc_MPS="infinite. If you are not aware of the consequences, you should probably not use "periodic" boundary conditions. (The MPS is still "open", so this will introduce long-range couplings between the first and last sites of the MPS!)

init_sites(model_params)

Define the local Hilbert space and operators; needs to be implemented in subclasses.

This function gets called by init_lattice() to get the Site for the lattice unit cell.

Note: Initializing the sites requires to define the conserved quantum numbers. All pre-defined sites accept conserve=None to disable using quantum numbers. Many models in TeNPy read out the conserve model parameter, which can be set to "best" to indicate the optimal parameters.
If you need to initialize more than one site, the function `tenpy.networks.site.set_common_charges()` should be helpful.

**Parameters**

- model_params (dict) – The model parameters given to `__init__`.

**Returns**

- sites – The local sites of the lattice, defining the local basis states and operators.

**Return type** (tuple of) `Site`

`init_terms(model_params)`

Add the onsite and coupling terms to the model; subclasses should implement this.

`save_hdf5(hdf5_saver, h5gr, subpath)`

Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute `'format'`.

**Parameters**

- hdf5_saver (`Hdf5Saver`) – Instance of the saving engine.
- h5gr (:class:`Group`) – HDF5 group which is supposed to represent `self`.
- subpath (str) – The name of `h5gr` with a `'/'` in the end.

`test_sanity()`

Sanity check, raises ValueErrors, if something is wrong.

`trivial_like_NNModel()`

Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

FermiHubbardChain

- full name: `tenpy.models.hubbard.FermiHubbardChain`
- parent module: `tenpy.models.hubbard`
- type: class
Methods

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FermiHubbardChain.<strong>init</strong>(model_params)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>FermiHubbardChain.add_coupling(strength, u1,...)</td>
<td>Add two-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>FermiHubbardChain.add_coupling_term(...)</td>
<td>Add a two-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td>FermiHubbardChains.add_exponentially_decaying_coupling(...)</td>
<td>Add an exponentially decaying long-range coupling.</td>
</tr>
<tr>
<td>FermiHubbardChain.add_local_term(strength, term)</td>
<td>Add a single term to self.</td>
</tr>
<tr>
<td>FermiHubbardChain.add_multi_coupling(...)</td>
<td>Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.</td>
</tr>
<tr>
<td>FermiHubbardChain.add_multi_coupling_term(...)</td>
<td>Add a general M-site coupling term on given MPS sites.</td>
</tr>
</tbody>
</table>

continues on next page
Table 115 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>FermiHubbardChain.add_onsite_term(strength, opname)</code></td>
<td>Add onsite terms to <code>onsite_terms</code>.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.add_onsite_term(strength,...)</code></td>
<td>Add an onsite term on a given MPS site.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.all_coupling_terms()</code></td>
<td>Sum of all <code>coupling_terms</code>.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.all_onsite_terms()</code></td>
<td>Sum of all <code>onsite_terms</code>.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.bond_energies(psi)</code></td>
<td>Calculate bond energies $\langle \psi</td>
</tr>
<tr>
<td><code>FermiHubbardChain.calc_H_bond_from_MPO(...)</code></td>
<td>Calculate the MPO Hamiltonian from the bond Hamiltonian.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.calc_H_bond_from_MPO(tol_zero)</code></td>
<td>Calculate $H_{bond}$ from <code>coupling_terms</code> and <code>onsite_terms</code>.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.calc_H_MPO(...)</code></td>
<td>Calculate the MPO representation of the Hamiltonian.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.calc_H_MPO_from_bond(...)</code></td>
<td>Calculate the bond Hamiltonian from the MPO Hamiltonian.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.calc_H_onsite(...)</code></td>
<td>Calculate $H_{onsite}$ from <code>self.onsite_terms</code>.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.coupling_strength_add_ext_flux(...)</code></td>
<td>Add an external flux to the coupling strength.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.enlarge_mps_unit_cell(factor)</code></td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.from_MPIModel(mpo_model)</code></td>
<td>Initialize a NearestNeighborModel from a model class defining an MPO.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.from_hdf5(hdf5_loader,...)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.group_sites([n,...,grouped_sites])</code></td>
<td>Modify <code>self</code> in place to group sites.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.init_lattice(model_params)</code></td>
<td>Initialize a lattice for the given model parameters.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.init_lattice(model_params)</code></td>
<td>Initialize a lattice for the given model parameters.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.init_sites(model_params)</code></td>
<td>Define the local Hilbert space and operators; needs to be implemented in subclasses.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.init_terms(model_params)</code></td>
<td>Add the onsite and coupling terms to the model; subclasses should implement this.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.save_hdf5(hdf5_saver,...)</code></td>
<td>Export <code>self</code> into a HDF5 file.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td><code>FermiHubbardChain.trivial_like_NNModel()</code></td>
<td>Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.</td>
</tr>
</tbody>
</table>

**class** `tenpy.models.hubbard.FermiHubbardChain(model_params)`

**Bases:** `tenpy.models.hubbard.FermiHubbardModel`, `tenpy.models.model.NearestNeighborModel`

The `FermiHubbardModel` on a Chain, suitable for TEBD.

See the `FermiHubbardModel` for the documentation of parameters.

**add_coupling(strength, ul, op1, u2, op2, dx, op_string=None, str_on_first=True, raise_op2_left=False, category=None, plus_hc=False)**

Add two-site coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form $\sum_{x_0,...,x_{dim-1}} \text{strength} [\text{shift}(\vec{x})] \cdot O_0 \cdot O_1$, where $O_0 := \text{lat.unit_cell}[u0].\text{get_op}(op0)$ acts on the site $(x_0, ..., x_{(dim-1)}, u1)$, and $O_1 := \text{lat.unit_cell}[u1].\text{get_op}(op1)$ acts on the site $(x_0+dx[0], ...,
Possible combinations \( x_0, \ldots, x_{(\text{dim}-1)} \) are determined from the boundary conditions in possible_couplings().

The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_couplings() and depends on the boundary conditions. The shift(...) depends on \( dx \), and is chosen such that the first entry strength[0, 0, \ldots] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to coupling_terms; this function does not rebuild the MPO.

Deprecated since version 0.4.0: The arguments str_on_first and raise_op2_left will be removed in version 1.0.0.

**Parameters**

- **strength** (scalar / array) – Prefactor of the coupling. May vary spatially (see above). If an array of smaller size is provided, it gets tiled to the required shape.
- **u1** (int) – Picks the site \( \text{lat.unit_cell}[u1] \) for OP1.
- **op1** (str) – Valid operator name of an onsite operator in \( \text{lat.unit_cell}[u1] \) for OP1.
- **u2** (int) – Picks the site \( \text{lat.unit_cell}[u2] \) for OP2.
- **op2** (str) – Valid operator name of an onsite operator in \( \text{lat.unit_cell}[u2] \) for OP2.
- **dx** (iterable of int) – Translation vector (of the unit cell) between OP1 and OP2. For a 1D lattice, a single int is also fine.
- **op_string** (str / None) – Name of an operator to be used between the OP1 and OP2 sites. Typical use case is the phase for a Jordan-Wigner transformation. The operator should be defined on all sites in the unit cell. If None, auto-determine whether a Jordan-Wigner string is needed, using op_needs_JW().
- **str_on_first** (bool) – Whether the provided op_string should also act on the first site. This option should be chosen as True for Jordan-Wigner strings. When handling Jordan-Wigner strings we need to extend the op_string to also act on the ‘left’, first site (in the sense of the MPS ordering of the sites given by the lattice). In this case, there is a well-defined ordering of the operators in the physical sense (i.e. which of op1 or op2 acts first on a given state). We follow the convention that op2 acts first (in the physical sense), independent of the MPS ordering. Deprecated.
- **raise_op2_left** (bool) – Raise an error when op2 appears left of op1 (in the sense of the MPS ordering given by the lattice). Deprecated.
- **category** (str) – Descriptive name used as key for coupling_terms. Defaults to a string of the form "\( \{\text{op1}\}_i \quad \{\text{op2}\}_j \)".
- **plus_hc** (bool) – If True, the hermitian conjugate of the terms is added automatically.

**Examples**

When initializing a model, you can add a term \( J \sum_{<i,j>} S_i^z S_j^z \) on all nearest-neighbor bonds of the lattice like this:

```python
>>> J = 1.  # the strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(J, u1, 'Sz', u2, 'Sz', dx)
```
The strength can be an array, which gets tiled to the correct shape. For example, in a 1D `Chain` with an even number of sites and periodic (or infinite) boundary conditions, you can add alternating strong and weak couplings with a line like:

```python
>>> self.add_coupling([[1.5, 1.], u1, 'Sz', u2, 'Sz', dx)
```

Make sure to use the `plus_hc` argument if necessary, e.g. for hoppings:

```python
>>> t = 1. # hopping strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx, plus_hc=True)
```

Alternatively, you can add the hermitian conjugate terms explicitly. The correct way is to complex conjugate the strength, take the hermitian conjugate of the operators and swap the order (including a swap `u1 <-> u2`), and use the opposite direction `-dx`, i.e. the h.c. of `add_coupling(t, u1, 'A', u2, 'B', dx)` is `add_coupling(np.conj(t), u2, hc('B'), u1, hc('A'), -dx)`, where `hc` takes the hermitian conjugate of the operator names, see `get_hc_op_name()`. For spin-less fermions (`FermionSite`), this would be

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cd', u2, 'C', dx)
...     self.add_coupling(np.conj(t), u2, 'Cd', u1, 'C', -dx) # h.c.
```

With spin-full fermions (`SpinHalfFermions`), it could be:

```python
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     self.add_coupling(t, u1, 'Cdu', u2, 'Cd', dx) # Cdagger_up C_down
...     self.add_coupling(np.conj(t), u2, 'Cdd', u1, 'Cu', -dx) # h.c.
```

Note that the Jordan-Wigner strings for the fermions are added automatically!

See also:

- `add_onsite` Add terms acting on one site only.
- `add_multi_coupling_term` for terms on more than two sites.
- `add_coupling_term` Add a single term without summing over `vecc`

```python
add_coupling_term(strength, i, j, op_i, op_j, op_string='Id', category=None, plus_hc=False)
```

Add a two-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_coupling_term(…)`.

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use `add_local_term()` instead.

**Parameters**

- `strength` (float) – The strength of the coupling term.
- `i` (int) – The MPS indices of the two sites on which the operator acts. We require `0 <= i < N_sites` and `i < j`, i.e., `op_i` acts “left” of `op_j`. If `j >= N_sites`, it indicates couplings between unit cells of an infinite MPS.
• \( j \) (int) – The MPS indices of the two sites on which the operator acts. We require \( 0 \leq i < N_{\text{sites}} \) and \( i < j \), i.e., \( op_i \) acts “left” of \( op_j \). If \( j \geq N_{\text{sites}} \), it indicates couplings between unit cells of an infinite MPS.

• \( \text{op1} \) (str) – Names of the involved operators.

• \( \text{op2} \) (str) – Names of the involved operators.

• \( \text{op_string} \) (str) – The operator to be inserted between \( i \) and \( j \).

• \( \text{category} \) (str) – Descriptive name used as key for coupling_terms. Defaults to a string of the form \( \{\text{op1}\}_i \{\text{op2}\}_j \).

• \( \text{plus hc} \) (bool) – If True, the hermitian conjugate of the term is added automatically.

\begin{align*}
\text{add_exponentially_decaying_coupling} & \quad \text{(strength, lambda, \ op_i, \ op_j, \ subsites=None,} \\
& \quad \text{op_string=None, plus hc=False)} \\
\text{Add an exponentially decaying long-range coupling.} \\
& \quad \text{strength} \sum_{i,j} \lambda^{|i-j|} A_{\text{subsites}[i]} B_{\text{subsites}[j]}
\end{align*}

Where the operator \( A \) is given by \( op_i \), and \( B \) is given by \( op_j \). Note that the sum over \( i,j \) is long-range, for infinite systems going beyond the MPS unit cell. Moreover, note that the distance in the exponent is the distance within subsites.

Parameters

• \( \text{strength} \) (float) – Overall prefactor.

• \( \text{lambda} \) (float) – Decay-rate

• \( \text{op_i} \) (string) – Names for the operators.

• \( \text{op_j} \) (string) – Names for the operators.

• \( \text{subsites} \) (None | 1D array) – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. None selects all sites.

• \( \text{op_string} \) (None | str) – The operator to be inserted between \( A \) and \( B \); If None, this function checks whether a fermionic "JW" string is needed for the given operators; in this case the right \( op_j \) acts first.

• \( \text{plus hc} \) (bool) – If True, the hermitian conjugate of the term is added automatically.

Examples

At least for simple enough 1D chains (or ladders), you can use \text{fit_with_sum_of_exp()} to approximate a long-range function with a few sum of exponentials and then add them with this function.

```python
>>> def decay(x):
...     return np.exp(-0.1*x) / x**2
>>> from tenpy.tools.fit import fit_with_sum_of_exp, sum_of_exp
>>> n_exp = 5
>>> fit_range = 50
>>> lam, pref = fit_with_sum_of_exp(decay, n_exp, fit_range)
>>> x = np.arange(1, fit_range + 1)
>>> print('error in fit: {0:.3e}'.format(np.abs(decay(x) - sum_of_exp(lam, pref, x))))
error in fit: 1.073e-04
>>> for pr, la in zip(pref, lam):
...     self.add_exponentially_decaying_coupling(pr, la, 'N', 'N')
```
add_local_term(strength, term, category=None, plus_hc=False)
Add a single term to self.

The represented term is strength times the product of the operators given in terms. Each operator is specified by the name and the site it acts on; the latter given by a lattice index, see Lattice.

Depending on the length of term, it can add an onsite term or a coupling term to onsite_terms or coupling_terms, respectively.

Parameters

- **strength** *(float/complex)* – The prefactor of the term.
- **term** *(list of (str, array_like))* – List of tuples *(opname, lat_idx)* where opname is a string describing the operator acting on the site given by the lattice index lat_idx. Here, lat_idx is for example *[x, y, u]* for a 2D lattice, with *u* being the index within the unit cell.
- **category** – Descriptive name used as key for onsite_terms or coupling_terms.
- **plus_hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

add_multi_coupling(strength, ops, _deprecate_1='DEPRECATED', _deprecate_2='DEPRECATED', op_string=None, category=None, plus_hc=False)
Add multi-site coupling terms to the Hamiltonian, summing over lattice sites.

Represented couplings of the form \( \sum_\vec{x} \text{strength}[[\text{shift}(\vec{x})] \cdot O_{P_0} \cdot O_{P_1} \cdot \ldots \cdot O_{P_{M-1}}, involving \( \( M \) operators. Here, \( O_{P_m} \) stands for the operator defined by the \( m \)-th tuple *(opname, dx, u)* given in the argument ops, which determines the position \( \vec{x} + \vec{dx} \) and unit-cell index \( u \) of the site it acts on; the actual operator is given by \( \text{self.lat.unit_cell}[u].get_op(opname) \).

The coupling strength may vary spatially if the given strength is a numpy array. The correct shape of this array is the coupling_shape returned by tenpy.models.lattice.possible_multi_couplings() and depends on the boundary conditions. The shift(...) depends on the dx entries of ops and is chosen such that the first entry strength*[0, 0, ...] of strength is the prefactor for the first possible coupling fitting into the lattice if you imagine open boundary conditions.

The necessary terms are just added to coupling_terms; this function does not rebuild the MPO.

Deprecated since version 0.6.0: We switched from the three arguments \( u0, op0 \) and other_op with other_ops=[*(u1, op1, dx1)*, *(op2, u2, dx2)*, ...] to a single, equivalent argument ops which should now read ops=[*(op0, dx0, u0)*, *(op1, dx1, u1)*, *(op2, dx2, u2)*, ...], where dx0 = *[0]*self.lat.dim. Note the changed order inside the tuples!

Parameters

- **strength** *(scalar | array)* – Prefactor of the coupling. May vary spatially, and is tiled to the required shape.
- **ops** *(list of (opname, dx, u))* – Each tuple determines one operator of the coupling, see the description above. opname (str) is the name of the operator, dx (list of length lat.dim) is a translation vector, and u (int) is the index of lat.unit.cell on which the operator acts. The first entry of ops corresponds to \( O_{P_0} \) and acts last in the physical sense.
- **op_string** *(str | None)* – If a string is given, we use this as the name of an operator to be used inbetween the operators, excluding the sites on which any operators act. This operator should be defined on all sites in the unit cell.
If None, auto-determine whether a Jordan-Wigner string is needed (using op_needs_JW()) for each of the segments inbetween the operators and also on the sites of the left operators.

- **category** *(str)* – Descriptive name used as key for coupling_terms. Defaults to a string of the form "\( \{\text{op0}\}_i \{\text{other_ops}[0]\}_j \{\text{other_ops}[1]\}_k \ldots \)."

- **plus_hc** *(bool)* – If True, the hermitian conjugate of the terms is added automatically.

**Examples**

A call to `add_coupling()` with arguments `add_coupling(strength, u1, 'A', u2, 'B', dx)` is equivalent to the following:

```python
>>> dx_0 = [0] * self.lat.dim  # = [0] for a 1D lattice, [0, 0] in 2D
>>> self.add_multi_coupling(strength, [('A', dx_0, u1), ('B', dx, u2)])
```

To explicitly add the hermitian conjugate (instead of simply using `plus_hc = True`), you need to take the complex conjugate of the strength, reverse the order of the operators and take the hermitian conjugates of the individual operator names (indicated by the `hc(...)`, see `get_hc_op_name()`):

```python
>>> self.add_multi_coupling(np.conj(strength), [(hc('B'), dx, u2), (hc('A'), ...
˓→dx_0, u1)])
```

**See also:**

- **add_onsite** Add terms acting on one site only.
- **add_coupling** Add terms acting on two sites.
- **add_multi_coupling_term** Add a single term, not summing over the possible \( \vec{x} \).

**add_multi_coupling_term** *(strength, ijk, ops_ijkl, op_string=None, category=None, plus_hc=False)*

Add a general M-site coupling term on given MPS sites.

Wrapper for `self.coupling_terms[category].add_multi_coupling_term(...)`.  

**Warning:** This function does not handle Jordan-Wigner strings! You might want to use `add_local_term()` instead.

**Parameters**

- **strength** *(float)* – The strength of the coupling term.

- **ijk** *(list of int)* – The MPS indices of the sites on which the operators acts. With \( i, j, k, \ldots = ijk \), we require that they are ordered ascending, \( i < j < k < \ldots \) and that \( 0 \leq i < N\text{sites} \). Inidces \( \geq N\text{sites} \) indicate couplings between different unit cells of an infinite MPS.

- **ops_ijkl** *(list of str)* – Names of the involved operators on sites \( i, j, k, \ldots \).

- **op_string** *(list of str)* – Names of the operator to be inserted between the operators, e.g., `op_string[0]` is inserted between \( i \) and \( j \).

- **category** *(str)* – Descriptive name used as key for coupling_terms. Defaults to a string of the form "\( \{\text{op0}\}_i \{\text{op1}\}_j \{\text{op2}\}_k \ldots \)."

- **plus_hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.
add_onsite (strength, u, opname, category=None, plus_hc=False)
Add onsite terms to onsite_terms.

Add \( \sum_{\vec{x}} \text{strength}[\vec{x}] \times \text{OP} \) to the represented Hamiltonian, where the operator \( \text{OP}=\text{lat}.unit\_cell[u].\text{get\_op}(\text{opname}) \) acts on the site given by a lattice index \( (x_0, \ldots, x_{\text{dim}-1}, u) \).

The necessary terms are just added to onsite_terms; doesn’t rebuild the MPO.

Parameters

- **strength** *(scalar | array)* – Prefactor of the onsite term. May vary spatially. If an array of smaller size is provided, it gets tiled to the required shape.
- **u** *(int)* – Picks a Site \( \text{lat}.\text{unit}\_\text{cell}[u] \) out of the unit cell.
- **opname** *(str)* – valid operator name of an onsite operator in \( \text{lat}.\text{unit}\_\text{cell}[u] \).
- **category** *(str)* – Descriptive name used as key for onsite_terms. Defaults to opname.
- **plus_hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.

See also:

add_coupling Add a terms acting on two sites.

add_onsite_term Add an onsite term on a given MPS site.

Wrapper for \( \text{self.onsite\_terms[category]}.\text{add\_onsite\_term}(\ldots) \).

Parameters

- **strength** *(float)* – The strength of the term.
- **i** *(int)* – The MPS index of the site on which the operator acts. We require \( 0 \leq i < L \).
- **op** *(str)* – Name of the involved operator.
- **category** *(str)* – Descriptive name used as key for onsite_terms. Defaults to op.
- **plus_hc** *(bool)* – If True, the hermitian conjugate of the term is added automatically.

all_coupling_terms ()
Sum of all coupling_terms.

all_onsite_terms ()
Sum of all onsite_terms.

bond_energies (psi)
Calculate bond energies \( <\psi|H_{\text{bond}}|\psi> \).

Parameters psi (MPS) – The MPS for which the bond energies should be calculated.

Returns E_bond – List of bond energies: for finite bc, \( E_{\text{Bond}[i]} \) is the energy of bond \( i, i+1 \) (i.e. we omit bond 0 between sites L-1 and 0); for infinite bc \( E_{\text{bond}[i]} \) is the energy of bond \( i-1, i \).

Return type 1D ndarray
calc_H_MPO (tol_zero=1e-15)
Calculate MPO representation of the Hamiltonian.

Uses onsite_terms and coupling_terms to build an MPOGraph (and then an MPO).

Parameters tol_zero (float) – Prefactors with abs(strength) < tol_zero are considered to be zero.

Returns H_MPO – MPO representation of the Hamiltonian.

Return type MPO

calc_H_MPO_from_bond (tol_zero=1e-15)
Calculate the MPO Hamiltonian from the bond Hamiltonian.

Parameters tol_zero (float) – Arrays with norm < tol_zero are considered to be zero.

Returns H_MPO – MPO representation of the Hamiltonian.

Return type MPO

calc_H_bond (tol_zero=1e-15)
calculate H_bond from coupling_terms and onsite_terms.

Parameters tol_zero (float) – prefactors with abs(strength) < tol_zero are considered to be zero.

Returns H_bond – Bond terms as required by the constructor of NearestNeighborModel.
Legs are ['p0', 'p0*', 'p1', 'p1*']

Return type list of Array
:raises ValueError : if the Hamiltonian contains longer-range terms.

calc_H_bond_from_MPO (tol_zero=1e-15)
Calculate the bond Hamiltonian from the MPO Hamiltonian.

Parameters tol_zero (float) – Arrays with norm < tol_zero are considered to be zero.

Returns H_bond – Bond terms as required by the constructor of NearestNeighborModel.
Legs are ['p0', 'p0*', 'p1', 'p1*']

Return type list of Array
:raises ValueError : if the Hamiltonian contains longer-range terms.

calc_H_onsite (tol_zero=1e-15)
Calculate H_onsite from self.onsite_terms.

Deprecated since version 0.4.0: This function will be removed in 1.0.0. Replace calls to this function by self.all_onsite_terms().remove_zeros(tol_zero).to_Arrays(self.lat.mps_sites()). You might also want to take explicit_plus_hc into account.

Parameters tol_zero (float) – prefactors with abs(strength) < tol_zero are considered to be zero.

Returns

* H_onsite (list of npc.Array)

  onsite terms of the Hamiltonian. If explicit_plus_hc is True, – Hermitian conjugates of the onsite terms will be included.

coupling_strength_add_ext_flux (strength, dx, phase)
Add an external flux to the coupling strength.
When performing DMRG on a “cylinder” geometry, it might be useful to put an “external flux” through the cylinder. This means that a particle hopping around the cylinder should pick up a phase given by the external flux [resta1998]. This is also called “twisted boundary conditions” in literature. This function adds a complex phase to the \texttt{strength} array on some bonds, such that particles hopping in positive direction around the cylinder pick up \( \exp(i \ \text{phase}) \).

**Warning:** For the sign of \texttt{phase} it is important that you consistently use the creation operator as \texttt{op1} and the annihilation operator as \texttt{op2} in \texttt{add_coupling()}.  

**Parameters**

- **\texttt{strength} (scalar / array)** – The strength to be used in \texttt{add_coupling()}, when no external flux would be present.
- **\texttt{dx} (iterable of int)** – Translation vector (of the unit cell) between \texttt{op1} and \texttt{op2} in \texttt{add_coupling()}.  
- **\texttt{phase} (iterable of float)** – The phase of the external flux for hopping in each direction of the lattice. E.g., if you want flux through the cylinder on which you have an infinite MPS, you should give \texttt{phase=[0, phi]} such that particles pick up a phase \( \text{phi} \) when hopping around the cylinder.

**Returns** \texttt{strength} – The strength array to be used as \texttt{strength} in \texttt{add_coupling()} with the given \texttt{dx}.

**Return type** complex array

**Examples**

Let’s say you have an infinite MPS on a cylinder, and want to add nearest-neighbor hopping of fermions with the \texttt{FermionSite}. The cylinder axis is the \texttt{x}-direction of the lattice, so to put a flux through the cylinder, you want particles hopping \textit{around} the cylinder to pick up a phase \( \text{phi} \) given by the external flux.

```python
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0, phi])
...     self.add_coupling(strength_with_flux, u1, 'Cd', u2, 'C', dx)
...     self.add_coupling(np.conj(strength_with_flux), u2, 'Cd', u1, 'C', -dx)
```

**enlarge_mps_unit_cell** \((\texttt{factor=2})\)

Repeat the unit cell for infinite MPS boundary conditions; in place.

This has to be done after finishing initialization and can not be reverted.

**Parameters** \texttt{factor} (\texttt{int}) – The new number of sites in the MPS unit cell will be increased from \(N_{\text{sites}}\) to \(\text{factor}\times N_{\text{sites}}\). Since MPS unit cells are repeated in the \texttt{x}-direction in our convention, the lattice shape goes from \((L_x, L_y, \ldots, L_u)\) to \((L_x\times\text{factor}, L_y, \ldots, L_u)\).

**classmethod** \texttt{from_MPOModel} \((\texttt{mpo_model})\)

Initialize a NearestNeighborModel from a model class defining an MPO.

This is especially useful in combination with \texttt{MPOModel.group_sites()}.  

---

*TeNPy, Release 0.7.2.dev55+68eae2c*
Parameters `mpo_model` (MPOModel) – A model instance implementing the MPO. Does not need to be a NearestNeighborModel, but should only have nearest-neighbor couplings.

Examples

The SpinChainNNN2 has next-nearest-neighbor couplings and thus only implements an MPO:

```python
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20, 'verbose': 0})
>>> print(isinstance(nnn_chain, NearestNeighborModel))
False
>>> print("range before grouping:", nnn_chain.H_MPO.max_range)
range before grouping: 2
```

By grouping each two neighboring sites, we can bring it down to nearest neighbors.

```python
>>> grouped_sites = nnn_chain.group_sites(2)
>>> print("range after grouping:", nnn_chain.H_MPO.max_range)
range after grouping: 1
```

Yet, TEBD will not yet work, as the model doesn’t define $H_{\text{bond}}$. However, we can initialize a Nearest-NeighborModel from the MPO:

```python
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
>>> isinstance(nnn_chain_for_tebd, NearestNeighborModel)
True
```

classmethod `from_hdf5` (hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

Parameters

- `hdf5_loader` (Hdf5Loader) – Instance of the loading engine.
- `h5gr` (Group) – HDF5 group which is represent the object to be constructed.
- `subpath` (str) – The name of `h5gr` with a ‘/’ in the end.

Returns `obj` – Newly generated class instance containing the required data.

Return type `cls`

group_sites (n=2, grouped_sites=\text{None})
Modify self in place to group sites.

Group each $n$ sites together using the `GroupedSite`. This might allow to do TEBD with a Trotter decomposition, or help the convergence of DMRG (in case of too long range interactions).

This has to be done after finishing initialization and can not be reverted.

Parameters

- `n` (int) – Number of sites to be grouped together.
- `grouped_sites` (\text{None} | list of GroupedSite) – The sites grouped together.

Returns `grouped_sites` – The sites grouped together.

Return type list of `GroupedSite`
init_lattice(model_params)
Initialize a lattice for the given model parameters.

This function reads out the model parameter `lattice`. This can be a full `Lattice` instance, in which case it is just returned without further action. Alternatively, the `lattice` parameter can be a string giving the name of one of the predefined lattices, which then gets initialized. Depending on the dimensionality of the lattice, this requires different model parameters.

Parameters

- **model_params** (dict) – The model parameters given to `__init__`.

Returns

- **lat** – An initialized lattice.

Return type

- `Lattice`

Options

- **option** CouplingMPOModel.lattice: str | Lattice
  The name of a lattice pre-defined in TeNPy to be initialized. Alternatively, a (possibly self-defined) Lattice instance. In the latter case, no further parameters are read out.

- **option** CouplingMPOModel.bc_MPS: str
  Boundary conditions for the MPS.

- **option** CouplingMPOModel.order: str
  The order of sites within the lattice for non-trivial lattices, e.g., 'default', 'snake', see `ordering()`. Only used if `lattice` is a string.

- **option** CouplingMPOModel.L: int
  The length in x-direction; only read out for 1D lattices. For an infinite system the length of the unit cell.

- **option** CouplingMPOModel.Lx: int

- **option** CouplingMPOModel.Ly: int
  The length in x- and y-direction; only read out for 2D lattices. For "infinite" `bc_MPS`, the system is infinite in x-direction and `Lx` is the number of “rings” in the infinite MPS unit cell, while `Ly` gives the circumference around the cylinder or width of th te rung for a ladder (depending on `bc_y`).

- **option** CouplingMPOModel.bc_y: str
  "cylinder" | "ladder"; only read out for 2D lattices. The boundary conditions in y-direction.

- **option** CouplingMPOModel.bc_x: str
  "open" | "periodic". Can be used to force “periodic” boundaries for the lattice, i.e., for the couplings in the Hamiltonian, even if the MPS is finite. Defaults to "open" for `bc_MPS="finite"` and "periodic" for `bc_MPS="infinite"`. If you are not aware of the consequences, you should probably not use “periodic” boundary conditions. (The MPS is still “open”, so this will introduce long-range couplings between the first and last sites of the MPS!)

init_sites(model_params)
Define the local Hilbert space and operators; needs to be implemented in subclasses.

This function gets called by `init_lattice()` to get the `Site` for the lattice unit cell.

Note: Initializing the sites requires to define the conserved quantum numbers. All pre-defined sites accept `conserve=None` to disable using quantum numbers. Many models in TeNPy read out the `conserve` model parameter, which can be set to "best" to indicate the optimal parameters.

If you need to initialize more than one site, the function `tenpy.networks.site.set_common_charges()` should be helpful.
Parameters **model_params** *(dict)* – The model parameters given to *__init__*.  

Returns **sites** – The local sites of the lattice, defining the local basis states and operators.  

Return type *(tuple of)* **Site**  

**init_terms** *(model_params)*  
Add the onsite and coupling terms to the model; subclasses should implement this.  

**save_hdf5** *(hdf5_saver, h5gr, subpath)*  
Export *self* into a HDF5 file.  

This method saves all the data it needs to reconstruct *self* with *from_hdf5()* .  

This implementation saves the content of *__dict__* with *save_dict_content()* , storing the format under the attribute *'format'*.  

Parameters  

• **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.  

• **h5gr** *(<class`Group`>)* – HDF5 group which is supposed to represent *self*.  

• **subpath** *(str)* – The name of *h5gr* with a '/ ' in the end.  

**test_sanity** ()  
Sanity check, raises ValueErrors, if something is wrong.  

**trivial_like_NNModel** ()  
Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.  

Module description  

Bosonic and fermionic Hubbard models.  

7.11.9 hofstadter  

• full name: tenpy.models.hofstadter  

• parent module: tenpy.models  

• type: module
Classes

Hdf5Exportable

Model

CouplingModel MPOModel

CouplingMPOModel

HofstadterBosons HofstadterFermions

HofstadterBosons(model_params) Bosons on a square lattice with magnetic flux.
HofstadterFermions(model_params) Fermions on a square lattice with magnetic flux.

Functions

gauge_hopping(model_params) Compute hopping amplitudes for the Hofstadter models based on a gauge choice.

**gauge_hopping**

- full name: tenpy.models.hofstadter.gauge_hopping
- parent module: tenpy.models.hofstadter
- type: function

    tenpy.models.hofstadter.gauge_hopping(model_params)
    Compute hopping amplitudes for the Hofstadter models based on a gauge choice.

    In the Hofstadter model, the magnetic field enters as an Aharonov-Bohm phase. This phase is dependent on a choice of gauge, which simultaneously defines a ‘magnetic unit cell’ (MUC).
The magnetic unit cell is the smallest set of lattice plaquettes that encloses an integer number of flux quanta. It can be user-defined by setting mx and my, but for common gauge choices is computed based on the flux density.

**The gauge choices are:**

- **‘landau_x’**: Landau gauge along the x-axis. The magnetic unit cell will have shape \( \text{max}(mx, 1) \). For flux densities \( p/q, mx \) will default to \( q \). Example: at a flux density \( 1/3 \), the magnetic unit cell will have shape \( (3, 1) \), so it encloses exactly 1 flux quantum.

- **‘landau_y’**: Landau gauge along the y-axis. The magnetic unit cell will have shape \( (1, \text{my}) \). For flux densities \( p/q, my \) will default to \( q \). Example: at a flux density \( 3/7 \), the magnetic unit cell will have shape \( (1, 7) \), so it encloses exactly 3 flux quanta.

- **‘symmetric’**: symmetric gauge. The magnetic unit cell will have shape \( (mx, my) \), with \( mx = my \). For flux densities \( p/q, mx \) and \( my \) will default to \( q \) Example: at a flux density \( 4/9 \), the magnetic unit cell will have shape \( (9, 9) \).

**Parameters**

- **gauge** ('landau_x' | 'landau_y' | 'symmetric') – Choice of the gauge, see table above.

- **mx** (int | None) – Dimensions of the magnetic unit cell in terms of lattice sites. None defaults to the minimal choice compatible with gauge and \( \phi_{pq} \).

- **my** (int | None) – Dimensions of the magnetic unit cell in terms of lattice sites. None defaults to the minimal choice compatible with gauge and \( \phi_{pq} \).

- **Jx** (float) – ‘Bare’ hopping amplitudes (without phase). Without any flux we have \( \text{hop}_x = -Jx \) and \( \text{hop}_y = -Jy \).

- **Jy** (float) – ‘Bare’ hopping amplitudes (without phase). Without any flux we have \( \text{hop}_x = -Jx \) and \( \text{hop}_y = -Jy \).

- **phi_pq** (tuple (int, int)) – Magnetic flux as a fraction \( p/q \), defined as \( (p, q) \)

**Returns** \( \text{hop}_x, \text{hop}_y \) – Hopping amplitudes to be used as prefactors for \( c_{x,y}^\dagger c_{x+1,y} \) (\( \text{hop}_x \)) and \( c_{x,y}^\dagger c_{x,y+1} \) (\( \text{hop}_y \)), respectively, with the necessary phases for the gauge.

**Return type** float | array

**Module description**

Cold atomic (Harper-)Hofstadter model on a strip or cylinder.

**Todo:** WARNING: These models are still under development and not yet tested for correctness. Use at your own risk! Replicate known results to confirm models work correctly. Long term: implement different lattices. Long term: implement variable hopping strengths \( Jx, Jy \).
7.11.10 haldane

- full name: tenpy.models.haldane
- parent module: tenpy.models
- type: module

**Classes**

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BosonicHaldaneModel(model_params)</td>
<td>Hardcore bosonic Haldane model.</td>
</tr>
<tr>
<td>FermionicHaldaneModel(model_params)</td>
<td>Spinless fermionic Haldane model.</td>
</tr>
</tbody>
</table>

**Module description**

Bosonic and fermionic Haldane models.
7.11.11 toric_code

- full name: tenpy.models.toric_code
- parent module: tenpy.models
- type: module

Classes

---

**DualSquare**

- **(Lx, Ly, sites, **kwargs)**
  - The dual lattice of the square lattice (again square).

**ToricCode**

- **(model_params)**
  - Toric code model.

---

- full name: tenpy.models.toric_code.DualSquare
- parent module: tenpy.models.toric_code
- type: class
## Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>DualSquare.__init__(Lx, Ly, sites, **kwargs)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>DualSquare.count_neighbors([u, key])</code></td>
<td>Count e.g.</td>
</tr>
<tr>
<td><code>DualSquare.coupling_shape(dx)</code></td>
<td>Calculate correct shape of the strengths for a coupling.</td>
</tr>
<tr>
<td><code>DualSquare.enlarge_mps_unit_cell([factor])</code></td>
<td>Repeat the unit cell for infinite MPS boundary conditions; in place.</td>
</tr>
<tr>
<td><code>DualSquare.from_hdf5(hdf5_loader, h5gr, subpath)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>DualSquare.lat2mps_idx(lat_idx)</code></td>
<td>Translate lattice indices ((x_0, \ldots, x_{(D-1)}, u)) to MPS index (i).</td>
</tr>
<tr>
<td><code>DualSquare.mps2lat_idx(i)</code></td>
<td>Translate MPS index (i) to lattice indices ((x_0, \ldots, x_{(dim-1)}, u)).</td>
</tr>
<tr>
<td><code>DualSquare.mps2lat_values(A[, axes, u])</code></td>
<td>Reshape/reorder (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td><code>DualSquare.mps2lat_values_masked(A[, axes, ...])</code></td>
<td>Reshape/reorder an array (A) to replace an MPS index by lattice indices.</td>
</tr>
<tr>
<td><code>DualSquare.mps_idx_fix_u([u])</code></td>
<td>Return an index array of MPS indices for which the site within the unit cell is (u).</td>
</tr>
<tr>
<td><code>DualSquare.mps_lat_idx_fix_u([u])</code></td>
<td>Similar as <code>mps_idx_fix_u()</code>, but return also the corresponding lattice indices.</td>
</tr>
<tr>
<td><code>DualSquare.mps_sites()</code></td>
<td>Return a list of sites for all MPS indices.</td>
</tr>
<tr>
<td><code>DualSquare.multi_coupling_shape(dx)</code></td>
<td>Calculate correct shape of the strengths for a multi_coupling.</td>
</tr>
<tr>
<td><code>DualSquare.number_nearest_neighbors([u])</code></td>
<td>Deprecated.</td>
</tr>
<tr>
<td><code>DualSquare.number_next_nearest_neighbors([u])</code></td>
<td>Deprecated.</td>
</tr>
<tr>
<td><code>DualSquare.ordering(order)</code></td>
<td>Provide possible orderings of the (N) lattice sites.</td>
</tr>
<tr>
<td><code>DualSquare.plot_basis(ax[, origin, shade])</code></td>
<td>Plot arrows indicating the basis vectors of the lattice.</td>
</tr>
<tr>
<td><code>DualSquare.plot_bc_identified(ax[, ...])</code></td>
<td>Mark two sites identified by periodic boundary conditions.</td>
</tr>
<tr>
<td><code>DualSquare.plot_coupling(ax[, coupling, wrap])</code></td>
<td>Plot lines connecting nearest neighbors of the lattice.</td>
</tr>
<tr>
<td><code>DualSquare.plot_order(ax[, order, textkwargs])</code></td>
<td>Plot a line connecting sites in the specified “order” and text labels enumerating them.</td>
</tr>
</tbody>
</table>

continues on next page
Table 120 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>DualSquare.plot_sites(ax[, markers])</code></td>
<td>Plot the sites of the lattice with markers.</td>
</tr>
<tr>
<td><code>DualSquare.position(lat_idx)</code></td>
<td>return ‘space’ position of one or multiple sites.</td>
</tr>
<tr>
<td><code>DualSquare.possible_couplings(u1, u2, dx)</code></td>
<td>Find possible MPS indices for two-site couplings.</td>
</tr>
<tr>
<td><code>DualSquare.possible_multi_couplings(ops)</code></td>
<td>Generalization of <code>possible_couplings()</code> to couplings with more than 2 sites.</td>
</tr>
<tr>
<td><code>DualSquare.save_hdf5(hdf5_saver, h5gr, sub-path)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>DualSquare.site(i)</code></td>
<td>return <code>Site</code> instance corresponding to an MPS index i</td>
</tr>
<tr>
<td><code>DualSquare.test_sanity()</code></td>
<td>Sanity check.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

- `DualSquare.Lu`
- `DualSquare.boundary_conditions` Human-readable list of boundary conditions from `bc` and `bc_shift`.
- `DualSquare.dim` The dimension of the lattice.
- `DualSquare.nearest_neighbors`
- `DualSquare.next_nearest_neighbors`
- `DualSquare.next_next_nearest_neighbors`
- `DualSquare.order` Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

```python
class tenpy.models.toric_code.DualSquare(Lx, Ly, sites, **kwargs)
    Bases: tenpy.models.lattice.Lattice

    The dual lattice of the square lattice (again square).

    The sites in this lattice correspond to the vertical and horizontal (nearest neighbor) bonds of a common Square lattice with the same dimensions Lx, Ly.

    Parameters

    - `Lx (int)` – Dimensions of the original lattice. This lattice has 2*Lx*Ly sites.
    - `Ly (int)` – Dimensions of the original lattice. This lattice has 2*Lx*Ly sites.
    - `sites (Site)` – The sites for the horizontal (first entry) and vertical (second entry) bonds.
    - `**kwargs` – Additional keyword arguments given to the `Lattice`. `basis`, `pos` and `pairs` are set accordingly.

    `ordering(order)` Provide possible orderings of the N lattice sites.

    The following orders are defined in this method compared to `tenpy.models.lattice.Lattice. ordering()`:

    | order | equivalent priority | equivalent snake_winding |
    |-------|---------------------|--------------------------|
    | 'default' | (0, 2, 1) | (False, False, False) |

    `property boundary_conditions` Human-readable list of boundary conditions from `bc` and `bc_shift`. |
Returns `boundary_conditions` – List of "open" or "periodic", one entry for each direction of the lattice.

Return type list of str

`count_neighbors`(u=0, key='nearest_neighbors')
Count e.g. the number of nearest neighbors for a site in the bulk.

Parameters
- `u` (int) – Specifies the site in the unit cell, for which we should count the number of neighbors (or whatever `key` specifies).
- `key` (str) – Key of pairs to select what to count.

Returns `number` – Number of nearest neighbors (or whatever `key` specified) for the `u`-th site in the unit cell, somewhere in the bulk of the lattice. Note that it might not be the correct value at the edges of a lattice with open boundary conditions.

Return type int

`coupling_shape`(dx)
Calculate correct shape of the strengths for a coupling.

Parameters `dx` (tuple of int) – Translation vector in the lattice for a coupling of two operators. Corresponds to `dx` argument of `tenpy.models.model.CouplingModel.add_multi_coupling()`.

Returns
- `coupling_shape` (tuple of int) – Len `dim`. The correct shape for an array specifying the coupling strength. `lat_indices` has only rows within this shape.
- `shift_lat_indices`(array) – Translation vector from origin to the lower left corner of box spanned by `dx`.

property `dim` The dimension of the lattice.

`enlarge_mps_unit_cell`(factor=2)
Repeat the unit cell for infinite MPS boundary conditions; in place.

Parameters `factor` (int) – The new number of sites in the MPS unit cell will be increased from `N_sites` to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the x-direction in our convention, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

classmethod `from_hdf5`(hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

Parameters
- `hdf5_loader` (Hdf5Loader) – Instance of the loading engine.
- `h5gr` (Group) – HDF5 group which is represent the object to be constructed.
- `subpath` (str) – The `name` of `h5gr` with a '/' in the end.

Returns `obj` – Newly generated class instance containing the required data.

Return type cls

`lat2mps_idx`(lat_idx)
Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index `i`.

7.11. models 521
Parameters `lat_idx` (array_like [.., dim+1]) – The last dimension corresponds to lattice indices \((x_0, \ldots, x_{(D-1)}, u)\). All lattice indices should be positive and smaller than the corresponding entry in `self.shape`. Exception: for “infinite” `bc_MPS`, an \(x_0\) outside indicates shifts across the boundary.

Returns `i` – MPS index/indices corresponding to `lat_idx`. Has the same shape as `lat_idx` without the last dimension.

Return type array_like

`mps2lat_idx(i)`

Translate MPS index `i` to lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\).

Parameters `i` (int | array_like of int) – MPS index/indices.

Returns `lat_idx` – First dimensions like `i`, last dimension has len `dim+1` and contains the lattice indices \((x_0, \ldots, x_{(dim-1)}, u)\) corresponding to `i`. For `i` across the MPS unit cell and “infinite” `bc_MPS`, we shift \(x_0\) accordingly.

Return type array

`mps2lat_values(A, axes=0, u=None)`

Reshape/reorder `A` to replace an MPS index by lattice indices.

Parameters
- `A` (ndarray) – Some values. Must have `A.shape[axes] = self.N_sites` if `u` is None, or `A.shape[axes] = self.N_cells` if `u` is an int.
- `axes` ((iterable of) int) – chooses the axis which should be replaced.
- `u` (None | int) – Optionally choose a subset of MPS indices present in the axes of `A`, namely the indices corresponding to `self.unit_cell[u]`, as returned by `mps_idx_fix_u()`. The resulting array will not have the additional dimension(s) of `u`.

Returns `res_A` – Reshaped and reordered versions of `A`. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index `j` maps to lattice site \((x0, x1, x2)\), then `res_A[..., x0, x1, x2, ...] = A[..., j, ...]`.

Return type ndarray

Examples

Say you measure exception values of an onsite term for an MPS, which gives you an 1D array `A`, where `A[i]` is the expectation value of the site given by `self.mps2lat_idx(i)`. Then this function gives you the expectation values ordered by the lattice:

```python
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[tuple(lat.mps2lat_idx(5))] == A[5]
True
```

If you have a correlation function `C[i, j]`, it gets just slightly more complicated:

```python
>>> print(lat.shape, C.shape)
(10, 3, 2) (60, 60)
```
If the unit cell consists of different physical sites, an onsite operator might be defined only on one of the sites in the unit cell. Then you can use `mps_idx_fix_u()` to get the indices of sites it is defined on, measure the operator on these sites, and use the argument `u` of this function.

```python
>>> u = 0
>>> idx_subset = lat.mps_idx_fix_u(u)
>>> A_u = A[idx_subset]
>>> A_u_res = lat.mps2lat_values(A_u, u=u)
>>> A_u_res.shape
(10, 3)
>>> np.all(A_res[:, :, u] == A_u_res[:, :])
True
```

**mps2lat_values_masked**

Reshape/reorder an array `A` to replace an MPS index by lattice indices.

This is a generalization of `mps2lat_values()` allowing for the case of an arbitrary set of MPS indices present in each axis of `A`.

**Parameters**

- `A` *(ndarray)* – Some values.
- `axes` *(iterable of int)* – Chooses the axis of `A` which should be replaced. If multiple axes are given, you also need to give multiple index arrays as `mps_inds`.
- `mps_inds` *(list of 1D ndarray)* – Specifies for each axis in `axes`, for which MPS indices we have values in the corresponding axis of `A`. Defaults to `[np.arange(A.shape[ax]) for ax in axes]`. For indices across the MPS unit cell and “infinite” `bc_MPS`, we shift `x_0` accordingly.
- `include_u` *(list of bool)* – Specifies for each axis in `axes`, whether the `u` index of the lattice should be included into the output array `res_A`. Defaults to `len(self.unit_cell) > 1`.

**Returns** `res_A` – Reshaped and reordered copy of `A`. Such that MPS indices along the specified axes are replaced by lattice indices, i.e., if MPS index `j` maps to lattice site `(x0, x1, x2)`, then `res_A[..., x0, x1, x2, ...] = A[..., mps_inds[j], ...].

**Return type** `np.ma.MaskedArray`

**mps_idx_fix_u** *(u=None)*

return an index array of MPS indices for which the site within the unit cell is `u`.

If you have multiple sites in your unit-cell, an onsite operator is in general not defined for all sites. This functions returns an index array of the mps indices which belong to sites given by `self.unit_cell[u].

**Parameters** `u` *(None / int)* – Selects a site of the unit cell. `None` (default) means all sites.

**Returns** `mps_idx` – MPS indices for which `self.site(i)` is `self.unit_cell[u]. Ordered ascending.

**Return type** `array`

**mps_lat_idx_fix_u** *(u=None)*

Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
Parameters  

\(u\) (None | int) – Selects a site of the unit cell. None (default) means all sites.

Returns

- **mps_idx** (array) – MPS indices \(i\) for which \(\text{self.site}(i)\) is \(\text{self.unit_cell}[u]\).
- **lat_idx** (2D array) – The row \(j\) contains the lattice index (without \(u\)) corresponding to \(\text{mps_idx}[j]\).

**mps_sites()**

Return a list of sites for all MPS indices.

Equivalent to \([\text{self.site}(i)\text{ for }i\text{ in range(self.N_sites)}]\).

This should be used for sites of 1D tensor networks (MPS, MPO,...).

**multi_coupling_shape** (\(dx\))

Calculate correct shape of the strengths for a multi_coupling.

Parameters  

\(dx\) (2D array, shape (N_ops, dim)) – \(dx[i, :]\) is the translation vector in the lattice for the \(i\)-th operator. Corresponds to the \(dx\) of each operator given in the argument \(ops\) of \(\text{tenpy.models.model.CouplingModel.add_multi_coupling()}\).

Returns

- **coupling_shape** (tuple of int) – Len \(dim\). The correct shape for an array specifying the coupling strength. \(lat_indices\) has only rows within this shape.
- **shift_lat_indices** (array) – Translation vector from origin to the lower left corner of box spanned by \(dx\). (Unlike for coupling_shape() it can also contain entries > 0)

**number_nearest_neighbors** (\(u=0\))

Deprecated.

Deprecated since version 0.5.0: Use count_neighbors() instead.

**number_next_nearest_neighbors** (\(u=0\))

Deprecated.

Deprecated since version 0.5.0: Use count_neighbors() instead.

**property order**

Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

Each row of the array contains the lattice indices for one site, the order of the rows thus specifies a path through the lattice, along which an MPS will wind through through the lattice.

You can visualize the order with plot_order().

**plot_basis** (\(ax\), origin=(0.0, 0.0), shade=None, **kwargs)

Plot arrows indicating the basis vectors of the lattice.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
- ****kwargs – Keyword arguments for ax.arrow.

**plot_bc_identified** (\(ax\), direction=- 1, origin=None, cylinder_axis=False, **kwargs)

Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

Parameters

- **ax** (matplotlib.axes.Axes) – The axes on which we should plot.
• **direction (int)** – The direction of the lattice along which we should mark the identified sites. If None, mark it along all directions with periodic boundary conditions.

• **cylinder_axis (bool)** – Whether to plot the cylinder axis as well.

• **origin (None | np.ndarray)** – The origin starting from where we mark the identified sites. Defaults to the first entry of `unit_cell_positions`.

• **kwargs** – Keyword arguments for the used `ax.plot`.

**plot_coupling (ax, coupling=None, wrap=False, **kwargs)**
Plot lines connecting nearest neighbors of the lattice.

Parameters

• **ax (matplotlib.axes.Axes)** – The axes on which we should plot.

• **coupling (list of (u1, u2, dx))** – By default (None), use `self.pairs['nearest_neighbors']`. Specifies the connections to be plotted; iterating over lattice indices `(i0, i1, ... )`, we plot a connection from the site `(i0, i1, ... , u1)` to the site `(i0+dx[0], i1+dx[1], ... , u2)`, taking into account the boundary conditions.

• **wrap (bool)** – If True, wrap

• **kwargs** – Further keyword arguments given to `ax.plot()`.

**plot_order (ax, order=None, textkwars={'color': 'r'}, **kwargs)**
Plot a line connecting sites in the specified “order” and text labels enumerating them.

Parameters

• **ax (matplotlib.axes.Axes)** – The axes on which we should plot.

• **order (None | 2D array (self.N_sites, self.dim+1))** – The order as returned by `ordering()`; by default (None) use `order`.

• **textkwars (None | dict)** – If not None, we add text labels enumerating the sites in the plot. The dictionary can contain keyword arguments for `ax.text()`.

• **kwargs** – Further keyword arguments given to `ax.plot()`.

**plot_sites (ax, markers=['o', '^', 's', 'p', 'h', 'D'], **kwargs)**
Plot the sites of the lattice with markers.

Parameters

• **ax (matplotlib.axes.Axes)** – The axes on which we should plot.

• **markers (list)** – List of values for the keyword marker of `ax.plot()` to distinguish the different sites in the unit cell, a site `u` in the unit cell is plotted with a marker `markers[u % len(markers)]`.

• **kwargs** – Further keyword arguments given to `ax.plot()`.

**position (lat_idx)**
return ‘space’ position of one or multiple sites.

Parameters **lat_idx (ndarray, (... , dim+1))** – Lattice indices.

Returns **pos** – The position of the lattice sites specified by `lat_idx` in real-space.

Return type **ndarray, (... , dim)**
possible_couplings \((u1, u2, dx)\)
Find possible MPS indices for two-site couplings.

For periodic boundary conditions \((bc[a] == \text{False})\) the index \(x_a\) is taken modulo \(Ls[a]\) and runs through \(\text{range}(Ls[a])\). For open boundary conditions, \(x_a\) is limited to \(0 <= x_a < Ls[a]\) and \(0 <= x_a+dx[a] < \text{lat}.Ls[a]\).

Parameters
- **u1** \((\text{int})\) – Indices within the unit cell; the \(u1\) and \(u2\) of \(\text{add_coupling()}\)
- **u2** \((\text{int})\) – Indices within the unit cell; the \(u1\) and \(u2\) of \(\text{add_coupling()}\)
- **dx** \((\text{array})\) – Length \(\text{dim}\). The translation in terms of basis vectors for the coupling.

Returns
- **mps1, mps2** \((\text{array})\) – For each possible two-site coupling the MPS indices for the \(u1\) and \(u2\).
- **lat_indices** \((2D \text{ int array})\) – Rows of **lat_indices** correspond to rows of **mps_ijkl** and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** \((\text{tuple of int})\) – Len \(\text{dim}\). The correct shape for an array specifying the coupling strength. **lat_indices** has only rows within this shape.

possible_multi_couplings \((ops)\)
Generalization of \(\text{possible_couplings()}\) to couplings with more than 2 sites.

Parameters **ops** \((\text{list of (opname, dx, u)})\) – Same as the argument **ops** of \(\text{add_multi_coupling()}\).

Returns
- **mps_ijkl** \((2D \text{ int array})\) – Each row contains MPS indices \(i,j,k,l,...\) for each of the operators positions. The positions are defined by \(dx\) \((j,k,l,...\) relative to \(i\)) and boundary conditions of \(self\) (how much the box for given \(dx\) can be shifted around without hitting a boundary - these are the different rows).
- **lat_indices** \((2D \text{ int array})\) – Rows of **lat_indices** correspond to rows of **mps_ijkl** and contain the lattice indices of the “lower left corner” of the box containing the coupling.
- **coupling_shape** \((\text{tuple of int})\) – Len \(\text{dim}\). The correct shape for an array specifying the coupling strength. **lat_indices** has only rows within this shape.

save_hdf5 \((\text{hdf5_saver, h5gr, subpath})\)
Export \(self\) into a HDF5 file.

This method saves all the data it needs to reconstruct \(self\) with \(\text{from_hdf5()}\).
Specifically, it saves **unit_cell**, **Ls**, **unit_cell_positions**, **basis**, **boundary_conditions**, **pairs** under their name, **bc_MPS** as "boundary_conditions_MPS", and **order** as "order_for_MPS". Moreover, it saves \(\text{dim}\) and **N_sites** as HDF5 attributes.

Parameters
- **hdf5_saver** \((\text{Hdf5Saver})\) – Instance of the saving engine.
- **h5gr** \((\text{class}`\text{Group}')\) – HDF5 group which is supposed to represent \(self\).
- **subpath** \((\text{str})\) – The name of **h5gr** with a ‘/’ in the end.

site \((i)\)

return **Site** instance corresponding to an MPS index \(i\)
**Module description**

Kitaev’s exactly solvable toric code model.

As we put the model on a cylinder, the name “toric code” is a bit misleading, but it is the established name for this model...

### 7.12 networks

- full name: tenpy.networks
- parent module: tenpy
- type: module

**Module description**

Definitions of tensor networks like MPS and MPO.

Here, ‘tensor network’ refers just to the (partial) contraction of tensors. For example an MPS represents the contraction along the ‘virtual’ legs/bonds of its $B$.

#### Submodules

<table>
<thead>
<tr>
<th>Submodule</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>site</td>
<td>Defines a class describing the local physical Hilbert space.</td>
</tr>
<tr>
<td>mps</td>
<td>This module contains a base class for a Matrix Product State (MPS).</td>
</tr>
<tr>
<td>mpo</td>
<td>Matrix product operator (MPO).</td>
</tr>
<tr>
<td>terms</td>
<td>Classes to store a collection of operator names and sites they act on, together with prefactors.</td>
</tr>
<tr>
<td>purification_mps</td>
<td>This module contains an MPS class representing an density matrix by purification.</td>
</tr>
</tbody>
</table>

#### 7.12.1 site

- full name: tenpy.networks.site
- parent module: tenpy.networks
- type: module
Classes

BosonSite([Nmax, conserve, filling]) Create a Site for up to Nmax bosons.
FermionSite([conserve, filling]) Create a Site for spin-less fermions.
GroupedSite(sites[, labels, charges]) Group two or more Site into a larger one.
Site(leg[, state_labels]) Collects necessary information about a single local site of a lattice.
SpinHalfFermionSite([cons_N, cons_Sz, filling]) Create a Site for spinful (spin-1/2) fermions.
SpinHalfSite([conserve]) Spin-1/2 site.
SpinSite([S, conserve]) General Spin S site.

BosonSite

• full name: tenpy.networks.site.BosonSite
• parent module: tenpy.networks.site
• type: class
# Inheritance Diagram

```
Hdf5Exportable
   ↓
Site
   ↓
BosonSite
```

## Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>BosonSite.<strong>init</strong></strong>([Nmax, conserve, filling])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td><strong>BosonSite.add_op</strong>(name, op[, need_JW, hc])</td>
<td>Add one on-site operators.</td>
</tr>
<tr>
<td><strong>BosonSite.change_charge</strong>([new_leg_charge, ...])</td>
<td>Change the charges of the site (in place).</td>
</tr>
<tr>
<td><strong>BosonSite.from_hdf5</strong>(hdf5_loader, h5gr, sub-path)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><strong>BosonSite.get_hc_op_name</strong>(name)</td>
<td>Return the hermitian conjugate of a given operator.</td>
</tr>
<tr>
<td><strong>BosonSite.get_op</strong>(name</td>
<td>Return operator of given name.</td>
</tr>
<tr>
<td><strong>BosonSite.multiply_op_names</strong>(names)</td>
<td>Multiply operator names together.</td>
</tr>
<tr>
<td><strong>BosonSite.multiply_operators</strong>(operators)</td>
<td>Multiply local operators (possibly given by their names) together.</td>
</tr>
<tr>
<td><strong>BosonSite.op_needs_JW</strong>(name)</td>
<td>Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.</td>
</tr>
<tr>
<td><strong>BosonSite.remove_op</strong>(name)</td>
<td>Remove an added operator.</td>
</tr>
<tr>
<td><strong>BosonSite.rename_op</strong>(old_name, new_name)</td>
<td>Rename an added operator.</td>
</tr>
<tr>
<td><strong>BosonSite.save_hdf5</strong>(hdf5_saver, h5gr, sub-path)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><strong>BosonSite.state_index</strong>(label)</td>
<td>Return index of a basis state from its label.</td>
</tr>
<tr>
<td><strong>BosonSite.state_indices</strong>(labels)</td>
<td>Same as state_index(), but for multiple labels.</td>
</tr>
<tr>
<td><strong>BosonSite.test_sanity</strong>()</td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td><strong>BosonSite.valid_opname</strong>(name)</td>
<td>Check whether ‘name’ labels a valid onsite-operator.</td>
</tr>
</tbody>
</table>
Class Attributes and Properties

<table>
<thead>
<tr>
<th>BosonSite.dim</th>
<th>Dimension of the local Hilbert space.</th>
</tr>
</thead>
<tbody>
<tr>
<td>BosonSite.onsite_ops</td>
<td>Dictionary of on-site operators for iteration.</td>
</tr>
</tbody>
</table>

```
class tenpy.networks.site.BosonSite(Nmax=1, conserve='N', filling=0.0)
    Bases: tenpy.networks.site.Site

Create a Site for up to Nmax bosons.
Local states are vac, 1, 2, ... , Nc. (Exception: for parity conservation, we sort as vac, 2, 4, ...
... 1, 3, 5, ...)

<table>
<thead>
<tr>
<th>operator</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Id, JW</td>
<td>Identity ( \mathbf{1} )</td>
</tr>
<tr>
<td>B</td>
<td>Annihilation operator ( b )</td>
</tr>
<tr>
<td>Bd</td>
<td>Creation operator ( b^\dagger )</td>
</tr>
<tr>
<td>N</td>
<td>Number operator ( n = b^\dagger b )</td>
</tr>
<tr>
<td>NN</td>
<td>( n^2 )</td>
</tr>
<tr>
<td>dN</td>
<td>( \delta n := n - \text{filling} )</td>
</tr>
<tr>
<td>dNdN</td>
<td>( \delta n^2 )</td>
</tr>
</tbody>
</table>
| P        | Parity \( \mathbf{1} - 2(n \mod 2) \).

<table>
<thead>
<tr>
<th>conserve</th>
<th>qmod</th>
<th>excluded onsite operators</th>
</tr>
</thead>
<tbody>
<tr>
<td>'N'</td>
<td>[1]</td>
<td>-</td>
</tr>
<tr>
<td>'parity'</td>
<td>[2]</td>
<td>-</td>
</tr>
<tr>
<td>None</td>
<td>[]</td>
<td>-</td>
</tr>
</tbody>
</table>
```

Parameters

- **Nmax** (**int**) – Cutoff defining the maximum number of bosons per site. The default \( Nmax=1 \) describes hard-core bosons.
- **conserve** (**str**) – Defines what is conserved, see table above.
- **filling** (**float**) – Average filling. Used to define \( dN \).

**conserve**

Defines what is conserved, see table above.

Type **str**

**filling**

Average filling. Used to define \( dN \).

Type **float**

```
def add_op(name, op, need_JW=False, hc=None)
    Add one on-site operators.
```

Parameters

- **name** (**str**) – A valid python variable name, used to label the operator. The name under which \( op \) is added as attribute to self.
• \textbf{op} (np.ndarray | \texttt{Array}) – A matrix acting on the local hilbert space representing the local operator. Dense numpy arrays are automatically converted to \texttt{Array}. LegCharges have to be \([\text{leg, leg.conj()}]\). We set labels ’p’, ’p∗’.

• \textbf{need\textunderscore JW} (bool) – Whether the operator needs a Jordan-Wigner string. If True, add \texttt{name} to \texttt{need\_JW\_string}.

• \textbf{hc} (None | False | str) – The name for the hermitian conjugate operator, to be used for \texttt{hc\_ops}. By default (None), try to auto-determine it. If False, disable adding antries to \texttt{hc\_ops}.

\textbf{change\_charge} (\texttt{new\_leg\_charge=\texttt{None}, permute=\texttt{\texttt{None})}}

Change the charges of the site (in place).

\textbf{Parameters}

• \textbf{new\_leg\_charge} (LegCharge | None) – The new charges to be used. If None, use trivial charges.

• \textbf{permute} (ndarray | None) – The permutation applied to the physical leg, which gets used to adjust \texttt{state\_labels} and \texttt{perm}. If you sorted the previous leg with \texttt{perm\_qind}, \texttt{new\_leg\_charge = leg.sort()}, use \texttt{old\_leg.perm\_flat\_from\_perm\_qind(perm\_qind)}. Ignored if None.

\textbf{property dim}

Dimension of the local Hilbert space.

\textbf{classmethod from\_hdf5} (\texttt{hdf5\_loader, h5\_grp, subpath})

Load instance from a HDF5 file. This method reconstructs a class instance from the data saved with \texttt{save\_hdf5()}.

\textbf{Parameters}

• \texttt{hdf5\_loader} (Hdf5Loader) – Instance of the loading engine.

• \texttt{h5\_grp} (Group) – HDF5 group which is represent the object to be constructed.

• \texttt{subpath} (str) – The name of \texttt{h5\_grp} with a ’/’ in the end.

\textbf{Returns} \texttt{obj} – Newly generated class instance containing the required data.

\textbf{Return type} cls

\textbf{get\_hc\_op\_name} (\texttt{name})

Return the hermitian conjugate of a given operator.

\textbf{Parameters} \texttt{name} (str) – The name of the operator to be returned. Multiple operators separated by whitespace are interpreted as an operator product, exactly as \texttt{get\_op()} does.

\textbf{Returns} \texttt{hc\_op\_name} – Operator name for the hermi such that \texttt{get\_op()} of

\textbf{Return type} str

\textbf{get\_op} (\texttt{name})

Return operator of given name.

\textbf{Parameters} \texttt{name} (str) – The name of the operator to be returned. In case of multiple operator names separated by whitespace, we multiply them together to a single on-site operator (with the one on the right acting first).

\textbf{Returns} \texttt{op} – The operator given by \texttt{name}, with labels ’p’, ’p∗’. If name already was an npc Array, it’s directly returned.

\textbf{Return type} np_conserved
multiply_op_names(names)
    Multiply operator names together.
    Join the operator names in names such that get_op returns the product of the corresponding operators.

    Parameters
    names (list of str) – List of valid operator labels.

    Returns
    combined_opname – A valid operator name Operatorname representing the product of operators in names.

    Return type
    str

multiply_operators(operators)
    Multiply local operators (possibly given by their names) together.

    Parameters
    operators (list of {str | Array}) – List of valid operator names (to be translated with get_op()) or directly on-site operators in the form of npc arrays with 'p', 'p*' label. The operators are multiplied left-to-right.

    Returns
    combined_operator – The product of the given operators in a left-to-right multiplication following the usual mathematical convention. For example, if operators=['Sz', 'Sp', 'Sx'], the final operator is equivalent to site.get_op('Sz Sp Sx'), with the 'Sx' operator acting first on any physical state.

    Return type
    Array

property onsite_ops
    Dictionary of on-site operators for iteration.
    Single operators are accessible as attributes.

op_needs_JW(name)
    Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.

    Parameters
    name (str) – The name of the operator, as in get_op().

    Returns
    needs_JW – Whether the operator needs a Jordan-Wigner string, judging from need_JW_string.

    Return type
    bool

remove_op(name)
    Remove an added operator.

    Parameters
    name (str) – The name of the operator to be removed.

rename_op(old_name, new_name)
    Rename an added operator.

    Parameters
    old_name (str) – The old name of the operator.
    new_name (str) – The new name of the operator.

save_hdf5(hdf5_saver, h5gr, subpath)
    Export self into a HDF5 file.
    This method saves all the data it needs to reconstruct self with from_hdf5().
    This implementation saves the content of __dict__ with save_dict_content(), storing the format under the attribute 'format'.

    Parameters
    hdf5_saver (Hdf5Saver) – Instance of the saving engine.
- **h5gr**: HDF5 group which is supposed to represent `self`.
- **subpath**: The name of `h5gr` with a '/' in the end.

**state_index** *(label)*
Return index of a basis state from its label.

  **Parameters**
  - `label` *(int | string)* – Either the index directly or a label (string) set before.

  **Returns**
  - `state_index` – the index of the basis state associated with the label.

  **Return type**
  - `int`

**state_indices** *(labels)*
Same as `state_index()`, but for multiple labels.

**test_sanity** *
Sanity check, raises ValueErrors, if something is wrong.

**valid_opname** *(name)*
Check whether `name` labels a valid onsite-operator.

  **Parameters**
  - `name` *(str)* – Label for the operator. Can be multiple operator(labels) separated by whitespace, indicating that they should be multiplied together.

  **Returns**
  - `valid` – True if `name` is a valid argument to `get_op()`.

  **Return type**
  - `bool`

**FermionSite**

- full name: tenpy.networks.site.FermionSite
- parent module: `tenpy.networks.site`
- type: class

**Inheritance Diagram**

```
Hdf5Exportable
  ↓
 Site
  ↓
FermionSite
```
Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FermionSite.<strong>init</strong>([conserve, filling])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>FermionSite.add_op(name, op[, need_JW, hc])</td>
<td>Add one on-site operators.</td>
</tr>
<tr>
<td>FermionSite.change_charge([new_leg_charge, ...])</td>
<td>Change the charges of the site (in place).</td>
</tr>
<tr>
<td>FermionSite.from_hdf5(hdf5_loader, h5gr, sub-path)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>FermionSite.get_hc_op_name(name)</td>
<td>Return the hermitian conjugate of a given operator.</td>
</tr>
<tr>
<td>FermionSite.get_op(name)</td>
<td>Return operator of given name.</td>
</tr>
<tr>
<td>FermionSite.multiply_op_names(names)</td>
<td>Multiply operator names together.</td>
</tr>
<tr>
<td>FermionSite.multiply_operators(operators)</td>
<td>Multiply local operators (possibly given by their names) together.</td>
</tr>
<tr>
<td>FermionSite.op_needs_JW(name)</td>
<td>Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.</td>
</tr>
<tr>
<td>FermionSite.remove_op(name)</td>
<td>Remove an added operator.</td>
</tr>
<tr>
<td>FermionSite.rename_op(old_name, new_name)</td>
<td>Rename an added operator.</td>
</tr>
<tr>
<td>FermionSite.save_hdf5(hdf5_saver, h5gr, sub-path)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>FermionSite.state_index(label)</td>
<td>Return index of a basis state from its label.</td>
</tr>
<tr>
<td>FermionSite.state_indices(labels)</td>
<td>Same as state_index(), but for multiple labels.</td>
</tr>
<tr>
<td>FermionSite.test_sanity()</td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td>FermionSite.valid_opname(name)</td>
<td>Check whether ‘name’ labels a valid onsite-operator.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>FermionSite.dim</td>
<td>Dimension of the local Hilbert space.</td>
</tr>
<tr>
<td>FermionSite.onsite_ops</td>
<td>Dictionary of on-site operators for iteration.</td>
</tr>
</tbody>
</table>

class tenpy.networks.site.FermionSite (conserve='N', filling=0.5)

    Bases: tenpy.networks.site.Site

    Create a Site for spin-less fermions.
    Local states are empty and full.

    Warning: Using the Jordan-Wigner string (JW) is crucial to get correct results, otherwise you just describe hardcore bosons! Further details in Fermions and the Jordan-Wigner transformation.

<table>
<thead>
<tr>
<th>operator</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Id</td>
<td>Identity (\mathbb{I})</td>
</tr>
<tr>
<td>JW</td>
<td>Sign for the Jordan-Wigner string.</td>
</tr>
<tr>
<td>C</td>
<td>Annihilation operator (c) (up to ‘JW’-string left of it)</td>
</tr>
<tr>
<td>Cd</td>
<td>Creation operator (c^\dagger) (up to ‘JW’-string left of it)</td>
</tr>
<tr>
<td>N</td>
<td>Number operator (n = c^\dagger c)</td>
</tr>
<tr>
<td>dN</td>
<td>(dn := n - \text{filling})</td>
</tr>
<tr>
<td>dNdN</td>
<td>((dn)^2)</td>
</tr>
<tr>
<td>conserve</td>
<td>qmod</td>
</tr>
<tr>
<td>----------</td>
<td>------</td>
</tr>
<tr>
<td>'N'</td>
<td>[1]</td>
</tr>
<tr>
<td>'parity'</td>
<td>[2]</td>
</tr>
<tr>
<td>None</td>
<td>[1]</td>
</tr>
</tbody>
</table>

Parameters

- **conserve** *(str)* – Defines what is conserved, see table above.
- **filling** *(float)* – Average filling. Used to define $dN$.

**conserve**

Defines what is conserved, see table above.

Type *str*

**filling**

Average filling. Used to define $dN$.

Type *float*

**add_op** *(name, op, need_JW=False, hc=None)*

Add one on-site operators.

Parameters

- **name** *(str)* – A valid python variable name, used to label the operator. The name under which *op* is added as attribute to self.
- **op** *(np.ndarray | Array)* – A matrix acting on the local hilbert space representing the local operator. Dense numpy arrays are automatically converted to *Array*. LegCharges have to be [leg, leg.conj()]. We set labels 'p', 'p*'.
- **need_JW** *(bool)* – Whether the operator needs a Jordan-Wigner string. If True, add *name* to *need_JW_string*.
- **hc** *(None | False | str)* – The name for the hermitian conjugate operator, to be used for *hc_ops*. By default (None), try to auto-determine it. If False, disable adding entries to *hc_ops*.

**change_charge** *(new_leg_charge=None, permute=None)*

Change the charges of the site (in place).

Parameters

- **new_leg_charge** *(LegCharge | None)* – The new charges to be used. If None, use trivial charges.
- **permute** *(ndarray | None)* – The permutation applied to the physical leg, which gets used to adjust state_labels and perm. If you sorted the previous leg with perm_qind, new_leg_charge = leg.sort(), use old_leg. perm_flat_from_perm_qind(perm_qind). Ignored if None.

**property dim**

Dimension of the local Hilbert space.

**classmethod from_hdf5** *(hdf5_loader, h5gr, subpath)*

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with *save_hdf5()*.

Parameters
• **hdf5_loader** (Hdf5Loader) – Instance of the loading engine.

• **h5gr** (Group) – HDF5 group which is represent the object to be constructed.

• **subpath** (**str**) – The name of h5gr with a '/' in the end.

**Returns** obj – Newly generated class instance containing the required data.

**Return type** cls

get_hc_op_name(**name**)  
Return the hermitian conjugate of a given operator.

**Parameters** name (**str**) – The name of the operator to be returned. Multiple operators separated by whitespace are interpreted as an operator product, exactly as get_op() does.

**Returns** hc_op_name – Operator name for the hermi such that get_op() of

**Return type** str

get_op(**name**)  
Return operator of given name.

**Parameters** name (**str**) – The name of the operator to be returned. In case of multiple operator names separated by whitespace, we multiply them together to a single on-site operator (with the one on the right acting first).

**Returns** op – The operator given by name, with labels 'p', 'p*'. If name already was an npc Array, it's directly returned.

**Return type** np_conserved

multiply_op_names(**names**)  
Multiply operator names together.

Join the operator names in names such that get_op returns the product of the corresponding operators.

**Parameters** names (**list of str**) – List of valid operator labels.

**Returns** combined_opname – A valid operator name Operatorname representing the product of operators in names.

**Return type** str

multiply_operators(**operators**)  
Multiply local operators (possibly given by their names) together.

**Parameters** operators (**list of {str | Array}**) – List of valid operator names (to be translated with get_op()) or directly on-site operators in the form of npc arrays with 'p', 'p*' label. The operators are multiplied left-to-right.

**Returns** combined_operator – The product of the given operators in a left-to-right multiplication following the usual mathematical convention. For example, if operators=['Sz', 'Sp', 'Sx'], the final operator is equivalent to site.get_op('Sz Sp Sx'), with the 'Sx' operator acting first on any physical state.

**Return type** Array

**property onsite_ops**  
Dictionary of on-site operators for iteration.

Single operators are accessible as attributes.

op_needs_JW(**name**)  
Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.
Parameters name (str) – The name of the operator, as in get_op().

Returns needs_JW – Whether the operator needs a Jordan-Wigner string, judging from need_JW_string.

Return type bool

remove_op (name)
Remove an added operator.

Parameters name (str) – The name of the operator to be removed.

rename_op (old_name, new_name)
Rename an added operator.

Parameters
• old_name (str) – The old name of the operator.
• new_name (str) – The new name of the operator.

save_hdf5 (hdf5_saver, h5gr, subpath)
Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5().

This implementation saves the content of __dict__ with save_dict_content(), storing the format under the attribute 'format'.

Parameters
• hdf5_saver (Hdf5Saver) – Instance of the saving engine.
• h5gr (:class:`Group`) – HDF5 group which is supposed to represent self.
• subpath (str) – The name of h5gr with a '/' in the end.

state_index (label)
Return index of a basis state from its label.

Parameters label (int | string) – Either the index directly or a label (string) set before.

Returns state_index – the index of the basis state associated with the label.

Return type int

state_indices (labels)
Same as state_index(), but for multiple labels.

test_sanity ()
Sanity check, raises ValueErrors, if something is wrong.

valid_opname (name)
Check whether ‘name’ labels a valid onsite-operator.

Parameters name (str) – Label for the operator. Can be multiple operator(labels) separated by whitespace, indicating that they should be multiplied together.

Returns valid – True if name is a valid argument to get_op().

Return type bool
GroupedSite

- full name: tenpy.networks.site.GroupedSite
- parent module: tenpy.networks.site
- type: class

Inheritance Diagram

![Inheritance Diagram](image)

Methods

<table>
<thead>
<tr>
<th>Method Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>GroupedSite.__init__</code>([sites[, labels, charges]])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>GroupedSite.add_op</code>(name, op[, need_JW, hc])</td>
<td>Add one on-site operators.</td>
</tr>
<tr>
<td><code>GroupedSite.change_charge</code>([new_leg_charge, ...])</td>
<td>Change the charges of the site (in place).</td>
</tr>
<tr>
<td><code>GroupedSite.from_hdf5</code>(hdf5_loader, h5gr, sub-path)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>GroupedSite.get_hc_op_name</code>(name)</td>
<td>Return the hermitian conjugate of a given operator.</td>
</tr>
<tr>
<td><code>GroupedSite.get_op</code>(name)</td>
<td>Return operator of given name.</td>
</tr>
<tr>
<td><code>GroupedSite.kroneckerproduct</code>(ops)</td>
<td>Return the Kronecker product $\mathcal{O}_0 \otimes \mathcal{O}_1$ of local operators.</td>
</tr>
<tr>
<td><code>GroupedSite.multiply_op_names</code>(names)</td>
<td>Multiply operator names together.</td>
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<tr>
<td><code>GroupedSite.multiply_operators</code>(operators)</td>
<td>Multiply local operators (possibly given by their names) together.</td>
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<tr>
<td><code>GroupedSite.op_needs_JW</code>(name)</td>
<td>Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.</td>
</tr>
<tr>
<td><code>GroupedSite.remove_op</code>(name)</td>
<td>Remove an added operator.</td>
</tr>
<tr>
<td><code>GroupedSite.rename_op</code>(old_name, new_name)</td>
<td>Rename an added operator.</td>
</tr>
<tr>
<td><code>GroupedSite.save_hdf5</code>(hdf5_saver, h5gr, sub-path)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>GroupedSite.state_index</code>(label)</td>
<td>Return index of a basis state from its label.</td>
</tr>
</tbody>
</table>

continues on next page
Table 128 – continued from previous page

<table>
<thead>
<tr>
<th>Method/Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>GroupedSite.state_indices(labels)</code></td>
<td>Same as <code>state_index()</code>, but for multiple labels.</td>
</tr>
<tr>
<td><code>GroupedSite.test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td><code>GroupedSite.valid_opname(name)</code></td>
<td>Check whether ‘name’ labels a valid onsite-operator.</td>
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### Class Attributes and Properties

<table>
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<tr>
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<th>Description</th>
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<td>Dimension of the local Hilbert space.</td>
</tr>
<tr>
<td><code>GroupedSite.onsite_ops</code></td>
<td>Dictionary of on-site operators for iteration.</td>
</tr>
</tbody>
</table>

```python
class tenpy.networks.site.GroupedSite(sites, labels=None, charges='same')
    Bases: tenpy.networks.site.Site

Group two or more Site into a larger one.

A typical use-case is that you want a NearestNeighborModel for TEBD although you have next-nearest neighbor interactions: you just double your local Hilbertspace to consist of two original sites. Note that this is a ‘hack’ at the cost of other things (e.g., measurements of ‘local’ operators) getting more complicated/computationally expensive.

If the individual sites indicate fermionic operators (with entries in `need_JW_string`), we construct the new on-site operators of `site1` to include the JW string of `site0`, i.e., we use the Kronecker product of `[JW, op]` instead of `[Id, op]` if necessary (but always `[op, Id]`). In that way the onsite operators of this DoubleSite automatically fulfill the expected commutation relations. See also Fermions and the Jordan-Wigner transformation.

**Parameters**

- **sites** (list of `Site`) – The individual sites being grouped together. Copied before use if `charges!='same'`.
- **labels** – Include the Kronecker product of the each onsite operator `op` on `sites[i]` and identities on other sites with the name `opname+labels[i]`. Similarly, set state labels for `''.join(state[i]+'_'+labels[i])`. Defaults to `[str(i) for i in range(n_sites)]`, which for example grouping two SpinSites gives operators name like "Sz0" and sites labels like 'up_0 down_1'.
- **charges** ('same' | 'drop' | 'independent') – How to handle charges, defaults to 'same'. 'same' means that all `sites` have the same `ChargeInfo`, and the total charge is the sum of the charges on the individual `sites`. 'independent' means that the `sites` have possibly different `ChargeInfo`, and the charges are conserved separately, i.e., we have `n_sites` conserved charges. For 'drop', we drop any charges, such that the remaining legcharges are trivial. For more complex situations, you can call `multi_sites_combine_charges()` beforehand.

**n_sites**

The number of sites grouped together, i.e. `len(sites)`.

**sites**

The sites grouped together into self.

**labels**

The labels using which the single-site operators are added during construction.
```
**kroneckerproduct** *(ops)*

Return the Kronecker product $o_0 \otimes o_1$ of local operators.

- **Parameters**
  - *ops* (list of *Array*) – One operator (or operator name) on each of the ungrouped sites. Each operator should have labels [‘p’, ‘p*’].

- **Returns**
  - *prod* – Kronecker product $o_0 \otimes o_1 \otimes \cdots$, with labels [‘p’, ‘p*’].

- **Return type** *Array*

**add_op** *(name, op, need_JW=False, hc=None)*

Add one on-site operators.

- **Parameters**
  - *name* *(str)* – A valid python variable name, used to label the operator. The name under which *op* is added as attribute to self.
  - *op* *(np.ndarray | Array)* – A matrix acting on the local hilbert space representing the local operator. Dense numpy arrays are automatically converted to *Array*. LegCharges have to be [leg, leg.conj()]. We set labels 'p', 'p*'.
  - *need_JW* *(bool)* – Whether the operator needs a Jordan-Wigner string. If True, add *name* to need_JW_string.
  - *hc* *(None | False | str)* – The name for the hermitian conjugate operator, to be used for *hc_ops*. By default (None), try to auto-determine it. If False, disable adding antries to *hc_ops*.

**change_charge** *(new_leg_charge=None, permute=None)*

Change the charges of the site (in place).

- **Parameters**
  - *new_leg_charge* *(LegCharge | None)* – The new charges to be used. If None, use trivial charges.
  - *permute* *(ndarray | None)* – The permutation applied to the physical leg, which gets used to adjust state_labels and perm. If you sorted the previous leg with *perm_qind*, new_leg_charge = leg.sort(), use old_leg.perm_flat_from_perm_qind(*perm_qind*). Ignored if None.

**property dim**

Dimension of the local Hilbert space.

**classmethod from_hdf5** *(hdf5_loader, h5gr, subpath)*

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with *save_hdf5()*.

- **Parameters**
  - *hdf5_loader* *(Hdf5Loader)* – Instance of the loading engine.
  - *h5gr* *(Group)* – HDF5 group which is represent the object to be constructed.
  - *subpath* *(str)* – The name of *h5gr* with a ’/’ in the end.

- **Returns**
  - *obj* – Newly generated class instance containing the required data.

- **Return type** *cls*

**get_hc_op_name** *(name)*

Return the hermitian conjugate of a given operator.
**Parameters** name *(str)* — The name of the operator to be returned. Multiple operators separated by whitespace are interpreted as an operator product, exactly as `get_op()` does.

**Returns** hc_op_name — Operator name for the hermi such that `get_op()` of

**Return type** str

`get_op(name)`

Return operator of given name.

**Parameters** name *(str)* — The name of the operator to be returned. In case of multiple operator names separated by whitespace, we multiply them together to a single on-site operator (with the one on the right acting first).

**Returns** op — The operator given by name, with labels 'p', 'p*'. If name already was an npc Array, it's directly returned.

**Return type** np_conserved

`multiply_op_names(names)`

Multiply operator names together.

Join the operator names in names such that `get_op` returns the product of the corresponding operators.

**Parameters** names *(list of str)* — List of valid operator labels.

**Returns** combined_opname — A valid operator name Operatorname representing the product of operators in names.

**Return type** str

`multiply_operators(operators)`

Multiply local operators (possibly given by their names) together.

**Parameters** operators *(list of {str | Array})* — List of valid operator names (to be translated with `get_op()`) or directly on-site operators in the form of npc arrays with 'p', 'p*' label. The operators are multiplied left-to-right.

**Returns** combined_operator — The product of the given operators in a left-to-right multiplication following the usual mathematical convention. For example, if `operators=['Sz', 'Sp', 'Sx']`, the final operator is equivalent to `site.get_op('Sz Sp Sx')`, with the 'Sx' operator acting first on any physical state.

**Return type** Array

`property onsite_ops`  
Dictionary of on-site operators for iteration.

Single operators are accessible as attributes.

`op_needs_JW(name)`

Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.

**Parameters** name *(str)* — The name of the operator, as in `get_op()`.

**Returns** needs_JW — Whether the operator needs a Jordan-Wigner string, judging from need_JW_string.

**Return type** bool

`remove_op(name)`

Remove an added operator.

**Parameters** name *(str)* — The name of the operator to be removed.
rename_op (old_name, new_name)
    Rename an added operator.

    Parameters
    • old_name (str) – The old name of the operator.
    • new_name (str) – The new name of the operator.

save_hdf5 (hdf5_saver, h5gr, subpath)
    Export self into a HDF5 file.
    This method saves all the data it needs to reconstruct self with from_hdf5().
    This implementation saves the content of __dict__ with save_dict_content(), storing the format
    under the attribute 'format'.

    Parameters
    • hdf5_saver (Hdf5Saver) – Instance of the saving engine.
    • h5gr (:class:`Group`) – HDF5 group which is supposed to represent self.
    • subpath (str) – The name of h5gr with a '/' in the end.

state_index (label)
    Return index of a basis state from its label.
    Parameters label (int | string) – either the index directly or a label (string) set before.
    Returns state_index – the index of the basis state associated with the label.
    Return type int

state_indices (labels)
    Same as state_index(), but for multiple labels.

test_sanity ()
    Sanity check, raises ValueErrors, if something is wrong.

valid_opname (name)
    Check whether 'name' labels a valid onsite-operator.
    Parameters name (str) – Label for the operator. Can be multiple operator(labels) separated
    by whitespace, indicating that they should be multiplied together.
    Returns valid – True if name is a valid argument to get_op().
    Return type bool

Site

- full name: tenpy.networks.site.Site
- parent module: tenpy.networks.site
- type: class
Inheritance Diagram

```
Hdf5Exportable
  └── Site
```

Methods

- `Site.__init__(leg[, state_labels])`: Initialize self.
- `Site.add_op(name, op[, need_JW, hc])`: Add one on-site operators.
- `Site.change_charge([new_leg_charge, permute])`: Change the charges of the site (in place).
- `Site.from_hdf5(hdf5_loader, h5gr, subpath)`: Load instance from a HDF5 file.
- `Site.get_hc_op_name(name)`: Return the hermitian conjugate of a given operator.
- `Site.get_op(name)`: Return operator of given name.
- `Site.multiply_op_names(names)`: Multiply operator names together.
- `Site.multiply_operators(operators)`: Multiply local operators (possibly given by their names) together.
- `Site.op_needs_JW(name)`: Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.
- `Site.remove_op(name)`: Remove an added operator.
- `Site.rename_op(old_name, new_name)`: Rename an added operator.
- `Site.save_hdf5(hdf5_saver, h5gr, subpath)`: Export self into a HDF5 file.
- `Site.state_index(label)`: Return index of a basis state from its label.
- `Site.state_indices(labels)`: Same as `state_index()`, but for multiple labels.
- `Site.test_sanity()`: Sanity check, raises ValueErrors, if something is wrong.
- `Site.valid_opname(name)`: Check whether `name` labels a valid onsite-operator.

Class Attributes and Properties

- `Site.dim`: Dimension of the local Hilbert space.
- `Site.onsite_ops`: Dictionary of on-site operators for iteration.

```python
class tenpy.networks.site.Site(leg, state_labels=None, **site_ops)
    Bases: tenpy.tools.hdf5_io.Hdf5Exportable

    Collects necessary information about a single local site of a lattice.

    This class defines what the local basis states are: it provides the `leg` defining the charges of the physical leg for this site. Moreover, it stores (local) on-site operators, which are directly available as attribute, e.g., `self.Sz`
```

7.12. networks 543
is the $Sz$ operator for the $\text{SpinSite}$. Alternatively, operators can be obtained with $\text{get\_op()}$. The operator names $\text{Id}$ and $\text{JW}$ are reserved for the identity and Jordan-Wigner strings.

**Warning:** The order of the local basis can change depending on the charge conservation! This is a necessary feature since we need to sort the basis by charges for efficiency. We use the $\text{state\_labels}$ and $\text{perm}$ to keep track of these permutations.

### Parameters

- **leg** (*LegCharge*) – Charges of the physical states, to be used for the physical leg of MPS.
- **state\_labels** (*None | list of str*) – Optionally a label for each local basis states. None entries are ignored / not set.
- **site\_ops** – Additional keyword arguments of the form name=$\text{op}$ given to $\text{add\_op()}$. The identity operator 'Id' is automatically included. If no 'JW' for the Jordan-Wigner string is given, 'JW' is set as an alias to 'Id'.

#### leg

Charges of the local basis states.

**Type** $\text{LegCharge}$

#### state\_labels

(Optional) labels for the local basis states.

**Type** $\{\text{str: int}\}$

#### opnames

Labels of all onsite operators (i.e. $self\_op$ exists if 'op' in $self\_opnames$). Note that $\text{get\_op()}$ allows arbitrary concatenations of them.

**Type** $\text{set}$

#### need\_JW\_string

Labels of all onsite operators that need a Jordan-Wigner string. Used in $\text{op\_needs\_JW()}$ to determine whether an operator anticommutes or commutes with operators on other sites.

**Type** $\text{set}$

#### ops

Onsite operators are added directly as attributes to $self$. For example after $self\_add\_op('Sz', Sz)$ you can use $self.Sz$ for the $Sz$ operator. All onsite operators have labels 'p', 'p*'.

**Type** $\text{Array}$

#### perm

Index permutation of the physical leg compared to $\text{conserve=None}$, i.e. \[ \text{OP\_conserved} = \text{OP\_nonconserved[np.ix_}(\text{perm,perm}) \land \text{perm[state\_labels\_conserved["some\_state"]]} == \text{state\_labels\_nonconserved["some\_state"]} \].

**Type** $1\text{D array}$

#### JW\_exponent

Exponents of the 'JW' operator, such that $self.JW.to\_ndarray() = \text{np.diag(np.exp(1. j*np.pi* JW\_exponent))}$

**Type** $1\text{D array}$

#### hc\_ops

Mapping from operator names to their hermitian conjugates. Use $\text{get\_hc\_op\_name()}$ to obtain entries.
Type `dict(str->str)`

Examples
The following generates a site for spin-1/2 with Sz conservation. Note that $S_x = (S_p + S_m)/2$ violates Sz conservation and is thus not a valid on-site operator.

```python
>>> chinfo = npc.ChargeInfo([1], ['Sz'])
```
```python
>>> ch = npc.LegCharge.from_qflat(chinfo, [1, -1])
```
```python
>>> Sp = [[0, 1.], [0, 0]]
```
```python
>>> Sm = [[0, 0], [1., 0]]
```
```python
>>> Sz = [[0.5, 0], [0, -0.5]]
```
```python
>>> site = tenpy.networks.site.Site(ch, ['up', 'down'], Splus=Sp, Sminus=Sm, Sz=Sz)
```
```python
>>> print(site.Splus.to_ndarray())
[[0. 1.]
 [0. 0.]]
```
```python
>>> print(site.get_op('Sminus').to_ndarray())
[[0. 0.]
 [1. 0.]]
```
```python
>>> print(site.get_op('Splus Sminus').to_ndarray())
[[1. 0.]
 [0. 0.]]
```

`change_charge (new_leg_charge=None, permute=None)`
Change the charges of the site (in place).

Parameters
- `new_leg_charge (LegCharge | None)` – The new charges to be used. If None, use trivial charges.
- `permute (ndarray | None)` – The permutation applied to the physical leg, which gets used to adjust `state_labels` and `perm`. If you sorted the previous leg with `perm_qind`, `new_leg_charge = leg.sort()`, use `old_leg. perm_flat_from_perm_qind(perm_qind). Ignored if None.

`test_sanity()`
Sanity check, raises ValueErrors, if something is wrong.

property `dim`
Dimension of the local Hilbert space.

property `onsite_ops`
Dictionary of on-site operators for iteration.
Single operators are accessible as attributes.

`add_op (name, op, need_JW=False, hc=None)`
Add one on-site operators.

Parameters
- `name (str)` – A valid python variable name, used to label the operator. The name under which `op` is added as attribute to self.
- `op (np.ndarray | Array)` – A matrix acting on the local hilbert space representing the local operator. Dense numpy arrays are automatically converted to Array. LegCharges have to be `[leg, leg.conj()]. We set labels 'p', 'p*'.

7.12. networks 545
• **need_JW (bool)** – Whether the operator needs a Jordan-Wigner string. If True, add `name` to `need_JW_string`.

• **hc (None | False | str)** – The name for the hermitian conjugate operator, to be used for `hc_ops`. By default (None), try to auto-determine it. If False, disable adding antries to `hc_ops`.

rename_op (`old_name, new_name`)
rename_op (`old_name, new_name`)
rename an added operator.

Parameters

• **old_name (str)** – The old name of the operator.

• **new_name (str)** – The new name of the operator.

remove_op (`name`)
remove_op (`name`)
Remove an added operator.

Parameters **name (str)** – The name of the operator to be removed.

state_index (`label`)
state_index (`label`)
Return index of a basis state from its label.

Parameters **label (int | string)** – Either the index directly or a label (string) set before.

Returns **state_index** – the index of the basis state associated with the label.

Return type int

state_indices (`labels`)
state_indices (`labels`)
Same as `state_index()`, but for multiple labels.

get_op (`name`)
get_op (`name`)
Return operator of given name.

Parameters **name (str)** – The name of the operator to be returned. In case of multiple operator names separated by whitespace, we multiply them together to a single on-site operator (with the one on the right acting first).

Returns **op** – The operator given by `name`, with labels `'p'`, `'p*'`. If name already was an npc Array, it’s directly returned.

Return type np_conserved

get_hc_op_name (`name`)
get_hc_op_name (`name`)
Return the hermitian conjugate of a given operator.

Parameters **name (str)** – The name of the operator to be returned. Multiple operators separated by whitespace are interpreted as an operator product, exactly as `get_op()` does.

Returns **hc_op_name** – Operator name for the hermi such that `get_op()` of

Return type str

op_needs_JW (`name`)
op_needs_JW (`name`)
Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.

Parameters **name (str)** – The name of the operator, as in `get_op()`.

Returns **needs_JW** – Whether the operator needs a Jordan-Wigner string, judging from `need_JW_string`.

Return type bool
**valid_opname** *(name)*  
Check whether 'name' labels a valid onsite-operator.

**Parameters**  
- **name** *(str)* – Label for the operator. Can be multiple operator(labels) separated by whitespace, indicating that they should be multiplied together.

**Returns**  
- **valid** – True if *name* is a valid argument to *get_op()*.

**Return type**  
**bool**

**multiply_op_names** *(names)*  
Multiply operator names together.

Join the operator names in *names* such that *get_op* returns the product of the corresponding operators.

**Parameters**  
- **names** *(list of str)* – List of valid operator labels.

**Returns**  
- **combined_opname** – A valid operator name Operatorname representing the product of operators in *names*.

**Return type**  
**str**

**multiply_operators** *(operators)*  
Multiply local operators (possibly given by their names) together.

**Parameters**  
- **operators** *(list of {str | Array})* – List of valid operator names (to be translated with *get_op()* or directly on-site operators in the form of npc arrays with 'p', 'p*' label. The operators are multiplied left-to-right.

**Returns**  
- **combined_operator** – The product of the given *operators* in a left-to-right multiplication following the usual mathematical convention. For example, if *operators*=['Sz', 'Sp', 'Sx'], the final operator is equivalent to *site.get_op*('Sz Sp Sx'), with the 'Sx' operator acting first on any physical state.

**Return type**  
**Array**

**classmethod from_hdf5** *(hdf5_loader, h5gr, subpath)*  
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with *save_hdf5()*.

**Parameters**  
- **hdf5_loader** *(Hdf5Loader)* – Instance of the loading engine.
- **h5gr** *(Group)* – HDF5 group which is represent the object to be constructed.
- **subpath** *(str)* – The *name* of *h5gr* with a '/ ' in the end.

**Returns**  
- **obj** – Newly generated class instance containing the required data.

**Return type**  
**cls**

**save_hdf5** *(hdf5_saver, h5gr, subpath)*  
Export *self* into a HDF5 file.

This method saves all the data it needs to reconstruct *self* with *from_hdf5()*.

This implementation saves the content of __dict__ with *save_dict_content()* , storing the format under the attribute 'format'.

**Parameters**  
- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.
- **h5gr** *(class `Group`)* – HDF5 group which is supposed to represent *self*. 

---

**7.12. networks**
• **subpath** (*str*) – The *name* of *h5gr* with a ‘/’ in the end.

**SpinHalfFermionSite**

- full name: *tenpy.networks.site.SpinHalfFermionSite*
- parent module: *tenpy.networks.site*
- type: class

**Inheritance Diagram**

```
Hdf5Exportable
  ↓
Site
  ↓
SpinHalfFermionSite
```

**Methods**

```
SpinHalfFermionSite.__init__([cons_N, ...]) Initialize self.

SpinHalfFermionSite.add_op(name, op[, ...]) Add one on-site operators.

SpinHalfFermionSite.change_charge([...]) Change the charges of the site (in place).

SpinHalfFermionSite.from_hdf5(hdf5_loader, ...) Load instance from a HDF5 file.

SpinHalfFermionSite.get_hc_op_name(name) Return the hermitian conjugate of a given operator.

SpinHalfFermionSite.get_op(name) Return operator of given name.

SpinHalfFermionSite.multiply_op_names(names) Multiply operator names together.

SpinHalfFermionSite.multiply_operators(operators) Multiply local operators (possibly given by their names) together.

SpinHalfFermionSite.op_needs_JW(name) Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.

SpinHalfFermionSite.remove_op(name) Remove an added operator.
```

continues on next page
Table 132 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpinHalfFermionSite.rename_op( old_name, new_name )</td>
<td>Rename an added operator.</td>
</tr>
<tr>
<td>SpinHalfFermionSite.save_hdf5(hdf5_saver,...)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>SpinHalfFermionSite.state_index(label)</td>
<td>Return index of a basis state from its label.</td>
</tr>
<tr>
<td>SpinHalfFermionSite.state_indices(labels)</td>
<td>Same as state_index(), but for multiple labels.</td>
</tr>
<tr>
<td>SpinHalfFermionSite.test_sanity()</td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td>SpinHalfFermionSite.valid_opname(name)</td>
<td>Check whether ‘name’ labels a valid on-site-operator.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpinHalfFermionSite.dim</td>
<td>Dimension of the local Hilbert space.</td>
</tr>
<tr>
<td>SpinHalfFermionSite.onsite_ops</td>
<td>Dictionary of on-site operators for iteration.</td>
</tr>
</tbody>
</table>

class tenpy.networks.site.SpinHalfFermionSite (cons_N='N', cons_Sz='Sz', filling=1.0)

Bases: tenpy.networks.site.Site

Create a Site for spinful (spin-1/2) fermions.

Local states are: empty (vacuum), up (one spin-up electron), down (one spin-down electron), and full (both electrons)

Local operators can be built from creation operators.

**Warning:** Using the Jordan-Wigner string (JW) in the correct way is crucial to get correct results, otherwise you just describe hardcore bosons!

<table>
<thead>
<tr>
<th>operator</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Id</td>
<td>Identity ^F</td>
</tr>
<tr>
<td>JW</td>
<td>Sign for the Jordan-Wigner string ((-1)^{n_\uparrow \downarrow})</td>
</tr>
<tr>
<td>JWu</td>
<td>Partial sign for the Jordan-Wigner string ((-1)^{n_\uparrow})</td>
</tr>
<tr>
<td>JWed</td>
<td>Partial sign for the Jordan-Wigner string ((-1)^{n_\downarrow})</td>
</tr>
<tr>
<td>Cu</td>
<td>Annihilation operator spin-up (c_\uparrow) (up to ‘JW’-string on sites left of it).</td>
</tr>
<tr>
<td>Cdu</td>
<td>Creation operator spin-up (c_\downarrow^\dagger) (up to ‘JW’-string on sites left of it).</td>
</tr>
<tr>
<td>Cd</td>
<td>Annihilation operator spin-down (c_\downarrow) (up to ‘JW’-string on sites left of it). Includes JWu such that it anti-commutes onsite with Cu, Cdu.</td>
</tr>
<tr>
<td>Cdd</td>
<td>Creation operator spin-down (c_\downarrow^\dagger) (up to ‘JW’-string on sites left of it). Includes JWu such that it anti-commutes onsite with Cu, Cdu.</td>
</tr>
<tr>
<td>Nu</td>
<td>Number operator (n_\uparrow = c_\uparrow^\dagger c_\uparrow)</td>
</tr>
<tr>
<td>Nd</td>
<td>Number operator (n_\downarrow = c_\downarrow^\dagger c_\downarrow)</td>
</tr>
<tr>
<td>NuNd</td>
<td>Dotted number operators (n_\uparrow n_\downarrow)</td>
</tr>
<tr>
<td>Ntot</td>
<td>Total number operator (n_t = n_\uparrow + n_\downarrow)</td>
</tr>
<tr>
<td>dN</td>
<td>Total number operator compared to the filling (\Delta n = n_t - \text{filling})</td>
</tr>
<tr>
<td>Sx, Sy, Sz</td>
<td>Spin operators (S^{x,y,z}), in particular (S^z = \frac{1}{2}(n_\uparrow - n_\downarrow))</td>
</tr>
<tr>
<td>Sp, Sm</td>
<td>Spin flips (S^x \pm iS^y), e.g. (S^+ = c_\uparrow^\dagger c_\downarrow)</td>
</tr>
</tbody>
</table>
The spin operators are defined as \( S^\gamma = (c_\uparrow, c_\downarrow)\sigma^\gamma (c_\uparrow, c_\downarrow)^T \), where \( \sigma^\gamma \) are spin-1/2 matrices (i.e. half the pauli matrices).

<table>
<thead>
<tr>
<th>cons_N</th>
<th>cons_Sz</th>
<th>qmod</th>
<th>excluded onsite operators</th>
</tr>
</thead>
<tbody>
<tr>
<td>‘N’</td>
<td>'Sz'</td>
<td>[1,1]</td>
<td>Sx, Sy</td>
</tr>
<tr>
<td>‘N’</td>
<td>'parity'</td>
<td>[1,2]</td>
<td>–</td>
</tr>
<tr>
<td>‘N’</td>
<td>None</td>
<td>[1]</td>
<td>–</td>
</tr>
<tr>
<td>'parity'</td>
<td>'Sz'</td>
<td>[2,1]</td>
<td>Sx, Sy</td>
</tr>
<tr>
<td>'parity'</td>
<td>'parity'</td>
<td>[2,2]</td>
<td>–</td>
</tr>
<tr>
<td>None</td>
<td>'Sz'</td>
<td>[1]</td>
<td>Sx, Sy</td>
</tr>
<tr>
<td>None</td>
<td>'parity'</td>
<td>[2]</td>
<td>–</td>
</tr>
<tr>
<td>None</td>
<td>None</td>
<td>[1]</td>
<td>–</td>
</tr>
</tbody>
</table>

Parameters

- **cons_N (‘N’ | ‘parity’ | None)** – Whether particle number is conserved, c.f. table above.
- **cons_Sz (‘Sz’ | ‘parity’ | None)** – Whether spin is conserved, c.f. table above.
- **filling (float)** – Average filling. Used to define \( dN \).

**cons_N**

Whether particle number is conserved, c.f. table above.

Type 'N' | 'parity' | None

**cons_Sz**

Whether spin is conserved, c.f. table above.

Type 'Sz' | 'parity' | None

**filling**

Average filling. Used to define \( dN \).

Type float

**add_op (name, op, need_JW=False, hc=None)**

Add one on-site operators.

Parameters

- **name (str)** – A valid python variable name, used to label the operator. The name under which \( op \) is added as attribute to self.
- **op (np.ndarray | Array)** – A matrix acting on the local hilbert space representing the local operator. Dense numpy arrays are automatically converted to Array. LegCharges have to be \( [\text{leg}, \text{leg}.\text{conj()}]) \). We set labels ‘p’, ‘p*’.
- **need_JW (bool)** – Whether the operator needs a Jordan-Wigner string. If True, add \( name \) to need_JW_string.
- **hc (None / False / str)** – The name for the hermitian conjugate operator, to be used for hc_ops. By default (None), try to auto-determine it. If False, disable adding entries to hc_ops.

**change_charge (new_leg_charge=None, permute=None)**

Change the charges of the site (in place).

Parameters
• **new_leg_charge** (LegCharge | None) – The new charges to be used. If None, use trivial charges.

• **permute** (ndarray | None) – The permutation applied to the physical leg, which gets used to adjust state_labels and perm. If you sorted the previous leg with perm_qind, new_leg_charge = leg.sort(), use old_leg.perm_flat_from_perm_qind(perm_qind). Ignored if None.

**property dim**
Dimension of the local Hilbert space.

**classmethod from_hdf5** (hdf5_loader, h5gr, subpath)
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

Parameters

• **hdf5_loader** (Hdf5Loader) – Instance of the loading engine.

• **h5gr** (Group) – HDF5 group which is represent the object to be constructed.

• **subpath** (str) – The name of h5gr with a '/' in the end.

Returns **obj** – Newly generated class instance containing the required data.

Return type **cls**

**get_hc_op_name** (name)
Return the hermitian conjugate of a given operator.

Parameters **name** (str) – The name of the operator to be returned. Multiple operators separated by whitespace are interpreted as an operator product, exactly as `get_op()` does.

Returns **hc_op_name** – Operator name for the hermi such that `get_op()` of

Return type **str**

**get_op** (name)
Return operator of given name.

Parameters **name** (str) – The name of the operator to be returned. In case of multiple operator names separated by whitespace, we multiply them together to a single on-site operator (with the one on the right acting first).

Returns **op** – The operator given by name, with labels 'p', 'p*'. If name already was an npc Array, it's directly returned.

Return type **np_conserved**

**multiply_op_names** (names)
Multiply operator names together.

Join the operator names in names such that `get_op` returns the product of the corresponding operators.

Parameters **names** (list of str) – List of valid operator labels.

Returns **combined_opname** – A valid operator name Operatorname representing the product of operators in names.

Return type **str**

**multiply_operators** (operators)
Multiply local operators (possibly given by their names) together.
Parameters **operators** *(list of \{str, Array\})* – List of valid operator names (to be translated with `get_op()`) or directly on-site operators in the form of npc arrays with 'p', 'p*' label. The operators are multiplied left-to-right.

Returns **combined_operator** – The product of the given `operators` in a left-to-right multiplication following the usual mathematical convention. For example, if `operators=['Sz', 'Sp', 'Sx']`, the final operator is equivalent to `site.get_op('Sz Sp Sx')`, with the 'Sx' operator acting first on any physical state.

Return type **Array**

**property onsite_ops**
Dictionary of on-site operators for iteration.

Single operators are accessible as attributes.

**op_needs_JW**(name)
Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.

Parameters **name** *(str)* – The name of the operator, as in `get_op()`.

Returns **needs_JW** – Whether the operator needs a Jordan-Wigner string, judging from `need_JW_string`.

Return type **bool**

**remove_op**(name)
Remove an added operator.

Parameters **name** *(str)* – The name of the operator to be removed.

**rename_op**(old_name, new_name)
Rename an added operator.

Parameters

- **old_name** *(str)* – The old name of the operator.
- **new_name** *(str)* – The new name of the operator.

**save_hdf5**(hdf5_saver, h5gr, subpath)
Export `self` into a HDF5 file.

This method saves all the data it needs to reconstruct `self` with `from_hdf5()`.

This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute 'format'.

Parameters

- **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.
- **h5gr** *(class 'Group')* – HDF5 group which is supposed to represent `self`.
- **subpath** *(str)* – The name of `h5gr` with a '/' in the end.

**state_index**(label)
Return index of a basis state from its label.

Parameters **label** *(int / string)* – Either the index directly or a label (string) set before.

Returns **state_index** – the index of the basis state associated with the label.

Return type **int**

**state_indices**(labels)
Same as `state_index()`, but for multiple labels.
test_sanity()
Sanity check, raises ValueErrors, if something is wrong.

valid_opname(name)
Check whether ‘name’ labels a valid onsite-operator.

Parameters name (str) – Label for the operator. Can be multiple operator(labels) separated by whitespace, indicating that they should be multiplied together.

Returns valid – True if name is a valid argument to get_op().

Return type bool

SpinHalfSite

- full name: tenpy.networks.site.SpinHalfSite
- parent module: tenpy.networks.site
- type: class

Inheritance Diagram

```
Hdf5Exportable
   ↓
   Site
   ↓
SpinHalfSite
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpinHalfSite.<strong>init</strong></td>
<td>Initialize self.</td>
</tr>
<tr>
<td>SpinHalfSite.add_op</td>
<td>Add one on-site operators.</td>
</tr>
<tr>
<td>SpinHalfSite.change_charge</td>
<td>Change the charges of the site (in place).</td>
</tr>
<tr>
<td>SpinHalfSite.from_hdf5</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td>SpinHalfSite.get_hc_op_name</td>
<td>Return the hermitian conjugate of a given operator.</td>
</tr>
<tr>
<td>SpinHalfSite.get_op</td>
<td>Return operator of given name.</td>
</tr>
<tr>
<td>SpinHalfSite.multiply_op_names</td>
<td>Multiply operator names together.</td>
</tr>
</tbody>
</table>

continues on next page
Table 134 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
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<tbody>
<tr>
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<td>Multiply local operators (possibly given by their names) together.</td>
</tr>
<tr>
<td><code>SpinHalfSite.op_needs_JW</code></td>
<td>Whether an (composite) onsite operator is fermionic and needs a JW string.</td>
</tr>
<tr>
<td><code>SpinHalfSite.remove_op</code></td>
<td>Remove an added operator.</td>
</tr>
<tr>
<td><code>SpinHalfSite.rename_op</code></td>
<td>Rename an added operator.</td>
</tr>
<tr>
<td><code>SpinHalfSite.save_hdf5</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>SpinHalfSite.state_index</code></td>
<td>Return index of a basis state from its label.</td>
</tr>
<tr>
<td><code>SpinHalfSite.state_indices</code></td>
<td>Same as <code>state_index()</code>, but for multiple labels.</td>
</tr>
<tr>
<td><code>SpinHalfSite.test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td><code>SpinHalfSite.valid_opname</code></td>
<td>Check whether 'name' labels a valid onsite-operator.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>SpinHalfSite.dim</code></td>
<td>Dimension of the local Hilbert space.</td>
</tr>
<tr>
<td><code>SpinHalfSite.onsite_ops</code></td>
<td>Dictionary of on-site operators for iteration.</td>
</tr>
</tbody>
</table>

```python
class tenpy.networks.site_spinHalfSite (conserve='Sz')
Bases: tenpy.networks.site.Site
```

Spin-1/2 site.
Local states are up (0) and down (1). Local operators are the usual spin-1/2 operators, e.g. \( S_z = \begin{bmatrix} 0.5, 0. \end{bmatrix}, \begin{bmatrix} 0., -0.5 \end{bmatrix} \), \( S_x = 0.5 \times \sigma_x \) for the Pauli matrix \( \sigma_x \).

<table>
<thead>
<tr>
<th>operator</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Id, JW</td>
<td>Identity ( \mathbb{1} )</td>
</tr>
<tr>
<td>Sx, Sy, Sz</td>
<td>Spin components ( S_x, y, z ), equal to half the Pauli matrices.</td>
</tr>
<tr>
<td>Sigmax, Sigmay, Sigmaz</td>
<td>Pauli matrices ( \sigma_x, y, z )</td>
</tr>
<tr>
<td>Sp, Sm</td>
<td>Spin flips ( S^x = S_x \pm iS_y )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>conserve</th>
<th>qmod</th>
<th>excluded onsite operators</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Sz'</td>
<td>[1]</td>
<td>Sx, Sy, Sigmax, Sigmay</td>
</tr>
<tr>
<td>None</td>
<td>[1]</td>
<td>–</td>
</tr>
</tbody>
</table>

Parameters `conserve (str)` – Defines what is conserved, see table above.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>conserve</td>
<td>Defines what is conserved, see table above.</td>
</tr>
</tbody>
</table>

Type `str`

### `add_op` 

`add_op (name, op, need_JW=False, hc=None)`

Add one on-site operator.

Parameters

- `name (str)` – A valid python variable name, used to label the operator. The name under which `op` is added as attribute to self.
• **op** (np.ndarray | Array) – A matrix acting on the local hilbert space representing the local operator. Dense numpy arrays are automatically converted to `Array`. LegCharges have to be `[leg, leg.conj()]`. We set labels 'p', 'p*'.

• **need_JW** (bool) – Whether the operator needs a Jordan-Wigner string. If True, add name to need_JW_string.

• **hc** (None / False / str) – The name for the hermitian conjugate operator, to be used for hc_ops. By default (None), try to auto-determine it. If False, disable adding antries to hc_ops.

**change_charge** (new_leg_charge=None, permute=None)

Change the charges of the site (in place).

Parameters

• **new_leg_charge** (LegCharge | None) – The new charges to be used. If None, use trivial charges.

• **permute** (ndarray | None) – The permutation applied to the physical leg, which gets used to adjust state_labels and perm. If you sorted the previous leg with perm_qind, new_leg_charge = leg.sort(), use old_leg. perm_flat_from_perm_qind(perm_qind). Ignored if None.

property **dim**

Dimension of the local Hilbert space.

**classmethod from_hdf5** (hdf5_loader, h5gr, subpath)

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

Parameters

• **hdf5_loader** (Hdf5Loader) – Instance of the loading engine.

• **h5gr** (Group) – HDF5 group which is represent the object to be constructed.

• **subpath** (str) – The name of h5gr with a '/' in the end.

Returns **obj** – Newly generated class instance containing the required data.

Return type **cls**

**get_hc_op_name** (name)

Return the hermitian conjugate of a given operator.

Parameters **name** (str) – The name of the operator to be returned. Multiple operators separated by whitespace are interpreted as an operator product, exactly as `get_op()` does.

Returns **hc_op_name** – Operator name for the hermi such that `get_op()` of

Return type **str**

**get_op** (name)

Return operator of given name.

Parameters **name** (str) – The name of the operator to be returned. In case of multiple operator names separated by whitespace, we multiply them together to a single on-site operator (with the one on the right acting first).

Returns **op** – The operator given by name, with labels 'p', 'p*'. If name already was an npc Array, it's directly returned.

Return type **np_conserved**
**multiply_op_names** *(names)*

Multiply operator names together.

Join the operator names in *names* such that *get_op* returns the product of the corresponding operators.

**Parameters**

*names* *(list of str)* – List of valid operator labels.

**Returns**

*combined_opname* – A valid operator name Operatorname representing the product of operators in *names*.

**Return type**

str

**multiply_operators** *(operators)*

Multiply local operators (possibly given by their names) together.

**Parameters**

*operators* *(list of {str | Array})* – List of valid operator names (to be translated with *get_op()*) or directly on-site operators in the form of npc arrays with 'p', 'p*' label. The operators are multiplied left-to-right.

**Returns**

*combined_operator* – The product of the given *operators* in a left-to-right multiplication following the usual mathematical convention. For example, if *operators*=['Sz', 'Sp', 'Sx'], the final operator is equivalent to *site.get_op('Sz Sp Sx'),* with the 'Sx' operator acting first on any physical state.

**Return type**

Array

**property onsite_ops**

Dictionary of on-site operators for iteration.

Single operators are accessible as attributes.

**op_needs_JW** *(name)*

Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.

**Parameters**

*name* *(str)* – The name of the operator, as in *get_op()*.

**Returns**

*needs_JW* – Whether the operator needs a Jordan-Wigner string, judging from *need JW_string*.

**Return type**

bool

**remove_op** *(name)*

Remove an added operator.

**Parameters**

*name* *(str)* – The name of the operator to be removed.

**rename_op** *(old_name, new_name)*

Rename an added operator.

**Parameters**

*old_name* *(str)* – The old name of the operator.

*new_name* *(str)* – The new name of the operator.

**save_hdf5** *(hdf5_saver, h5gr, subpath)*

Export *self* into a HDF5 file.

This method saves all the data it needs to reconstruct *self* with *from_hdf5()*.

This implementation saves the content of __dict__ with *save_dict_content()*, storing the format under the attribute 'format'.

**Parameters**

*hdf5_saver* *(Hdf5Saver)* – Instance of the saving engine.
• **h5gr** (*class* `Group`) – HDF5 group which is supposed to represent `self`.

• **subpath** (*str*) – The name of `h5gr` with a `/` in the end.

**state_index** (*label*)
Return index of a basis state from its label.

- **Parameters**
  - `label` (*int | string*) – either the index directly or a label (string) set before.

- **Returns**
  - `state_index` – the index of the basis state associated with the label.

- **Return type**
  - `int`

**state_indices** (*labels*)
Same as `state_index()`, but for multiple labels.

**test_sanity**()
Sanity check, raises ValueErrors, if something is wrong.

**valid_opname** (*name*)
Check whether `name` labels a valid onsite-operator.

- **Parameters**
  - `name` (*str*) – Label for the operator. Can be multiple operator(labels) separated by whitespace, indicating that they should be multiplied together.

- **Returns**
  - `valid` – True if `name` is a valid argument to `get_op()`.

- **Return type**
  - `bool`

### SpinSite

- **full name**: `tenpy.networks.site.SpinSite`
- **parent module**: `tenpy.networks.site`
- **type**: class

### Inheritance Diagram

```
Hdf5Exportable  
|          |  
|          |  
|          |  
|          |  
|          |  
Site      |  
|          |  
|          |  
|          |  
SpinSite  |  
```

7.12. networks
Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpinSite.<strong>init</strong>(S, conserve)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>SpinSite.add_op(name, op[, need_JW, hc])</td>
<td>Add one on-site operators.</td>
</tr>
<tr>
<td>SpinSite.change_charge([new_leg_charge, permute])</td>
<td>Change the charges of the site (in place).</td>
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<td>SpinSite.from_hdf5(hdf5_loader, h5gr, subpath)</td>
<td>Load instance from a HDF5 file.</td>
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<td>SpinSite.get_op(name)</td>
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<td>Multiply operator names together.</td>
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<tr>
<td>SpinSite.save_hdf5(hdf5_saver, h5gr, subpath)</td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td>SpinSite.state_index(label)</td>
<td>Return index of a basis state from its label.</td>
</tr>
<tr>
<td>SpinSite.state_indices(labels)</td>
<td>Same as state_index(), but for multiple labels.</td>
</tr>
<tr>
<td>SpinSite.test_sanity()</td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
<tr>
<td>SpinSite.valid_opname(name)</td>
<td>Check whether 'name' labels a valid onsite-operator.</td>
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<td>Dimension of the local Hilbert space.</td>
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<tr>
<td>SpinSite.onsite_ops</td>
<td>Dictionary of on-site operators for iteration.</td>
</tr>
</tbody>
</table>

class tenpy.networks.site.SpinSite(S=0.5, conserve='Sz')

Bases: tenpy.networks.site.Site

General Spin S site.

There are 2S+1 local states range from down (0) to up (2S+1), corresponding to Sz=-S, -S+1, ..., S-1, S. Local operators are the spin-S operators, e.g. \( S_z = \begin{bmatrix} 0.5, 0. \\ 0., -0.5 \end{bmatrix} \), \( S_x = 0.5 \sigma_x \) for the Pauli matrix \( \sigma_x \).

<table>
<thead>
<tr>
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<th>description</th>
</tr>
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<tbody>
<tr>
<td>Id, JW</td>
<td>Identity ( \mathbb{1} )</td>
</tr>
<tr>
<td>Sx, Sy, Sz</td>
<td>Spin components ( S_x, y, z ) equal to half the Pauli matrices.</td>
</tr>
<tr>
<td>Sp, Sm</td>
<td>Spin flips ( S_x^\perp = S_x \pm iS_y )</td>
</tr>
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<tr>
<th>conserve</th>
<th>qmod</th>
<th>excluded onsite operators</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Sz'</td>
<td>[1]</td>
<td>Sx, Sy</td>
</tr>
<tr>
<td>'parity'</td>
<td>[2]</td>
<td>-</td>
</tr>
<tr>
<td>None</td>
<td>[1]</td>
<td>-</td>
</tr>
</tbody>
</table>

Parameters conserve (str) – Defines what is conserved, see table above.

\( S \)

The 2S+1 states range from \( m = -S, -S+1, \ldots +S \).
Type \{0.5, 1, 1.5, 2, ..\}

**conserve**
Defines what is conserved, see table above.

Type `str`

**add_op** `(name, op, need_JW=False, hc=None)`
Add one on-site operators.

Parameters

- `name` (`str`) – A valid python variable name, used to label the operator. The name under which `op` is added as attribute to self.
- `op` (`np.ndarray` | `Array`) – A matrix acting on the local hilbert space representing the local operator. Dense numpy arrays are automatically converted to `Array`. LegCharges have to be `[leg, leg.conj()]`. We set labels 'p', 'p*'.
- `need_JW` (`bool`) – Whether the operator needs a Jordan-Wigner string. If True, add `name` to `need_JW_string`.
- `hc` (`None` | `False` | `str`) – The name for the hermitian conjugate operator, to be used for `hc_ops`. By default (`None`), try to auto-determine it. If `False`, disable adding antaries to `hc_ops`.

**change_charge** `(new_leg_charge=None, permute=None)`
Change the charges of the site (in place).

Parameters

- `new_leg_charge` (`LegCharge` | `None`) – The new charges to be used. If `None`, use trivial charges.
- `permute` (`ndarray` | `None`) – The permutation applied to the physical leg, which gets used to adjust `state_labels` and `perm`. If you sorted the previous leg with `perm_qind`, `new_leg_charge = leg.sort()`, use `old_leg.perm_flat_from_perm_qind(perm_qind)`. Ignored if `None`.

**property dim**
Dimension of the local Hilbert space.

**classmethod from_hdf5** `(hdf5_loader, h5gr, subpath)`
Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with `save_hdf5()`.

Parameters

- `hdf5_loader` (`Hdf5Loader`) – Instance of the loading engine.
- `h5gr` (`Group`) – HDF5 group which is represent the object to be constructed.
- `subpath` (`str`) – The name of `h5gr` with a ' / ' in the end.

Returns `obj` – Newly generated class instance containing the required data.

Return type `cls`

**get_hc_op_name** `(name)`
Return the hermitian conjugate of a given operator.

Parameters `name` (`str`) – The name of the operator to be returned. Multiple operators separated by whitespace are interpreted as an operator product, exactly as `get_op()` does.

Returns `hc_op_name` – Operator name for the hermi such that `get_op()` of
Return type str

get_op(name)
Return operator of given name.

Parameters name (str) – The name of the operator to be returned. In case of multiple operator names separated by whitespace, we multiply them together to a single on-site operator (with the one on the right acting first).

Returns op – The operator given by name, with labels 'p', 'p*'. If name already was an npc Array, it's directly returned.

Return type np_conserved

multiply_op_names(names)
Multiply operator names together.
Join the operator names in names such that get_op returns the product of the corresponding operators.

Parameters names (list of str) – List of valid operator labels.

Returns combined_opname – A valid operator name Operatorname representing the product of operators in names.

Return type str

multiply_operators(operators)
Multiply local operators (possibly given by their names) together.

Parameters operators (list of {str | Array}) – List of valid operator names (to be translated with get_op()) or directly on-site operators in the form of npc arrays with 'p', 'p*' label. The operators are multiplied left-to-right.

Returns combined_operator – The product of the given operators in a left-to-right multiplication following the usual mathematical convention. For example, if operators=['Sz', 'Sp', 'Sx'], the final operator is equivalent to site.get_op('Sz Sp Sx'), with the 'Sx' operator acting first on any physical state.

Return type Array

property onsite_ops
Dictionary of on-site operators for iteration.
Single operators are accessible as attributes.

op_needs_JW(name)
Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.

Parameters name (str) – The name of the operator, as in get_op().

Returns needs_JW – Whether the operator needs a Jordan-Wigner string, judging from need_JW_string.

Return type bool

remove_op(name)
Remove an added operator.

Parameters name (str) – The name of the operator to be removed.

rename_op(old_name, new_name)
Rename an added operator.

Parameters
• old_name (str) – The old name of the operator.
new_name (str) – The new name of the operator.

save_hdf5 (hdf5_saver, h5gr, subpath)
Export self into a HDF5 file.
This method saves all the data it needs to reconstruct self with from_hdf5().
This implementation saves the content of __dict__ with save_dict_content(), storing the format under the attribute 'format'.

Parameters
- hdf5_saver (Hdf5Saver) – Instance of the saving engine.
- h5gr (class `Group`) – HDF5 group which is supposed to represent self.
- subpath (str) – The name of h5gr with a '/' in the end.

state_index (label)
Return index of a basis state from its label.

Parameters label (int | string) – Either the index directly or a label (string) set before.

Returns state_index – the index of the basis state associated with the label.

Return type int

state_indices (labels)
Same as state_index(), but for multiple labels.

test_sanity()
Sanity check, raises ValueErrors, if something is wrong.

valid_opname (name)
Check whether ‘name’ labels a valid onsite-operator.

Parameters name (str) – Label for the operator. Can be multiple operator(labels) separated by whitespace, indicating that they should be multiplied together.

Returns valid – True if name is a valid argument to get_op().

Return type bool

Functions

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>group_sites</td>
<td>Given a list of sites, group each n sites together.</td>
</tr>
<tr>
<td>multi_sites_combine_charges</td>
<td>Adjust the charges of the given sites (in place) such that they can be used together.</td>
</tr>
<tr>
<td>set_common_charges</td>
<td>Adjust the charges of the given sites in place such that they can be used together.</td>
</tr>
</tbody>
</table>
group_sites

- full name: tenpy.networks.site.group_sites
- parent module: tenpy.networks.site
- type: function

```python
def group_sites(sites, n=2, labels=None, charges='same'):
    # Given a list of sites, group each n sites together.
    # Parameters
    # - sites (list of Site) – The sites to be grouped together.
    # - n (int) – We group each n consecutive sites from sites together in a GroupedSite.
    # - labels – See GroupedSites.
    # - charges – See GroupedSites.
    # Returns grouped_sites – The grouped sites. Has length (len(sites)-1)//n + 1.
    # Return type list of GroupedSite
```

multi_sites_combine_charges

- full name: tenpy.networks.site.multi_sites_combine_charges
- parent module: tenpy.networks.site
- type: function

```python
def multi_sites_combine_charges(sites, same_charges=[]):
    # Adjust the charges of the given sites (in place) such that they can be used together.
    # When we want to contract tensors corresponding to different Site instances, these sites need to share a single ChargeInfo. This function adjusts the charges of these sites such that they can be used together.
    # Deprecated since version 0.7.3: Deprecated in favore of the new, more powerful set_common_charges(). Be aware of the slightly different argument structure though, namely that this function keeps charges not included in same_charges, whereas you need to include them explicitly into the new_charges argument of set_common_charges.
    # Parameters
    # - sites (list of Site) – The sites to be combined. Modified in place.
    # - same_charges ([(int, int|str), (int, int|str), ...], ...) – Defines which charges actually are the same, i.e. their quantum numbers are added up. Each charge is specified by a tuple (s, i) = (int, int|str), where s gives the index of the site within sites and i the index or name of the charge in the ChargeInfo of this site.
    # Returns perms – For each site the permutation performed on the physical leg to sort by charges.
    # Return type list of ndarray
```

Examples
```python
>>> from tenpy.networks.site import *
>>> ferm = SpinHalfFermionSite(cons_N='N', cons_Sz='Sz')
>>> spin = SpinSite(1.0, 'Sz')
>>> ferm.leg.chinfo is spin.leg.chinfo
False
>>> print(spin.leg)
+1
0 [-2]
1 [ 0]
2 [ 2]
3
>>> multi_sites_combine_charges([ferm, spin], same_charges=[[0, 1], [1, 0]])
[array([0, 1, 2, 3]), array([0, 1, 2])]
>>> # no permutations where needed
>>> ferm.leg.chinfo is spin.leg.chinfo
True
>>> print(spin.leg)
+1
0 [[ 0 -2]
1 [ 0 0]
2 [ 0 2]]
3
```

---

**set_common_charges**

- full name: `tenpy.networks.site.set_common_charges`
- parent module: `tenpy.networks.site`
- type: function

```python
from tenpy.networks.site import set_common_charges
```

Adjust the charges of the given sites in place such that they can be used together.

Before we can contract operators (and tensors) corresponding to different `Site` instances, we first need to define the overall conserved charges, i.e., we need to merge the `ChargeInfo` of them to a single, global `chinfo` and adjust the charges of the physical legs. That's what this function does.

A typical place to do this would be in `tenpy.models.model.CouplingMPOModel.init_sites()`.

(This function replaces the now deprecated `mutli_sites_combine_charges()`.)

**Parameters**

- `sites` (list of `Site`) – The sites to be combined. The sites are modified in place.
- `new_charges` ('same' | 'drop' | 'independent' | list of list of tuple) – Defines the new, common charges in terms of the old ones.

**list of lists of tuple** If a list is given, each entry `new_charge` of the list defines one new charge, i.e. the new number of charges is `qnumber=len(new_charges)`. Each entry `new_charge` of the outer list is itself a list of 3-tuples, `new_charge = [(factor, site_index, old_charge_index), ...]`. where the value of the new charge is the sum of `factor` times the value of the old charge, (specified by the `site_index` and the `old_charge_index` within that `site`), and the sum runs over all entries in that list.

---

7.12. networks 563
new_charge. old_charge_index can be an integer (=the index) or a string (=the name) of the charge in the corresponding sites[site_index].leg.chinfo.

'same' defaults to charges with the same name to match, and charges with different names to be independently conserved (see example below); None-set names are considered different.

'drop' Drop/remove all charges, equivalent to new_charges=[].

'independent' For the case that the charges of the different sites are independent and individually conserved, even if they have the same name.

• new_names (list of str) – Names for each of the new charges. Defaults to name of the first old charge specified.

• new_mod (list of int) – mod for the new charges, one entry for each list in new_charges. Defaults to the mod of the old charges, if not specified otherwise.

Returns perms – For each site the permutation performed on the physical leg to sort by charges.

Return type list of ndarray

Examples
When we just initialize some sites, they will in general have different charges. For example, we could have a SpinHalfFermionSite a spin-1 SpinSite. For reference, let’s also print the names and values of the charges.

```python
>>> from tenpy.networks.site import *
>>> ferm = SpinHalfFermionSite(cons_N='N', cons_Sz='Sz')
>>> ferm.leg.chinfo.names
['N', '2*Sz']
>>> print(ferm.leg.to_qflat())
[[ 1 -1]
 [ 0  0]
 [ 2  0]
 [ 1  1]]
```

```python
>>> spin = SpinSite(1.0, conserve='Sz')
>>> spin.leg.chinfo.names
['2*Sz']
>>> print(spin.leg.to_qflat())

```

With the default new_charges='same', this function will combine charges with the same name, and hence we will have two conserved quantities, namely the fermion particle number 'N' = N_(up_fermions) + N_(down-fermions), and the total Sz spin '2*Sz' = N_(up-fermions) + N_(up-spins) - N_(down-fermions) - N_(down-spins). In this case, there will only appear an extra column of zeros for the charges of the spin leg.

```python
>>> set_common_charges([ferm, spin], new_charges='same')
[array([[0, 1, 2, 3]]), array([[0, 1, 2]])]
```

```python
>>> ferm.leg.chinfo.names
['N', '2*Sz']
>>> print(ferm.leg.to_qflat())  # didn't change (except making a copy)
[[ 1 -1]
 [ 0  0]
 [ 2  0]]
```
With `new_charges='independent'`, we preserve the charges of the old sites individually. In this example, we get 3 conserved quantities, namely the fermion particle number `N_ferm = \text{N}_{\text{up-fermions}} + \text{N}_{\text{down-fermions}}`, and the fermionic Sz spin `2*Sz_ferm = \text{N}_{\text{up-fermions}} - \text{N}_{\text{down-fermions}}` and the Sz spin of the spin sites, `2*Sz_spin = \text{N}_{\text{up-spins}} - \text{N}_{\text{down-spins}}`. (We give the charges new names for clearer distinction.) Corresponding zero columns are added to the LegCharges.

```
>>> ferm = SpinHalfFermionSite(cons_N='N', cons_Sz='Sz')
>>> spin = SpinSite(1.0, conserve='Sz')
>>> set_common_charges([ferm, spin], new_charges='independent',
...                     new_names=['N_ferm', '2*Sz_ferm', '2*Sz_spin'])
[array([0, 1, 2, 3]), array([0, 1, 2])])
```

With the full specification of the `new_charges` through a list of list of tuples, you can create new charges as linear combinations of the charges of the individual sites. For example, the `SpinHalfFermionSite` is essentially the product of two `FermionSite`, one for the up electrons, and one for the down electrons. The `2*Sz` charge of the `SpinHalfFermionSite` is then equivalent to the difference of individual particle numbers, `2*Sz = N_{up} - N_{down}`.

```
>>> f_up = FermionSite(conserve='N')
>>> f_down = FermionSite(conserve='N')
>>> print(f_up.leg.to_qflat())
[[0]
 [1]]
>>> print(f_down.leg.to_qflat())
[[0]
 [1]]
>>> f_down.state_labels
{'empty': 0, 'full': 1}
>>> set_common_charges([f_up, f_down],
...                     new_charges=[[(1, 0, 'N')], (1, 1, 'N')],
...                     new_names=['N_tot', '2*Sz=(N_up-N_down)'])
[array([0, 1]), array([1, 0])])
```

With `new_charges='independent'`, we preserve the charges of the old sites individually. In this example, we get 3 conserved quantities, namely the fermion particle number `N_ferm = \text{N}_{\text{up-fermions}} + \text{N}_{\text{down-fermions}}`, and the fermionic Sz spin `2*Sz_ferm = \text{N}_{\text{up-fermions}} - \text{N}_{\text{down-fermions}}` and the Sz spin of the spin sites, `2*Sz_spin = \text{N}_{\text{up-spins}} - \text{N}_{\text{down-spins}}`. (We give the charges new names for clearer distinction.) Corresponding zero columns are added to the LegCharges.
Another example could be that you have both fermions and bosons, and that you have terms $c_i c_j b_k^\dagger + c_i^\dagger c_j^\dagger b_k$, where two fermions can merge into a pair forming a boson. In this case, neither the fermion number nor the boson number is preserved individually, but the combination $N_{\text{fermions}} + 2 \times N_{\text{bosons}}$ is preserved.

Finally, it can sometimes be convenient to change the charges of the The new_charges='drop' or new_charges=[] option is a quick way to remove any charges.

```
>>> ferm = SpinHalfFermionSite(cons_N='N', cons_Sz='Sz')
>>> spin = SpinSite(1.0, conserve='Sz')
>>> set_common_charges([ferm, spin], new_charges='drop')
[array([0, 1, 2, 3]), array([0, 1, 2])]
>>> assert ferm.leg.chinfo.qnumber == spin.leg.chinfo.qnumber == 0  # trivial: no charges
```
Classes

MPS(sites, Bs, SVs[, bc, form, norm]) A Matrix Product State, finite (MPS) or infinite (iMPS).

MPSEnvironment(bra, ket[, init_LP, init_RP, ...]) Stores partial contractions of $\langle bra | Op | ket \rangle$ for local operators $Op$.

TransferMatrix(bra, ket[, shift_bra, ...]) Transfer matrix of two MPS (bra & ket).

MPSEnvironment

• full name: tenpy.networks.mps.MPSEnvironment
• parent module: tenpy.networks.mps
• type: class

Inheritance Diagram

Methods

MPSEnvironment.__init__(bra, ket[, init_LP, ...]) Initialize self.

MPSEnvironment.del_LP(i) Delete stored part strictly to the left of site $i$.

MPSEnvironment.del_RP(i) Delete stored part strictly to the right of site $i$.

MPSEnvironment.expectation_value(ops[, ...]) Expectation value $\langle bra | ops | ket \rangle$ of (n-site) operator(s).
Table 140 – continued from previous page

<table>
<thead>
<tr>
<th>Class Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>MPSEnvironment.full_contraction(i0)</code></td>
<td>Calculate the overlap by a full contraction of the network.</td>
</tr>
<tr>
<td><code>MPSEnvironment.get_LP(i[, store])</code></td>
<td>Calculate LP at given site from nearest available one.</td>
</tr>
<tr>
<td><code>MPSEnvironment.get_LP_age(i)</code></td>
<td>Return number of physical sites in the contractions of get_LP(i).</td>
</tr>
<tr>
<td><code>MPSEnvironment.get_RP(i[, store])</code></td>
<td>Calculate RP at given site from nearest available one.</td>
</tr>
<tr>
<td><code>MPSEnvironment.get_RP_age(i)</code></td>
<td>Return number of physical sites in the contractions of get_RP(i).</td>
</tr>
<tr>
<td><code>MPSEnvironment.get_initialization_data()</code></td>
<td>Return data for (re-)initialization.</td>
</tr>
<tr>
<td><code>MPSEnvironment.init_LP(i)</code></td>
<td>Build initial left part LP.</td>
</tr>
<tr>
<td><code>MPSEnvironment.init_RP(i)</code></td>
<td>Build initial right part RP for an MPS/MPOEnvironment.</td>
</tr>
<tr>
<td><code>MPSEnvironment.set_LP(i, LP, age)</code></td>
<td>Store part to the left of site i.</td>
</tr>
<tr>
<td><code>MPSEnvironment.set_RP(i, RP, age)</code></td>
<td>Store part to the right of site i.</td>
</tr>
<tr>
<td><code>MPSEnvironment.test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
</tbody>
</table>

```python
class tenpy.networks.mps.MPSEnvironment(bra, ket, init_LP=None, init_RP=None, age_LP=0, age_RP=0):
    Bases: object
    Stores partial contractions of < 𝑏𝑟𝑎 | 𝑂𝑝 | 𝑘𝑒𝑡 > for local operators Op.
    The network for a contraction < 𝑏𝑟𝑎 | 𝑂𝑝 | 𝑘𝑒𝑡 > of a local operator Op, say exemplary at sites i, i+1 looks like:

    | .-->- vR vL -->-.
    | | | |
    | LP | Op | RP |
    | | | |
    | .--<- vR* vL* <-. |
```

Of course, we can also calculate the overlap <bra|ket> by using the special case Op = Id.

We use the following label convention (where arrows indicate qconj):

```plaintext
| .-->- vR vL -->-.
| |
| LP | RP |
| |
| .--<- vR* vL* <-. |
```

To avoid recalculations of the whole network e.g. in the DMRG sweeps, we store the contractions up to some site index in this class. For bc='finite', 'segment', the very left and right part LP[0] and RP[-1] are trivial and don't change, but for bc='infinite' they are might be updated (by inserting another unit cell to the left/right).

The MPS bra and ket have to be in canonical form. All the environments are constructed without the singular values on the open bond. In other words, we contract left-canonical \( A \) to the left parts \( LP \) and right-canonical \( B \) to the right parts \( RP \). Thus, the special case ket=bra should yield identity matrices for \( LP \) and \( RP \).

Parameters:

- **bra** (MPS) – The MPS to project on. Should be given in usual ‘ket’ form; we call \( conj() \) on the matrices directly. Stored in place, without making copies. If necessary to match charges, we call `gauge_total_charge()`.
- **ket** (MPO | None) – The MPS on which the local operator acts. Stored in place, without making copies. If None, use `bra`.

- **init_LP** (None | Array) – Initial very left part LP. If None, build trivial one with `init_LP()`.

- **init_RP** (None | Array) – Initial very right part RP. If None, build trivial one with `init_RP()`.

- **age_LP** (int) – The number of physical sites involved into the contraction yielding `firstLP`.

- **age_RP** (int) – The number of physical sites involved into the contraction yielding `lastRP`.

\[ L \]
Number of physical sites involved into the Environment, i.e. the least common multiple of `bra.L` and `ket.L`.

  Type int

- **bra, ket**
  The two MPS for the contraction.

  Type MPS

- **dtype**
  The data type.

  Type type

- **_finite**
  Whether the boundary conditions of the MPS are finite.

  Type bool

- **_LP**
  Left parts of the environment, len \( L \). \( LP[i] \) contains the contraction strictly left of site \( i \) (or None, if we don’t have it calculated).

  Type list of {None | Array}

- **_RP**
  Right parts of the environment, len \( L \). \( RP[i] \) contains the contraction strictly right of site \( i \) (or None, if we don’t have it calculated).

  Type list of {None | Array}

- **_LP_age**
  Used for book-keeping, how large the DMRG system grew: \( _LP_age[i] \) stores the number of physical sites involved into the contraction network which yields `self._LP[i]`.

  Type list of int | None

- **_RP_age**
  Used for book-keeping, how large the DMRG system grew: \( _RP_age[i] \) stores the number of physical sites involved into the contraction network which yields `self._RP[i]`.

  Type list of int | None

- **test_sanity()**
  Sanity check, raises ValueErrors, if something is wrong.

- **init_LP(i)**
  Build initial left part LP.
Parameters: \(i (\text{int})\) – Build LP left of site \(i\).

Returns: \(\text{init\_LP}\) – Identity contractible with the \(vL\) leg of \(\text{ket\_get\_B}(i)\), labels ‘\(vR^*\)’, ‘\(vR\)’.

Return type: \(\text{Array}\)

\(\text{init\_RP}(i)\)

Build initial right part \(\text{RP}\) for an MPS/MPOEnvironment.

Parameters: \(i (\text{int})\) – Build RP right of site \(i\).

Returns: \(\text{init\_RP}\) – Identity contractible with the \(vR\) leg of \(\text{ket\_get\_B}(i)\), labels ‘\(vL^*\)’, ‘\(vL\)’.

Return type: \(\text{Array}\)

\(\text{get\_LP}(i, \text{store=True})\)

Calculate LP at given site from nearest available one.

The returned \(\text{LP}_i\) corresponds to the following contraction, where the M’s and the N’s are in the ‘A’ form:

```
|   \-------M[0]
| |      |   | vR
| LP[0] |   |
|   \-------N[0]
```

Parameters:

- \(i (\text{int})\) – The returned LP will contain the contraction \(\text{strictly}\) left of site \(i\).
- \(\text{store (bool)}\) – Whether to store the calculated LP in \(\text{self (True)}\) or discard them (False).

Returns: \(\text{LP}_i\) – Contraction of everything left of site \(i\), with labels ‘\(vR^*\)’, ‘\(vR\)’ for \(\text{bra, ket}\).

Return type: \(\text{Array}\)

\(\text{get\_RP}(i, \text{store=True})\)

Calculate RP at given site from nearest available one.

The returned \(\text{RP}_i\) corresponds to the following contraction, where the M’s and the N’s are in the ‘B’ form:

```
|\ 'vL' \->---M[i+1]
| |      |   | RP[-1]
|\ 'vL^*\ <----N[i+1]
```

Parameters:

- \(i (\text{int})\) – The returned RP will contain the contraction \(\text{strictly}\) right of site \(i\).
- \(\text{store (bool)}\) – Whether to store the calculated RP in \(\text{self (True)}\) or discard them (False).

Returns: \(\text{RP}_i\) – Contraction of everything left of site \(i\), with labels ‘\(vL^*\)’, ‘\(vL\)’ for \(\text{bra, ket}\).

Return type: \(\text{Array}\)
get_LP_age(i)
Return number of physical sites in the contractions of get_LP(i).
Might be None.

get_RP_age(i)
Return number of physical sites in the contractions of get_RP(i).
Might be None.

set_LP(i, LP, age)
Store part to the left of site i.

set_RP(i, RP, age)
Store part to the right of site i.

del_LP(i)
Delete stored part strictly to the left of site i.

del_RP(i)
Delete stored part strictly to the right of site i.

get_initialization_data()
Return data for (re-)initialization.

The returned parameters are collected in a dictionary with the following names.

Returns

• init_LP, init_RP (Array) – LP on the left of site 0 and RP on the right of site L-1, which can be used as init_LP and init_RP for the initialization of a new environment.

• age_LP, age_RP (int) – The number of physical sites involved into the contraction yielding init_LP and init_RP, respectively.

full_contraction(i0)
Calculate the overlap by a full contraction of the network.

The full contraction of the environments gives the overlap <bra|ket>, taking into account MPS.norm of both bra and ket. For this purpose, this function contracts get_LP(i0+1, store=False) and get_RP(i0, store=False) with appropriate singular values in between.

Parameters i0 (int) – Site index.

expectation_value(ops, sites=None, axes=None)
Expectation value <bra|ops|ket> of (n-site) operator(s).

Calculates n-site expectation values of operators sandwiched between bra and ket. For example, the contraction for a two-site operator on site i would look like:

```
  | .--S--B[i]--B[i+1]--.
  | | | | | | | | | | | | | | | | 
  | | | | | | | | | | | | | | | | 
  | LP[i] | op | RP[i+1]
  | | | | | | | | | | | | | | | | 
  | .--S--B*[i]--B*[i+1]--.
```

Here, the B are taken from ket, the B* from bra. The call structure is the same as for MPS.expectation_value().
Parameters

- **ops** ([list of] { `Array` | str }) – The operators, for which the expectation value should be taken. All operators should all have the same number of legs (namely 2 \( n \)). If less than \( \text{len(sites)} \) operators are given, we repeat them periodically. Strings (like 'Id', 'Sz') are translated into single-site operators defined by sites.

- **sites** ([list]) – List of site indices. Expectation values are evaluated there. If None (default), the entire chain is taken (clipping for finite b.c.)

- **axes** (None | ([list of str], [list of str])) – Two lists of each \( n \) leg labels giving the physical legs of the operator used for contraction. The first \( n \) legs are contracted with conjugated \( B \), the second \( n \) legs with the non-conjugated \( B \). None defaults to (['p'], ['p*']) for single site \( n=1 \), or (['p0', 'p1', ... 'p{n-1}'], ['p0*', 'p1*', .... 'p{n-1}*']) for \( n > 1 \).

Returns **exp_vals** – Expectation values, \( \text{exp_vals}[i] = \langle \text{bra}|\text{ops}[i]|\text{ket} \rangle \), where \( \text{ops}[i] \) acts on site(s) \( j, j+1, \ldots, j+{n-1} \) with \( j=\text{sites}[i] \).

Return type 1D ndarray

TransferMatrix

- full name: tenpy.networks.mps.TransferMatrix
- parent module: tenpy.networks.mps
- type: class

Inheritance Diagram
Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>TransferMatrix.<strong>init</strong>(bra, ket[...,])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>TransferMatrix.adjoint()</td>
<td>Return the hermitian conjugate of self</td>
</tr>
<tr>
<td>TransferMatrix.eigenvectors(*args, **kwargs)</td>
<td>Find (dominant) eigenvector(s) of self using scipy.sparse.</td>
</tr>
<tr>
<td>TransferMatrix.initial_guess([diag])</td>
<td>Return a diagonal matrix as initial guess for the eigenvector.</td>
</tr>
<tr>
<td>TransferMatrix.matvec(vec)</td>
<td>Given vec as an npc.Array, apply the transfer matrix.</td>
</tr>
<tr>
<td>TransferMatrix.to_matrix()</td>
<td>Contract self to a matrix.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

class tenpy.networks.mps.TransferMatrix(bra, ket, shift_bra=0, shift_ket=None, transpose=False, charge_sector=0, form='B')

Bases: tenpy.linalg.sparse.NpcLinearOperator

Transfer matrix of two MPS (bra & ket).

For an iMPS in the thermodynamic limit, we often need to find the ‘dominant RP’ (and LP). This means nothing else than to take the transfer matrix of the unit cell and find the (right/left) eigenvector with the largest (magnitude) eigenvalue, since it will dominate \((TM)^nRP\) (or \(LP(TM)^n\)) in the limit \(n \to \infty\) - whatever the initial RP is. This class provides exactly that functionality with eigenvectors().

Given two MPS, we define the transfer matrix as:

\[
\begin{array}{c|c|c|c|c|c}
|   | ---M[i]---M[i+1]--- \ldots ---M[i+L]--- |
|   |   |   |   |   |   |
|   | ---N[j]---N[j+1]--- \ldots ---N[j+L]--- |
\end{array}
\]

Here the \(M\) denotes the matrices of the bra and \(N\) the ones of the ket, respectively. To view it as a matrix, we combine the left and right indices to pipes:

\[
\begin{array}{c|c|c|c|c|c}
|   | (vL.vL*) \rightarrow TM \rightarrow (vR.vR*) acting on (vL.vL*) \rightarrow RP |
\end{array}
\]

Note that we keep all \(M\) and \(N\) as copies.

Deprecated since version 0.6.0: The default for \(shift\_ket\) was the value of \(shift\_bra\), this will be changed to 0.

Parameters

- **bra** *(MPS)* – The MPS which is to be (complex) conjugated.
- **ket** *(MPS)* – The MPS which is not (complex) conjugated.
- **shift_bra** *(int)* – We start the \(N\) of the bra at site \(shift\_bra\) (i.e. the \(j\) in the above network).
- **shift_ket** *(int | None)* – We start the \(M\) of the ket at site \(shift\_ket\) (i.e. the \(i\) in the above network). None is deprecated, default will be changed to 0 in the future.
- **transpose** *(bool)* – Whether self.matvec acts on \(RP\) (False) or \(LP\) (True).
• **charge_sector** (None | charges | 0) – Selects the charge sector of the vector onto which the Linear operator acts. **None** stands for all sectors, 0 stands for the zero-charge sector. Defaults to 0, i.e., **assumes** the dominant eigenvector is in charge sector 0.

• **form** ('B' | 'A' | 'C' | 'G' | 'Th' | None | tuple(float, float)) – In which canonical form we take the M and N matrices.

L
Number of physical sites involved in the transfer matrix, i.e. the least common multiple of bra.L and ket.L.

Type int

shift_bra
We start the N of the bra at site shift_bra.

Type int

shift_ket
We start the M of the ket at site shift_ket. None defaults to shift_bra.

Type int | None

transpose
Wheter self.matvec acts on RP (True) or LP (False).

Type bool

qtotal
Total charge of the transfer matrix (which is gauged away in matvec).

Type charges

form
In which canonical form (all of) the M and N matrices are.

Type tuple(float, float) | None

flat_linop
Class lifting matvec() to ndarrays in order to use speigs().

Type FlatLinearOperator

pipe
Pipe corresponding to ' (vL.vL*)' for transpose=False or ' (vR.vR*)' for transpose=True.

Type LegPipe

label_split
[ [ 'vL', 'vL*' ] if transpose=False or [ 'vR', 'vR*' ] if transpose=True.

_bra_N
Complex conjugated matrices of the bra, transposed for fast matvec.

Type list of npc.Array

_ket_M
The matrices of the ket, transposed for fast matvec.

Type list of npc.Array

matvec (vec)
Given vec as an npc.Array, apply the transfer matrix.
Parameters **vec** *(Array)* – Vector to act on with the transfer matrix. If not transposed, vec is the right part *RP* of an environment, with legs *(vL.vL\*)* in a pipe or split. If transposed, the left part *LP* of an environment with legs *(vR*.vR)*.

Returns **mat_vec** – The transfer matrix acted on *vec*, in the same form as given.

Return type *Array*

**initial_guess**(diag=1.0)

Return a diagonal matrix as initial guess for the eigenvector.

Parameters **diag** *(float | 1D ndarray)* – Should be 1. for the identity or some singular values squared.

Returns **mat** – A 2D array with *diag* on the diagonal such that *matvec()* can act on it.

Return type *Array*

**eigenvectors**(*args, **kwargs*)

Find (dominant) eigenvector(s) of self using *scipy.sparse*.

For arguments see *eigenvectors()*.

If no charge_sector was selected, we look in all charge sectors. The returned eigenvectors have combined legs *(vL.vL\*)* or *(vR*.vR)*.

**adjoint**()

Return the hermitian conjugate of self.

If *self* is hermitian, subclasses can choose to implement this to define the adjoint operator of *self*.

**to_matrix**()

Contract *self* to a matrix.

If *self* represents an operator with very small shape, e.g. because the MPS bond dimension is very small, an algorithm might choose to contract *self* to a single tensor.

Returns **matrix** – Contraction of the represented operator.

Return type *Array*

### Functions

**build_initial_state**(size, states, filling[, ...])  
Build an “initial state” list.

**build_initial_state**

- full name: tenpy.networks.mps.build_initial_state
- parent module: tenpy.networks.mps
- type: function

*tenpy.networks.mps.*build_initial_state*(size, states, filling[, ...])  
Build an “initial state” list.

Uses two iterables (‘states’ and ‘filling’) to determine how to fill the state. The two lists should have the same length as every element in ‘filling’ gives the filling fraction for the corresponding state in ‘states’.

Example
size = 6, states = [0, 1, 2], filling = [1./3, 2./3, 0.] n_states = size * filling = [2, 4, 0] ==> Two sites will get state 0, 4 sites will get state 1, 0 sites will get state 2.

Todo: Make more general: it should be possible to specify states as strings.

Parameters

- **size** *(int)* – length of state
- **states** *(iterable)* – Containing the possible local states
- **filling** *(iterable)* – Fraction of the total number of sites to get a certain state. If infinite fractions (e.g. 1/3) are needed, one should supply a fraction (1./3.)
- **mode** *(str | None)* – State filling pattern. Only ‘random’ is implemented
- **seed** *(int | None)* – Seed for random number generators

Returns `initial_state` *(list)*

Return type the initial state

Raises

- **ValueError** – If fractonal fillings are incommensurate with system size.
- **AssertionError** – If the total filling is not equal to 1, or the length of `filling` does not equal the length of `states`.

Module description

This module contains a base class for a Matrix Product State (MPS).

An MPS looks roughly like this:

```
| | | |
```

We use the following label convention for the B (where arrows indicate `qconj`):

```
| vL --> B --> vR
| |
```

We store one 3-leg tensor `_B[i]` with labels `vL`, `vR`, `p` for each of the `L` sites `0 <= i < L`. Additionally, we store `L+1` singular value arrays `_S[ib]` on each bond `0 <= ib <= L`, independent of the boundary conditions. `_S[ib]` gives the singlur values on the bond `i-1`, `i`. However, be aware that e.g. `chi` returns only the dimensions of the nontrivial_bonds depending on the boundary conditions.

The matrices and singular values always represent a normalized state (i.e. `np.linalg.norm(psi._S[ib]) == 1` up to roundoff errors), but (for finite MPS) we keep track of the norm in `norm` (which is respected by `overlap()`).

Valid MPS boundary conditions (not to confuse with `be_coupling` of `tenpy.models.model.CouplingModel`) are the following:
Finite MPS, \( s_0 G_0 s_1 G_1 \ldots s_{L-1} G_{L-1} \). This is achieved by using a trivial left and right bond \( s[0] = s[-1] = \text{np.array([1.])} \).

Generalization of 'finite', describes an MPS embedded in left and right environments. The left environment is described by \( \text{chi}[0] \) orthonormal states which are weighted by the singular values \( s[0] \). Similar, \( s[L] \) weight some right orthonormal states. You can think of the left and right states to be generated by additional MPS, such that the overall structure is something like \( \ldots s_L s_{L-1} s_{L-2} G_{L-2} s_{L-1} G_{L-1} s_{L-2} G_{L-2} \ldots \) (where we save the part in the brackets \( \ldots \)).

infinite MPS (iMPS): we save a 'MPS unit cell' \( [s_0 G_0 s_1 G_1 \ldots s_{L-1} G_{L-1}] \) which is repeated periodically, identifying all indices modulo \( self.L \). In particular, the last bond \( L \) is identified with 0. (The MPS unit cell can differ from a lattice unit cell). bond is identified with the first one.

<table>
<thead>
<tr>
<th>form</th>
<th>tuple</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>'B'</td>
<td>(0, 1)</td>
<td>right canonical: ( _B[i] = -- \text{Gamma}[i] -- s[i+1]-- ) The default form, which algorithms assume.</td>
</tr>
<tr>
<td>'C'</td>
<td>(0.5, 0.5)</td>
<td>symmetric form: ( _B[i] = -- s[i]^{0.5} -- \text{Gamma}[i] -- s[i+1]^{0.5}-- )</td>
</tr>
<tr>
<td>'A'</td>
<td>(1, 0)</td>
<td>left canonical: ( _B[i] = -- s[i] -- \text{Gamma}[i] -- )</td>
</tr>
<tr>
<td>'G'</td>
<td>(0, 0)</td>
<td>save only ( _B[i] = -- \text{Gamma}[i] -- )</td>
</tr>
<tr>
<td>'Th'</td>
<td>(1, 1)</td>
<td>Form of a local wave function ( \theta ) with singular value on both sides. psi.get_B(i, 'Th') is equivalent to <code>\psi.get_theta(i, n=1)</code>.</td>
</tr>
</tbody>
</table>
| None | None | General non-canonical form. Valid form for initialization, but you need to call 
canonical_form() (or similar) before using algorithms. |

An MPS can be in different 'canonical forms' (see [vidal2004][schollwoeck2011]). To take care of the different canonical forms, algorithms should use functions like get_theta(), get_B() and set_B() instead of accessing them directly, as they return the \( B \) in the desired form (which can be chosen as an argument). The values of the tuples for the form correspond to the exponent of the singular values on the left and right. To keep track of a “mixed” canonical form \( A A A s B B \), we save the tuples for each site of the MPS in \( \text{MPS.form} \).

7.12.3 mpo

- full name: tenpy.networks.mpo
- parent module: tenpy.networks
- type: module
Classes

MPO

MPOEnvironment

MPSEnvironment

MPOGraph

MPO

MPOEnvironment

MPSEnvironment

MPOGraph

MPOEnvironment

MPO(sites, Ws[, bc, IdL, IdR, max_range, ...])  Matrix product operator, finite (MPO) or infinite (iMPO).

MPOEnvironment(bra, H, ket[, init_LP, ...])  Stores partial contractions of \(< bra|H|ket >\) for an MPO \(H\).

MPSEnvironment(sites[, bc, max_range])  Representation of an MPO by a graph, based on a 'finite state machine'.

MPOEnvironment

• full name: tenpy.networks.mpo.MPOEnvironment
• parent module: tenpy.networks.mpo
• type: class

Inheritance Diagram
## Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>MPOEnvironment.__init__(bra, H, ket[, ...])</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>MPOEnvironment.del_LP(i)</code></td>
<td>Delete stored part strictly to the left of site $i$.</td>
</tr>
<tr>
<td><code>MPOEnvironment.del_RP(i)</code></td>
<td>Delete stored part strictly to the right of site $i$.</td>
</tr>
<tr>
<td><code>MPOEnvironment.expectation_value(ops[, ...])</code></td>
<td>(doesn’t make sense)</td>
</tr>
<tr>
<td><code>MPOEnvironment.full_contraction(i0)</code></td>
<td>Calculate the energy by a full contraction of the network.</td>
</tr>
<tr>
<td><code>MPOEnvironment.get_LP(i[, store])</code></td>
<td>Calculate LP at given site from nearest available one (including $i$).</td>
</tr>
<tr>
<td><code>MPOEnvironment.get_LP_age(i)</code></td>
<td>Return number of physical sites in the contractions of <code>get_LP(i)</code>.</td>
</tr>
<tr>
<td><code>MPOEnvironment.get_RP(i[, store])</code></td>
<td>Calculate RP at given site from nearest available one (including $i$).</td>
</tr>
<tr>
<td><code>MPOEnvironment.get_RP_age(i)</code></td>
<td>Return number of physical sites in the contractions of <code>get_RP(i)</code>.</td>
</tr>
<tr>
<td><code>MPOEnvironment.get_initialization_data()</code></td>
<td>Return data for (re-)initialization.</td>
</tr>
<tr>
<td><code>MPOEnvironment.init_LP(i)</code></td>
<td>Build initial left part LP.</td>
</tr>
<tr>
<td><code>MPOEnvironment.init_RP(i)</code></td>
<td>Build initial right part RP for an MPS/MPOEnvironment.</td>
</tr>
<tr>
<td><code>MPOEnvironment.set_LP(i, LP, age)</code></td>
<td>Store part to the left of site $i$.</td>
</tr>
<tr>
<td><code>MPOEnvironment.set_RP(i, RP, age)</code></td>
<td>Store part to the right of site $i$.</td>
</tr>
<tr>
<td><code>MPOEnvironment.test_sanity()</code></td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
</tbody>
</table>

### class tenpy.networks.mpo.MPOEnvironment (T)

Bases: `tenpy.networks.mps.MPSEnvironment`

Stores partial contractions of $< \text{bra}|H|\text{ket}>$ for an MPO $H$.

The network for a contraction $< \text{bra}|H|\text{ket}>$ of an MPO $H$ between two MPS looks like:

```
| .------>-M[0]-->-M[1]-->-M[2]--> ... -->-. |
| | | | | |
| | | ^ ^ ^ |
| | | | | |
| | | | | |
| LP[0] -->-W[0]-->-W[1]-->-W[2]--> ... --> RP[-1] |
| | | | | |
| | | | | |
| | | | | |
```

We use the following label convention (where arrows indicate $qconj$):

```
| .-->- vR vL -->-. |
| | | |
| LP-->- wR wL -->-RP |
| | | |
| .--<- vR* vL* -->-. |
```

To avoid recalculations of the whole network e.g. in the DMRG sweeps, we store the contractions up to some site index in this class. For `bc='finite', 'segment'`, the very left and right part $LP[0]$ and $RP[-1]$ are trivial and don’t change in the DMRG algorithm, but for `iDMRG (bc='infinite')` they are also updated (by inserting another unit cell to the left/right).
The MPS \textit{bra} and \textit{ket} have to be in canonical form. All the environments are constructed without the singular values on the open bond. In other words, we contract left-canonical \( A \) to the left parts \( \text{LP} \) and right-canonical \( B \) to the right parts \( \text{RP} \).

**Parameters**

- \textbf{\textit{bra}} (\textit{MPS}) – The MPS to project on. Should be given in usual ‘ket’ form; we call \texttt{conj()} on the matrices directly.
- \textbf{\textit{H}} (\textit{MPO}) – The MPO sandwiched between \textit{bra} and \textit{ket}. Should have ‘IdL’ and ‘IdR’ set on the first and last bond.
- \textbf{\textit{ket}} (\textit{MPS}) – The MPS on which \( H \) acts. May be identical with \textit{bra}.
- \textbf{\textit{init\_LP}} (\texttt{None} | \texttt{Array}) – Initial very left part \( \text{LP} \). If \texttt{None}, build trivial one with \texttt{init\_LP}.
- \textbf{\textit{init\_RP}} (\texttt{None} | \texttt{Array}) – Initial very right part \( \text{RP} \). If \texttt{None}, build trivial one with \texttt{init\_RP()}.
- \textbf{\textit{age\_LP}} (\texttt{int}) – The number of physical sites involved into the contraction yielding \( \text{firstLP} \).
- \textbf{\textit{age\_RP}} (\texttt{int}) – The number of physical sites involved into the contraction yielding \( \text{lastRP} \).

\( H \)

The MPO sandwiched between \textit{bra} and \textit{ket}.

Type \texttt{MPO}

\textbf{\texttt{test\_sanity}}()

Sanity check, raises ValueErrors, if something is wrong.

\textbf{\texttt{init\_LP}} (\texttt{i})

Build initial left part \( \text{LP} \).

Parameters \texttt{i} (\texttt{int}) – Build \( \text{LP} \) left of site \( i \).

Returns \texttt{init\_LP} – Identity contractible with the \texttt{vL} leg of \texttt{.ket.get\_B(i)}, multiplied with a unit vector nonzero in \texttt{H.IdL[i]}, with labels ‘\texttt{vR*}' , ‘\texttt{wR}', ‘\texttt{vR}'.

Return type \texttt{Array}

\textbf{\texttt{init\_RP}} (\texttt{i})

Build initial right part \( \text{RP} \) for an MPS/MPOEnvironment.

Parameters \texttt{i} (\texttt{int}) – Build \( \text{RP} \) right of site \( i \).

Returns \texttt{init\_RP} – Identity contractible with the \texttt{vR} leg of \texttt{self.get\_B(i)}, multiplied with a unit vector nonzero in \texttt{H.IdR[i]}, with labels ‘\texttt{vL*}' , ‘\texttt{wL}', ‘\texttt{vL}'.

Return type \texttt{Array}

\textbf{\texttt{get\_LP}} (\texttt{i, store=\texttt{True}})

Calculate \( \text{LP} \) at given site from nearest available one (including \texttt{i}).

The returned \( \text{LP}_i \) corresponds to the following contraction, where the M’s and the N’s are in the ‘A’ form:

```
| .-------M[0]--- ... -->M[i-1]-->-- 'vR'
|    |                  |                  |
| LP[0]-->W[0]--- ... -->W[i-1]-->-- 'wR'
|    |                  |                  |
| .-------N[0]--> ... -->N[i-1]-->-- 'vR*'
```
Parameters

- **i** (*int*) – The returned LP will contain the contraction strictly left of site i.
- **store** (*bool*) – Whether to store the calculated LP in self (True) or discard them (False).

Returns **LP_i** – Contraction of everything left of site i, with labels 'vR*', 'wR', 'vR' for bra, H, ket.

Return type **Array**

get_RP (i, store=True)

Calculate RP at given site from nearest available one (including i).

The returned RP_i corresponds to the following contraction, where the M’s and the N’s are in the ‘B’ form:

| 'vL' | 'wL' | 'vL*' |<--M[i+1]-- ... --M[L-1]----. |
| | | |<--W[i+1]-- ... --W[L-1]----RP[-1] |
| | | |<--N[i+1]-- ... --N[L-1]----. |

Parameters

- **i** (*int*) – The returned RP will contain the contraction strictly right of site i.
- **store** (*bool*) – Whether to store the calculated RP in self (True) or discard them (False).

Returns **RP_i** – Contraction of everything right of site i, with labels 'vL*', 'wL', 'vL' for bra, H, ket.

Return type **Array**

full_contraction (i0)

Calculate the energy by a full contraction of the network.

The full contraction of the environments gives the value <bra|H|ket> / (norm(|bra>) * norm(|ket>)), i.e. if bra is ket and normalized, the total energy. For this purpose, this function contracts get_LP(i0+1, store=False) and get_RP(i0, store=False).

Parameters **i0** (*int*) – Site index.

expectation_value (ops, sites=None, axes=None)

(del_LP (i)

Delete stored part strictly to the left of site i.

del_RP (i)

Delete stored part strictly to the right of site i.

get_LP_age (i)

Return number of physical sites in the contractions of get_LP(i).

Might be None.

get_RP_age (i)

Return number of physical sites in the contractions of get_RP(i).

Might be None.
get_initialization_data()
Return data for (re-)initialization.

The returned parameters are collected in a dictionary with the following names.

Returns

- **init_LP, init_RP** (*Array*) – LP on the left of site 0 and RP on the right of site \(L-1\), which can be used as init_LP and init_RP for the initialization of a new environment.
- **age_LP, age_RP** (*int*) – The number of physical sites involved into the contraction yielding init_LP and init_RP, respectively.

set_LP \((i, LP, age)\)
Store part to the left of site \(i\).

set_RP \((i, RP, age)\)
Store part to the right of site \(i\).

MPOGraph

- full name: tenpy.networks.mpo.MPOGraph
- parent module: tenpy.networks.mpo
- type: class

Inheritance Diagram

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPOGraph.<strong>init</strong>([sites[, bc, max_range]])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>MPOGraph.add(i, keyL, keyR, opname, strength)</td>
<td>Insert an edge into the graph.</td>
</tr>
<tr>
<td>MPOGraph.add_missing_IdL_IdR([insert_all_id])</td>
<td>Add missing identity ('Id') edges connecting 'IdL'-&gt;'IdL' and ```IdR'-&gt;'IdR'.</td>
</tr>
<tr>
<td>MPOGraph.add_string(i, j, key[, opname, ...])</td>
<td>Insert a bunch of edges for an 'operator string' into the graph.</td>
</tr>
<tr>
<td>MPOGraph.build_MPO([Ws_qtotal])</td>
<td>Build the MPO represented by the graph (<strong>self</strong>).</td>
</tr>
<tr>
<td>MPOGraph.from_term_list(term_list, sites, bc)</td>
<td>Initialize from a list of operator terms and prefactors.</td>
</tr>
<tr>
<td>MPOGraph.from_terms(terms, sites, bc[, ...])</td>
<td>Initialize an MPOGraph from OnsiteTerms and CouplingTerms.</td>
</tr>
<tr>
<td>MPOGraph.has_edge(i, keyL, keyR)</td>
<td>True if there is an edge from keyL on bond (i-1, i) to keyR on bond (i, i+1).</td>
</tr>
<tr>
<td>MPOGraph.test_sanity()</td>
<td>Sanity check, raises ValueErrors, if something is wrong.</td>
</tr>
</tbody>
</table>
Class Attributes and Properties

| MPOGraph.L | Number of physical sites; for infinite boundaries the length of the unit cell. |

```python
class tenpy.networks.mpo.MPOGraph(sites, bc='finite', max_range=None)
```

Representation of an MPO by a graph, based on a ‘finite state machine’.

This representation is used for building H_MPO from the interactions. The idea is to view the MPO as a kind of ‘finite state machine’. The **states** or **keys** of this finite state machine life on the MPO bonds between the Ws. They label the indices of the virtual bonds of the MPOs, i.e., the indices on legs wL and wR. They can be anything hash-able like a str, int or a tuple of them.

The **edges** of the graph are the entries W[keyL, keyR], which itself are onsite operators on the local Hilbert space. The indices keyL and keyR correspond to the legs 'wL', 'wR' of the MPO. The entry W[keyL, keyR] connects the state keyL on bond (i-1, i) with the state keyR on bond (i, i+1).

The keys 'IdR' (for ‘identity left’) and 'IdR' (for ‘identity right’) are reserved to represent only 'Id' (=identity) operators to the left and right of the bond, respectively.

**Todo:** might be useful to add a “cleanup” function which removes operators cancelling each other and/or unused states. Or better use a ‘compress’ of the MPO?

**Parameters**

- **sites** (list of Site) – Local sites of the Hilbert space.
- **bc** ({'finite', 'infinite'}) – MPO boundary conditions.
- **max_range** (int | np.inf | None) – Maximum range of hopping/interactions (in unit of sites) of the MPO. None for unknown.

**sites**

Defines the local Hilbert space for each site.

Type list of Site

**chinfo**

The nature of the charge.

Type ChargeInfo

**bc**

MPO boundary conditions.

Type {'finite', 'infinite'}

**max_range**

Maximum range of hopping/interactions (in unit of sites) of the MPO. None for unknown.

Type int | np.inf | None

**states**

states[i] gives the possible keys at the virtual bond (i-1, i) of the MPO. L+1 entries.

Type list of set of keys
For each site \( i \) a dictionary \{keyL: \{keyR: [(opname, strength)]\}\} with keyL in states[\( i \)] and keyR in states[\( i+1 \)].

**Type**: list of dict of dict of list of tuples

_**grid_legs**_

The charges for the MPO

**Type**: None | list of LegCharge

**classmethod from_terms**(\( \text{terms, sites, bc, insert_all_id=} \text{True} \))

Initialize an MPOGraph from OnsiteTerms and CouplingTerms.

**Parameters**

- **terms** (iterable of tenpy.networks.terms.*Terms classes) – Entries can be OnsiteTerms, CouplingTerms, MultiCouplingTerms or ExponentialCouplingTerms. All the entries get added to the new MPOGraph.
- **sites** (list of Site) – Local sites of the Hilbert space.
- **bc** (‘finite’ | ’infinite’) – MPO boundary conditions.
- **insert_all_id** (bool) – Whether to insert identities such that \( \text{IdL} \) and \( \text{IdR} \) are defined on each bond. See add_missing_IdL_IdR().

**Returns**: graph – Initialized with the given terms.

**Return type**: MPOGraph

See also:

**from_term_list** equivalent for representation by TermList.

**classmethod from_term_list**(\( \text{term_list, sites, bc, insert_all_id=} \text{True} \))

Initialize from a list of operator terms and prefactors.

**Parameters**

- **term_list** (TermList) – Terms to be added to the MPOGraph.
- **sites** (list of Site) – Local sites of the Hilbert space.
- **bc** (‘finite’ | ’infinite’) – MPO boundary conditions.
- **insert_all_id** (bool) – Whether to insert identities such that \( \text{IdL} \) and \( \text{IdR} \) are defined on each bond. See add_missing_IdL_IdR().

**Returns**: graph – Initialized with the given terms.

**Return type**: MPOGraph

See also:

**from_terms** equivalent for other representation of terms.

**test_sanity()**

Sanity check, raises ValueErrors, if something is wrong.

**property L**

Number of physical sites; for infinite boundaries the length of the unit cell.

**add**(\( i, \text{keyL, keyR, opname, strength, check_op=} \text{True, skip-existing=} \text{False} \))

Insert an edge into the graph.
Parameters

• $i$ (int) – Site index at which the edge of the graph is to be inserted.
• $\text{keyL}$ (hashable) – The state at bond $(i-1, i)$ to connect from.
• $\text{keyR}$ (hashable) – The state at bond $(i, i+1)$ to connect to.
• $\text{opname}$ (str) – Name of the operator.
• $\text{strength}$ (str) – Prefactor of the operator to be inserted.
• $\text{check_op}$ (bool) – Whether to check that ‘opname’ exists on the given site.
• $\text{skip_existing}$ (bool) – If True, skip adding the graph node if it exists (with same keys and $\text{opname}$).

add_string($i, j, \text{opname}=\text{Id}', \text{check_op}=\text{True}, \text{skip_existing}=\text{True}$)

Insert a bunch of edges for an ‘operator string’ into the graph.

Terms like $S_i^z S_j^z$ actually stand for $S_i^z \otimes \prod_{i<k<j} S_k^x \otimes S_j^z$. This function adds the $\otimes$ terms to the graph.

Parameters

• $i$ (int) – An edge is inserted on all bonds between $i$ and $j$, $i < j$. $j$ can be larger than $L$, in which case the operators are supposed to act on different MPS unit cells.
• $j$ (int) – An edge is inserted on all bonds between $i$ and $j$, $i < j$. $j$ can be larger than $L$, in which case the operators are supposed to act on different MPS unit cells.
• $\text{key}$ (hashable) – The state at bond $(i-1, i)$ to connect from and on bond $(j-1, j)$ to connect to. Also used for the intermediate states. No operator is inserted on a site $i < k < j$ if has_edge($k, \text{key}, \text{key}$).
• $\text{opname}$ (str) – Name of the operator to be used for the string. Useful for the Jordan-Wigner transformation to fermions.
• $\text{skip_existing}$ (bool) – Whether existing graph nodes should be skipped.

Returns $\text{label}_j$ – The key on the left of site $j$ to connect to. Usually the same as the parameter $\text{key}$, except if $j - i \geq self.L$, in which case we use the additional labels ($\text{key}$, 1), ($\text{key}$, 2),… to generate couplings over multiple unit cells.

Return type hashable

add_missing_IdL_IdR ($\text{insert_all_id}=\text{True}$)

Add missing identity (‘Id’) edges connecting ‘IdL’-$\rightarrow$‘IdL’ and ‘IdR’-$\rightarrow$‘IdR’.

This function should be called after all other operators have been inserted.

Parameters $\text{insert_all_id}$ (bool) – If True, insert ‘Id’ edges on all bonds. If False and boundary conditions are finite, only insert ‘IdL’-$\rightarrow$‘IdL’ to the left of the rightmost existing ‘IdL’ and ‘IdR’-$\rightarrow$‘IdR’ to the right of the leftmost existing ‘IdR’. The latter avoid “dead ends” in the MPO, but some functions (like make_WI) expect ‘IdL’/‘IdR’ to exist on all bonds.

has_edge($i, \text{keyL}, \text{keyR}$)

True if there is an edge from $\text{keyL}$ on bond $(i-1, i)$ to $\text{keyR}$ on bond $(i, i+1)$.

build_MPO ($Ws_qtotal=\text{None}$)

Build the MPO represented by the graph (self).

Parameters $Ws_qtotal$ (None / (list of) charges) – The qtotal for each of the Ws to be generated, default (None) means 0 charge. A single qtotal holds for each site.

Returns mpo – the MPO which self represents.
**grid_insert_ops**

- full name: `tenpy.networks.mpo.grid_insert_ops`
- parent module: `tenpy.networks.mpo`
- type: function

```python
tenpy.networks.mpo.grid_insert_ops(site, grid)
```

Replaces entries representing operators in a grid of $W[i]$ with npc.Arrays.

**Parameters**

- `site` (`site`) – The site on which the grid acts.
- `grid` (list of list of `entries`) – Represents a single matrix $W$ of an MPO, i.e. the lists correspond to the legs 'vL', 'vR', and entries to onsite operators acting on the given `site`. `entries` may be `None`, `Array`, a single string or of the form `[("opname", strength), ...]`, where 'opname' labels an operator in the `site`.

**Returns**

- `grid` – Copy of `grid` with entries `[("opname", strength), ...]` replaced by `sum([strength*site.get_op('opname') for opname, strength in entry])` and entries 'opname' replaced by `site.get_op('opname')`.

**Return type** list of list of {`None` | `Array`}

**make_W_II**

- full name: `tenpy.networks.mpo.make_W_II`
- parent module: `tenpy.networks.mpo`
- type: function

```python
tenpy.networks.mpo.make_W_II(t, A, B, C, D)
```

W_II approx to exp(t H) from MPO parts (A, B, C, D).

In the paper, we have two formal parameter “phi_{r/c}” which satisfies $\phi_r^2 = p\phi_c^2 = 0$. To implement this, we temporarily extend the virtual Hilbert space with two hard-core bosons “br, bl”. The components of Eqn (11) can be computed for each index of the virtual row/column independently The matrix exponential is done in the hard-core extended Hilbert space

**Parameters**

- `t` (`float`) – The time step per application of the propagator. Should be imaginary for real time evolution!
• **A** *(numpy.ndarray)* – Blocks of the MPO tensor to be exponentiated, as defined in [zaletel2015]. Legs 'wL', 'wR', 'p', 'p*'; legs projected to a single IdL/IdR can be dropped.

• **B** *(numpy.ndarray)* – Blocks of the MPO tensor to be exponentiated, as defined in [zaletel2015]. Legs 'wL', 'wR', 'p', 'p*'; legs projected to a single IdL/IdR can be dropped.

• **C** *(numpy.ndarray)* – Blocks of the MPO tensor to be exponentiated, as defined in [zaletel2015]. Legs 'wL', 'wR', 'p', 'p*'; legs projected to a single IdL/IdR can be dropped.

• **D** *(numpy.ndarray)* – Blocks of the MPO tensor to be exponentiated, as defined in [zaletel2015]. Legs 'wL', 'wR', 'p', 'p*'; legs projected to a single IdL/IdR can be dropped.

**Module description**

Matrix product operator (MPO).

An MPO is the generalization of an MPS to operators. Graphically:

```
| ^ ^ ^
| | | |
| | | |
| ^ ^ ^
```

So each ‘matrix’ has two physical legs p, p* instead of just one, i.e. the entries of the ‘matrices’ are local operators. Valid boundary conditions of an MPO are the same as for an MPS (i.e. ‘finite’ | ’segment’ | 'infinite’). (In general, you can view the MPO as an MPS with larger physical space and bring it into canonical form. However, unlike for an MPS, this doesn’t simplify calculations. Thus, an MPO has no form.)

We use the following label convention for the W (where arrows indicate qconj):

```
| p*
| ^
| wL -> W -> wR
| |
| ^
| p
```

If an MPO describes a sum of local terms (e.g. most Hamiltonians), some bond indices correspond to ‘only identities to the left/right’. We store these indices in IdL and IdR (if there are such indices).

Similar as for the MPS, a bond index i is left of site i, i.e. between sites i-1 and i.
7.12.4 terms

- full name: tenpy.networks.terms
- parent module: tenpy.networks
- type: module

**Classes**

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CouplingTerms(L)</td>
<td>Operator names, site indices and strengths representing two-site coupling terms.</td>
</tr>
<tr>
<td>ExponentiallyDecayingTerms(L)</td>
<td>Represent a sum of exponentially decaying (long-range) couplings.</td>
</tr>
<tr>
<td>MultiCouplingTerms(L)</td>
<td>Operator names, site indices and strengths representing general M-site coupling terms.</td>
</tr>
<tr>
<td>OnsiteTerms(L)</td>
<td>Operator names, site indices and strengths representing onsite terms.</td>
</tr>
<tr>
<td>TermList(terms[, strength])</td>
<td>A list of terms (=operator names and sites they act on) and associated strengths.</td>
</tr>
</tbody>
</table>

**CouplingTerms**

- full name: tenpy.networks.terms.CouplingTerms
- parent module: tenpy.networks.terms
- type: class
Inheritance Diagram

```
Hdf5Exportable
   └── CouplingTerms
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>CouplingTerms.__init__(L)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>CouplingTerms.add_coupling_term(strength, i, ...)</code></td>
<td>Add a two-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td><code>CouplingTerms.add_to_graph(graph)</code></td>
<td>Add terms from <code>coupling_terms</code> to an MPOGraph.</td>
</tr>
<tr>
<td><code>CouplingTerms.coupling_term_handle_JW(., . . . [,), . . . ])</code></td>
<td>Helping function to call before <code>add_multi_coupling_term()</code>.</td>
</tr>
<tr>
<td><code>CouplingTerms.from_hdf5(hdf5_loader, h5gr, ...)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>CouplingTerms.max_range()</code></td>
<td>Determine the maximal range in <code>coupling_terms</code>.</td>
</tr>
<tr>
<td><code>CouplingTerms.plot_coupling_terms(ax, lat[,...])</code></td>
<td>&quot;Plot coupling terms into a given lattice.</td>
</tr>
<tr>
<td><code>CouplingTerms.remove_zeros([tol_zero])</code></td>
<td>Remove entries close to 0 from <code>coupling_terms</code>.</td>
</tr>
<tr>
<td><code>CouplingTerms.save_hdf5(hdf5_saver, h5gr, ...)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>CouplingTerms.to_TermList()</code></td>
<td>Convert <code>onsite_terms</code> into a TermList.</td>
</tr>
<tr>
<td><code>CouplingTerms.to_nn_bond_Arrays(sites)</code></td>
<td>Convert the <code>coupling_terms</code> into Arrays on nearest neighbor bonds.</td>
</tr>
</tbody>
</table>

```python
class tenpy.networks.terms.CouplingTerms(L):
    Bases: tenpy.tools.hdf5_io.Hdf5Exportable

    Operator names, site indices and strengths representing two-site coupling terms.

    Parameters:
    L (int) – Number of sites.

    L
    Number of sites.

    Type  int

    coupling_terms
    Filled by `add_coupling_term()`. Nested dictionaries of the form `{i: {('opname_i', 'opname_string'): {j: {'opname_j': strength})}}`. Note that always `i < j`, but entries with `j >= L` are allowed for `bc_MPS == 'infinite'`, in which case they indicate couplings between different iMPS unit cells.
```
Type  dict of dict

max_range()

Determine the maximal range in coupling_terms.

Returns max_range – The maximum of \( j - i \) for the \( i, j \) occurring in a term of coupling_terms.

Return type  int

add_coupling_term(strength, i, j, op_i, op_j, op_string='Id')

Add a two-site coupling term on given MPS sites.

Parameters

- **strength** (float) – The strength of the coupling term.
- **i** (int) – The MPS indices of the two sites on which the operator acts. We require \( 0 \leq i < N_{\text{sites}} \) and \( i < j \), i.e., \( \text{op}_i \) acts “left” of \( \text{op}_j \). If \( j \geq N_{\text{sites}} \), it indicates couplings between unit cells of an infinite MPS.
- **j** (int) – The MPS indices of the two sites on which the operator acts. We require \( 0 \leq i < N_{\text{sites}} \) and \( i < j \), i.e., \( \text{op}_i \) acts “left” of \( \text{op}_j \). If \( j \geq N_{\text{sites}} \), it indicates couplings between unit cells of an infinite MPS.
- **op1** (str) – Names of the involved operators.
- **op2** (str) – Names of the involved operators.
- **op_string** (str) – The operator to be inserted between \( i \) and \( j \).

coupling_term_handle_JW(strength, term, sites, op_string=None)

Helping function to call before add_multi_coupling_term().

Parameters

- **strength** (float) – The strength of the coupling term.
- **term** ([(str, int), (str, int)]) – List of two tuples (op, i) where i is the MPS index of the site the operator named op acts on.
- **sites** (list of Site) – Defines the local Hilbert space for each site. Used to check whether the operators need Jordan-Wigner strings.
- **op_string** (None / str) – Operator name to be used as operator string between the operators, or None if the Jordan-Wigner string should be figured out.

Warning: None figures out for each segment between the operators, whether a Jordan-Wigner string is needed. This is different from a plain 'JW', which just applies a string on each segment!

Returns  Arguments for MultiCouplingTerms.add_multi_coupling_term() such that the added term corresponds to the parameters of this function.

Return type  strength, i, j, op_i, op_j, op_string

plot_coupling_terms(ax, lat, style_map='default', common_style={'linestyle': '--'}, text=None, text_pos=0.4)

“Plot coupling terms into a given lattice.

This function plots the coupling_terms

Parameters
• **ax** (matplotlib.axes.Axes) – The axes on which we should plot.

• **lat** (Lattice) – The lattice for plotting the couplings, most probably the M.lat of the corresponding model M, see lat.

• **style_map** (function | None) – Function which get’s called with arguments i, j, op_i, op_string, op_j, strength for each two-site coupling and should return a keyword-dictionary with the desired plot-style for this coupling. By default (None), the linewidth is given by the absolute value of strength, and the linecolor depends on the phase of strength (using the hsv colormap).

• **common_style** (dict) – Common style, which overwrites values of the dictionary returned by style_map. A ‘label’ is only used for the first plotted line.

• **text** (format_string | None) – If not None, we add text labeling the couplings in the plot. Available keywords are i, j, op_i, op_string, op_j, strength as well as strength_abs, strength_angle, strength_real.

• **text_pos** (float) – Specify where to put the text on the line between i (0.0) and j (1.0), e.g. 0.5 is exactly in the middle between i and j.

See also:

- **tenpy.models.lattice.Lattice.plot_sites** plot the sites of the lattice.

- **add_to_graph**(graph)
  Add terms from coupling_terms to an MPOGraph.

  **Parameters**
  - **graph** (MPOGraph) – The graph into which the terms from coupling_terms should be added.

- **to_nn_bond_Arrays**(sites)
  Convert the coupling_terms into Arrays on nearest neighbor bonds.

  **Parameters**
  - **sites** (list of Site) – Defines the local Hilbert space for each site. Used to translate the operator names into Array.

  **Returns** H_bond – The coupling_terms rewritten as sum_i H_bond[i] for MPS indices i. H_bond[i] acts on sites (i-1, i), None represents 0. Legs of each H_bond[i] are ['p0', 'p0*', 'p1', 'p1*'].

  **Return type** list of {Array | None}

- **remove_zeros**(tol_zero=1e-15)
  Remove entries close to 0 from coupling_terms.

  **Parameters**
  - **tol_zero** (float) – Entries in coupling_terms with strength < tol_zero are considered to be zero and removed.

- **to_TermList**()
  Convert onsite_terms into a TermList.

  **Returns** term_list – Representation of the terms as a list of terms.

  **Return type** TermList

- **classmethod from_hdf5**(hdf5_loader, h5gr, subpath)
  Load instance from a HDF5 file.

  This method reconstructs a class instance from the data saved with save_hdf5().

  **Parameters**
  - **hdf5_loader** (Hdf5Loader) – Instance of the loading engine.
• **h5gr** ([Group](#)) – HDF5 group which is represent the object to be constructed.

• **subpath** *(str)* – The *name* of *h5gr* with a '/' in the end.

**Returns** obj – Newly generated class instance containing the required data.

**Return type** cls

```python
save_hdf5(hdf5_saver, h5gr, subpath)
```

Export *self* into a HDF5 file.

This method saves all the data it needs to reconstruct *self* with *from_hdf5()*.

This implementation saves the content of *__dict__* with *save_dict_content()*; storing the format under the attribute 'format'.

**Parameters**

• **hdf5_saver** *(Hdf5Saver)* – Instance of the saving engine.

• **h5gr** *(:class:`Group`)* – HDF5 group which is supposed to represent *self*.

• **subpath** *(str)* – The *name* of *h5gr* with a '/' in the end.

---

**ExponentiallyDecayingTerms**

• full name: tenpy.networks.terms.ExponentiallyDecayingTerms

• parent module: tenpy.networks.terms

• type: class

---

**Inheritance Diagram**

```
Hdf5Exportable
    └─ ExponentiallyDecayingTerms
```
Methods

```python
 class tenpy.networks.terms.ExponentiallyDecayingTerms(L):
     Bases: tenpy.tools.hdf5_io.Hdf5Exportable

     Represent a sum of exponentially decaying (long-range) couplings.

     MPOs can represent translation invariant, exponentially decaying long-range terms of the following form with a single extra index of the virtual bonds:

     \[ \sum_{i \neq j} \lambda |i-j| A_i B_j \]

     For 2D cylinders (or ladders), we need a slight generalization of this, where the operators act only on a subset of the sites in each unit cell, given by a 1D array `subsites`:

     \[ \sum_{i<j} \lambda |i-j| A_{subsites[i]} B_{subsites[j]} \]

     Note that we still have \(|i-j|\), such that this will give uniformly decaying interactions, independent of the way the MPS winds through the 2D lattice, as long as `subsites` is sorted. An easy example would be a ladder, where we want the long-range interactions on the first rung only, `subsites = lat.mps_idx_fix_u(u=0)`, see mps_idx_fix_u().

     Parameters
     \[ \text{L (int)} \] – Number of sites.

     \[ \text{L} \]

     Number of sites.

     Type int

     exp_decaying_terms

     Each tuple (strength, opname_i, opname_j, lambda, subsites, opname_string) represents one of the terms as described above; see add_exponentially_decaying_coupling() for more details.

     Type list of tuples

     add_exponentially_decaying_coupling(strength, lambda_, op_i, op_j, subsites=None, op_string='Id')

     Add an exponentially decaying long-range coupling.

     \[ \sum_{i<j} \lambda |i-j| A_{subsites[i]} B_{subsites[j]} \]

     Where the operator \(A\) is given by \(op_i\) and \(B\) is given by \(op_j\). Note that the sum over \(ij\) is long-range, for infinite systems beyond the MPS unit cell.
```
Parameters

- **strength** (*float*) – Overall prefactor.
- **lambda** (*float*) – Decay-rate
- **op_i** (*string*) – Names for the operators.
- **op_j** (*string*) – Names for the operators.
- **subsites** (*None / 1D array*) – Selects a subset of sites within the MPS unit cell on which the operators act. Needs to be sorted. *None* selects all sites.
- **op_string** (*string*) – The operator to be inserted between $A$ and $B$; for Fermions this should be "JW".

**add_to_graph** (*graph*, *key='exp-decay'*)
Add terms from **onsite_terms** to an MPOGraph.

Parameters

- **graph** (*MPOGraph*) – The graph into which the terms from **exp_decaying_terms** should be added.
- **key** (*str*) – Key to distinguish from other **states** in the MPOGraph. We find integers **key_nr** and use (**key_nr**, **key**) as **state** for the different entries in **exp_decaying_terms**.

**to_TermList** (*cutoff=0.01, bc='finite'*)
Convert self into a **TermList**.

Parameters

- **cutoff** (*float*) – Drop terms where the overall prefactor is smaller then **cutoff**.
- **bc** (*"finite" | "infinite"*) – Boundary conditions to be used.

Returns **term_list** – Representation of the terms as a list of terms. For “infinite” **bc**, only terms starting in the first MPS unit cell are included.

Return type **TermList**

**max_range** ()
Maximum range of the couplings. In this case **np.inf**.

**classmethod from_hdf5** (*hdf5_loader, h5gr, subpath*)
Load instance from a HDF5 file.
This method reconstructs a class instance from the data saved with **save_hdf5()**.

Parameters

- **hdf5_loader** (*Hdf5Loader*) – Instance of the loading engine.
- **h5gr** (*Group*) – HDF5 group which is represent the object to be constructed.
- **subpath** (*str*) – The **name** of **h5gr** with a '/ ' in the end.

Returns **obj** – Newly generated class instance containing the required data.

Return type **cls**

**save_hdf5** (*hdf5_saver, h5gr, subpath*)
Export **self** into a HDF5 file.
This method saves all the data it needs to reconstruct **self** with **from_hdf5()**.
This implementation saves the content of `__dict__` with `save_dict_content()`, storing the format under the attribute 'format'.

**Parameters**
- `hdf5_saver` ([Hdf5Saver](Hdf5Saver)) – Instance of the saving engine.
- `h5gr` ([class `Group`]) – HDF5 group which is supposed to represent `self`.
- `subpath` (str) – The name of `h5gr` with a ' / ' in the end.

**MultiCouplingTerms**
- full name: `tenpy.networks.terms.MultiCouplingTerms`
- parent module: `tenpy.networks.terms`
- type: class

**Inheritance Diagram**

```
Hdf5Exportable
    ▼
   ▼
CouplingTerms
    ▼
MultiCouplingTerms
```

**Methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>MultiCouplingTerms.__init__(L)</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.add_coupling_term(...[...])</code></td>
<td>Add a two-site coupling term on given MPS sites.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.add_multi_coupling_term(...)</code></td>
<td>Add a multi-site coupling term.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.add_to_graph(graph[, _i,...])</code></td>
<td></td>
</tr>
<tr>
<td><code>MultiCouplingTerms.coupling_term_handle_JW(...)</code></td>
<td>Helping function to call before <code>add_multi_coupling_term()</code>.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.from_hdf5(hdf5_loader,...)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
</tbody>
</table>

continues on next page
Table 152 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>MultiCouplingTerms.max_range()</code></td>
<td>Determine the maximal range in <code>coupling_terms</code>.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.multi_coupling_term_handle_JW(...)</code></td>
<td>Helping function to call before <code>add_multi_coupling_term()</code>.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.plot_coupling_terms(ax, lat)</code></td>
<td>&quot;Plot coupling terms into a given lattice.&quot;</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.remove_zeros([tol_zero, _d0])</code></td>
<td>Remove entries close to 0 from <code>coupling_terms</code>.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.save_hdf5(hdf5_saver, ...)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.to_TermList()</code></td>
<td>Convert onsite_terms into a TermList.</td>
</tr>
<tr>
<td><code>MultiCouplingTerms.to_nn_bond_Arrays(sites)</code></td>
<td>Convert the coupling_terms into Arrays on nearest neighbor bonds.</td>
</tr>
</tbody>
</table>

**class** `tenpy.networks.terms.MultiCouplingTerms(L)`

**Bases:** `tenpy.networks.terms.CouplingTerms`

Operator names, site indices and strengths representing general $M$-site coupling terms.

Generalizes the `coupling_terms` of `CouplingTerms` to $M$-site couplings. The structure of the nested dictionary `coupling_terms` is similar, but we allow an arbitrary recursion depth of the dictionary.

**Parameters**

- **$L$** (`int`) – Number of sites.

  **Type** `int`

  `coupling_terms`

  Nested dictionaries of the following form:

  ```python
  {i: {'opname_i', 'opname_string_ij'};
   j: {'opname_j', 'opname_string_jk'};
   k: {'opname_k', 'opname_string_kl'};
   ...
   l: {'opname_l':
       strength
   }
   ...
  }
  }
  }
  }
  ```

  For a $M$-site coupling, this involves a nesting depth of $2\times M$ dictionaries. Note that always $i < j < k < \ldots < l$, but entries with $j, k, l \geq L$ are allowed for the case of `bc_MPS == 'infinite'`, when they indicate couplings between different iMPS unit cells.

  **Type** `dict of dict`

  `add_multi_coupling_term(strength, ijk, ops_ijkl, op_string='Id')`

  Add a multi-site coupling term.

  **Parameters**

  - **strength** (`float`) – The strength of the coupling term.

  - **ijk** (`list of int`) – The MPS indices of the sites on which the operators acts. With $i, j, k, \ldots = ijk$, we require that they are ordered ascending, $i < j < k < \ldots$ and
that $0 \leq i < N_{\text{sites}}$. Indices $\geq N_{\text{sites}}$ indicate couplings between different unit cells of an infinite MPS.

- **ops_ijkl** (*list of str*) – Names of the involved operators on sites $i, j, k, \ldots$.
- **op_string** (*list of str*) – Names of the operator to be inserted between the operators, e.g., op_string[0] is inserted between $i$ and $j$. A single name holds for all in-between segments.

### multi_coupling_term_handle_JW

Helping function to call before `add_multi_coupling_term()`.

Handle/figure out Jordan-Wigner strings if needed.

**Parameters**

- **strength** (*float*) – The strength of the term.
- **term** (*list of (str, int]*) – List of tuples (op_i, i) where $i$ is the MPS index of the site the operator named op_i acts on. We require the operators to be sorted (strictly ascending) by sites. If necessary, call `order_combine_term()` beforehand.
- **sites** (*list of Site*) – Defines the local Hilbert space for each site. Used to check whether the operators need Jordan-Wigner strings.
- **op_string** (None / str) – Operator name to be used as operator string between the operators, or None if the Jordan Wigner string should be figured out.

**Warning:** None figures out for each segment between the operators, whether a Jordan-Wigner string is needed. This is different from a plain 'JW', which just applies a string on each segment!

**Returns** Arguments for *MultiCouplingTerms.add_multi_coupling_term()* such that the added term corresponds to the parameters of this function.

**Return type** strength, ijkl, ops_ijkl, op_string

### max_range

Determine the maximal range in `coupling_terms`.

**Returns** max_range – The maximum of $j - i$ for the $i, j$ occurring in a term of `coupling_terms`.

**Return type** int

### add_to_graph

Add terms from `coupling_terms` to an MPOGraph.

**Parameters**

- **graph** (*MPOGraph*) – The graph into which the terms from `coupling_terms` should be added.
- **_i** (None) – Should not be given; only needed for recursion.
- **_d1** (None) – Should not be given; only needed for recursion.
- **_label_left** (None) – Should not be given; only needed for recursion.

### remove_zeros

Remove entries close to 0 from `coupling_terms`.

**Parameters**

- **tol_zero** = 1e-15, _d0=0
• **tol_zero** (*float*) – Entries in coupling_terms with strength < tol_zero are con-
sidered to be zero and removed.

• **_d0** (*None*) – Should not be given; only needed for recursion.

to_TermList()  
Convert onsite_terms into a TermList.

Returns term_list – Representation of the terms as a list of terms.

Return type TermList

add_coupling_term(*strength, i, j, op_i, op_j, op_string='Id')*

Add a two-site coupling term on given MPS sites.

Parameters

• **strength** (*float*) – The strength of the coupling term.

• **i** (*int*) – The MPS indices of the two sites on which the operator acts. We require 0 <= i < N_sites and i < j, i.e., op_i acts “left” of op_j. If j >= N_sites, it indicates couplings between unit cells of an infinite MPS.

• **j** (*int*) – The MPS indices of the two sites on which the operator acts. We require 0 <= i < N_sites and i < j, i.e., op_i acts “left” of op_j. If j >= N_sites, it indicates couplings between unit cells of an infinite MPS.

• **op1** (*str*) – Names of the involved operators.

• **op2** (*str*) – Names of the involved operators.

• **op_string** (*str*) – The operator to be inserted between i and j.

coupling_term_handle_JW(*strength, term, sites, op_string=None)*

Helping function to call before add_multi_coupling_term().

Parameters

• **strength** (*float*) – The strength of the coupling term.

• **term** ([(str, int), (str, int)]) – List of two tuples (op, i) where i is the MPS index of the site the operator named op acts on.

• **sites** (list of Site) – Defines the local Hilbert space for each site. Used to check whether the operators need Jordan-Wigner strings.

• **op_string** (*None / str*) – Operator name to be used as operator string between the operators, or None if the Jordan Wigner string should be figured out.

Warning: None figures out for each segment between the operators, whether a Jordan-Wigner string is needed. This is different from a plain 'JW', which just applies a string on each segment!

Returns Arguments for MultiCouplingTerms.add_multi_coupling_term() such that the added term corresponds to the parameters of this function.

Return type strength, i, j, op_i, op_j, op_string

classmethod from_hdf5(*hdf5_loader, h5gr, subpath)*

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with save_hdf5().

Parameters


• **hdf5_loader** (**Hdf5Loader**) – Instance of the loading engine.
• **h5gr** (**Group**) – HDF5 group which is represent the object to be constructed.
• **subpath** (**str**) – The name of h5gr with a '/' in the end.

**Returns** obj – Newly generated class instance containing the required data.

**Return type** cls

```python
plot_coupling_terms(ax, lat, style_map='default', common_style={'linestyle': '--'}, text=None, text_pos=0.4)
```

"Plot coupling terms into a given lattice.

This function plots the coupling terms

**Parameters**

- **ax** (**matplotlib.axes.Axes**) – The axes on which we should plot.
- **lat** (**Lattice**) – The lattice for plotting the couplings, most probably the M.lat of the corresponding model M, see lat.
- **style_map** (**function | None**) – Function which get's called with arguments i, j, op_i, op_string, op_j, strength for each two-site coupling and should return a keyword-dictionary with the desired plot-style for this coupling. By default (None), the linewidth is given by the absolute value of strength, and the linecolor depends on the phase of strength (using the hsv colormap).
- **common_style** (**dict**) – Common style, which overwrites values of the dictionary returned by style_map. A 'label' is only used for the first plotted line.
- **text** (**format_string | None**) – If not None, we add text labeling the couplings in the plot. Available keywords are i, j, op_i, op_string, op_j, strength as well as strength_abs, strength_angle, strength_real.
- **text_pos** (**float**) – Specify where to put the text on the line between i (0.0) and j (1.0), e.g. 0.5 is exactly in the middle between i and j.

See also:

tenpy.models.lattice.Lattice.plot_sites plot the sites of the lattice.

```python
save_hdf5(hdf5_saver, h5gr, subpath)
```

Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5().

This implementation saves the content of __dict__ with save_dict_content(), storing the format under the attribute 'format'.

**Parameters**

- **hdf5_saver** (**Hdf5Saver**) – Instance of the saving engine.
- **h5gr** (**:class:`Group`**) – HDF5 group which is supposed to represent self.
- **subpath** (**str**) – The name of h5gr with a '/' in the end.

```python
to_nn_bond_Arrays(sites)
```

Convert the coupling_terms into Arrays on nearest neighbor bonds.

**Parameters** sites (list of **Site**) – Defines the local Hilbert space for each site. Used to translate the operator names into Array.
Returns **H\_bond** – The *coupling\_terms* rewritten as \( \sum_i H_{\text{bond}[i]} \) for MPS indices \( i \). \( H_{\text{bond}[i]} \) acts on sites \( (i-1, i) \), \text{None} represents 0. Legs of each \( H_{\text{bond}[i]} \) are \[ 'p0', 'p0*', 'p1', 'p1*'. \]

**Return type** list of \{Array | None\}

### OnsiteTerms

- full name: tenpy.networks.terms.OnsiteTerms
- parent module: tenpy.networks.terms
- type: class

#### Inheritance Diagram

```
Hdf5Exportable
   ↓
OnsiteTerms
```

#### Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>OnsiteTerms._init_</strong>(L)</td>
<td>Initialize self.</td>
</tr>
<tr>
<td><strong>OnsiteTerms.add_onsite_term</strong>(strength, i, op)</td>
<td>Add a onsite term on a given MPS site.</td>
</tr>
<tr>
<td><strong>OnsiteTerms.add_to_graph</strong>(graph)</td>
<td>Add terms from ( \text{onsite_terms} ) to an MPOGraph.</td>
</tr>
<tr>
<td><strong>OnsiteTerms.add_to_nn_bond_Arrays</strong>(H_bond)</td>
<td>Add ( \text{self.onsite_terms} ) into nearest-neighbor bond arrays.</td>
</tr>
<tr>
<td><strong>OnsiteTerms.from_hdf5</strong>(hdf5_loader, h5gr, sub_path)</td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><strong>OnsiteTerms.max_range</strong>()</td>
<td>Maximum range of the terms.</td>
</tr>
<tr>
<td><strong>OnsiteTerms.remove_zeros</strong>([tol_zero])</td>
<td>Remove entries close to 0 from ( \text{onsite_terms} ).</td>
</tr>
<tr>
<td><strong>OnsiteTerms.save_hdf5</strong>(hdf5_saver, h5gr, sub_path)</td>
<td>Export ( \text{self} ) into a HDF5 file.</td>
</tr>
<tr>
<td><strong>OnsiteTerms.to_Arrays</strong>(sites)</td>
<td>Convert the ( \text{onsite_terms} ) into a list of np_conserved Arrays.</td>
</tr>
<tr>
<td><strong>OnsiteTerms.to_TermList</strong>()</td>
<td>Convert ( \text{onsite_terms} ) into a TermList.</td>
</tr>
</tbody>
</table>

**class** `tenpy.networks.terms.OnsiteTerms\( L \)`

**Bases**: `tenpy.tools.hdf5_io.Hdf5Exportable`

Operator names, site indices and strengths representing onsite terms.
Represents a sum of onsite terms where the operators are only given by their name (in the form of a string). What the operator represents is later given by a list of `Site` with `get_op()`.

**Parameters**

- `L (int)` – Number of sites.

**L**

Number of sites.

**Type** int

**onsite_terms**

Filled by method `add_onsite_term`. For each index `i` a dictionary `{'opname': strength}` defining the onsite terms.

**Type** list of dict

**max_range()**

Maximum range of the terms. In this case 0.

**add_onsite_term**(strength, i, op)

Add a onsite term on a given MPS site.

**Parameters**

- `strength (float)` – The strength of the term.
- `i (int)` – The MPS index of the site on which the operator acts. We require `0 <= i < L`.
- `op (str)` – Name of the involved operator.

**add_to_graph**(graph)

Add terms from `onsite_terms` to an MPOGraph.

**Parameters**

- `graph (MPOGraph)` – The graph into which the terms from `onsite_terms` should be added.

**to_Arrays**(sites)

Convert the `onsite_terms` into a list of np_conserved Arrays.

**Parameters**

- `sites` (list of `Site`) – Defines the local Hilbert space for each site. Used to translate the operator names into `Array`.

**Returns**

- `onsite_arrays` – Onsite terms represented by `self`. Entry `i` of the list lives on `sites[i]`.

**Return type** list of `Array`

**remove_zeros**(tol_zero=1e-15)

Remove entries close to 0 from `onsite_terms`.

**Parameters**

- `tol_zero (float)` – Entries in `onsite_terms` with `strength < tol_zero` are considered to be zero and removed.

**add_to_nn_bond_Arrays**(H_bond, sites, finite, distribute=(0.5, 0.5))

Add `self.onsite_terms` into nearest-neighbor bond arrays.

**Parameters**

- `H_bond` (list of `{Array | None}`) – The coupling_terms rewritten as `\sum_i H_{bond[i]}` for MPS indices `i`. `H_{bond[i]}` acts on sites `(i-1, i)`. `None` represents 0. Legs of each `H_{bond[i]}` are `['p0', 'p0*', 'p1', 'p1*']`. Modified in place.
• **sites** (list of *Site*) – Defines the local Hilbert space for each site. Used to translate the operator names into *Array*.

• **distribute** (*float, float*) – How to split the onsite terms (in the bulk) into the bond terms to the left (*distribute[0]*) and right (*distribute[1]*)

• **finite** (*bool*) – Boundary conditions of the MPS, *MPS.finite*. If finite, we distribute the onsite term of the

    to_TermList()
    Convert *onsite_terms* into a *TermList*.

    Returns *term_list* – Representation of the terms as a list of terms.

    Return type *TermList*

    **classmethod from_hdf5** (*hdf5_loader, h5gr, subpath*)
    Load instance from a HDF5 file.
    This method reconstructs a class instance from the data saved with *save_hdf5()*.

    Parameters
    • **hdf5_loader** (*Hdf5Loader*) – Instance of the loading engine.
    • **h5gr** (*Group*) – HDF5 group which is represent the object to be constructed.
    • **subpath** (*str*) – The name of *h5gr* with a '/* in the end.

    Returns *obj* – Newly generated class instance containing the required data.

    Return type *cls*

    **save_hdf5** (*hdf5_saver, h5gr, subpath*)
    Export *self* into a HDF5 file.
    This method saves all the data it needs to reconstruct *self* with *from_hdf5()*.
    This implementation saves the content of __dict__ with *save_dict_content()*, storing the format under the attribute 'format'.

    Parameters
    • **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.
    • **h5gr** (*class`Group`) – HDF5 group which is supposed to represent *self*.
    • **subpath** (*str*) – The name of *h5gr* with a '/* in the end.

    **TermList**

    • full name: tenpy.networks.terms.TermList
    • parent module: *tenpy.networks.terms*
    • type: class
Inheritance Diagram

```
  Hdf5Exportable
   ↓
  TermList
```

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>TermList.__init__(terms[, strength])</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>TermList.from_hdf5(hdf5_loader, h5gr, subpath)</code></td>
<td>Load instance from a HDF5 file.</td>
</tr>
<tr>
<td><code>TermList.from_lattice_locations(lattice, terms)</code></td>
<td>Initialize from a list of terms given in lattice indices instead of MPS indices.</td>
</tr>
<tr>
<td><code>TermList.order_combine(sites)</code></td>
<td>Order and combine operators in each term.</td>
</tr>
<tr>
<td><code>TermList.save_hdf5(hdf5_saver, h5gr, subpath)</code></td>
<td>Export self into a HDF5 file.</td>
</tr>
<tr>
<td><code>TermList.to_OnsiteTerms_CouplingTerms(sites)</code></td>
<td>Convert to OnsiteTerms and CouplingTerms</td>
</tr>
</tbody>
</table>

```
class tenpy.networks/terms.TermList (terms, strength=1.0)  
Bases: tenpy.tools.hdf5_io.Hdf5Exportable
```

A list of terms (=operator names and sites they act on) and associated strengths. A representation of terms, similar as `OnsiteTerms`, `CouplingTerms` and `MultiCouplingTerms`. This class does not store operator strings between the sites. Jordan-Wigner strings of fermions are added during conversion to (Multi)CouplingTerms.

**Warning:** Since this class does **not** store the operator string between the sites, conversion from `CouplingTerms` or `MultiCouplingTerms` to `TermList` is lossy!

**Parameters**

- **terms** *(list of list of (str, int))* – List of terms where each term is a list of tuples (opname, i) of an operator name and a site i it acts on. For Fermions, the order is the order in the mathematic sense, i.e., the right-most/last operator in the list acts last.
- **strengths** *(list of float/complex)* – For each term in terms an associated prefactor or strength. A single number holds for all terms equally.

**terms**

List of terms where each term is a tuple (opname, i) of an operator name and a site i it acts on.

**Type** list of list of (str, int)
**strengths**

For each term in *terms* an associated prefactor or strength.

*Type* 1D ndarray

**Examples**

For fermions, the term \(0.5(c_0^\dagger c_2 + h.c.) + 1.3 \ast n_1\) can be represented by:

```python
>>> t = TermList([(('Cd', 0), ('C', 2)), [('Cd', 2), ('C', 0)], [('N', 1)]),
... [0.5, 0.5, 1.3])
```

```python
>>> print(t)
0.50000 * Cd_0 C_2 +
0.50000 * Cd_2 C_0 +
1.30000 * N_1
```

If you have a *Lattice*, you might also want to specify the location of the operators by lattice indices instead of MPS indices. For example, you can obtain the nearest-neighbor density terms **without double counting each pair** on a *TriangularLattice*:

```python
>>> lat = tenpy.models.lattice.Triangular(6, 6, None, bc_MPS='infinite', bc=˓
... 'periodic')
>>> t2_terms = [(('N', [0, 0, u1]), ('N', [dx[0], dx[1], u2]))
... for (u1, u2, dx) in lat.pairs['nearest_neighbors']]
>>> t2 = TermList.from_lattice_locations(lat, t2_terms)
>>> print(t2)
1.00000 * N_0 N_6 +
1.00000 * N_0 N_-5 +
1.00000 * N_0 N_5
```

The negative index -5 here indicates a tensor left of the current MPS unit cell.

**classmethod from_lattice_locations** (*lattice, terms, strength=1.0, shift=None*)

Initialize from a list of terms given in lattice indices instead of MPS indices.

**Parameters**

- **lattice** (*Lattice*) – The underlying lattice to be used for conversion, e.g. `M.lat` from a *Model*.
- **terms** ([list of list of (str, tuple)]) – List of terms, where each term is a tuple `(opname, lat_idx)` with `lat_idx` itself being a tuple `(x, y, u)` (for a 2D lattice) of the lattice coordinates.
- **strengths** ([list of float/complex]) – For each term in *terms* an associated prefactor or strength. A single number holds for all terms equally.
- **shift** (`None` / tuple of int) – Overall shift added to all lattice coordinates `lat_idx` in *terms* before conversion. None defaults to no shift.

**Returns** *term_list* – Representation of the terms.

**Return type** *TermList*

**to_OnsiteTerms_CouplingTerms** (*sites*)

Convert to *OnsiteTerms* and *CouplingTerms*

Performs Jordan-Wigner transformation for fermionic operators.
**Parameters**

- **sites** (list of *Site*) – Defines the local Hilbert space for each site. Used to check whether the operators need Jordan-Wigner strings. The length is used as $L$ for the *onsite_terms* and *coupling_terms*.

**Returns**

- **onsite_terms** (*OnsiteTerms*) – Onsite terms.
- **coupling_terms** (*CouplingTerms | MultiCouplingTerms*) – Coupling terms. If *self* contains terms involving more than two operators, a *MultiCouplingTerms* instance, otherwise just *CouplingTerms*.

**order_combine**(*sites*)

Order and combine operators in each term.

- **sites** (list of *Site*) – Defines the local Hilbert space for each site. Used to check whether the operators anticommute (= whether they need Jordan-Wigner strings) and for multiplication rules.

See also:

- **order_and_combine_term** does it for a single term.

**classmethod from_hdf5** (*hdf5_loader*, *h5gr*, *subpath*)

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with *save_hdf5()*.  

**Parameters**

- **hdf5_loader** (*Hdf5Loader*) – Instance of the loading engine.
- **h5gr** (*Group*) – HDF5 group which is represent the object to be constructed.
- **subpath** (*str*) – The name of *h5gr* with a ‘/’ in the end.

**Returns** *obj* – Newly generated class instance containing the required data.

**Return type** cls

**save_hdf5** (*hdf5_saver*, *h5gr*, *subpath*)

Export *self* into a HDF5 file.

This method saves all the data it needs to reconstruct *self* with *from_hdf5()*.  

This implementation saves the content of *__dict__* with *save_dict_content()*, storing the format under the attribute 'format'.

**Parameters**

- **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.
- **h5gr** (*class `Group`*) – HDF5 group which is supposed to represent *self*.
- **subpath** (*str*) – The name of *h5gr* with a ‘/’ in the end.
Functions

order_combine_term (term, sites) Combine operators in a term to one terms per site.

order_combine_term

- full name: tenpy.networks.terms.order_combine_term
- parent module: tenpy.networks.terms
- type: function


tenpy.networks.terms.order_combine_term (term, sites)

Combine operators in a term to one terms per site.

Takes in a term of operators and sites they acts on, commutes operators to order them by site and combines operators acting on the same site with multiply_op_names().

Parameters

- term (a list of (opname_i, i) tuples) – Represents a product of onsite operators with site indices i they act on. Needs not to be ordered and can have multiple entries acting on the same site.
- sites (list of Site) – Defines the local Hilbert space for each site. Used to check whether the operators anticommute (= whether they need Jordan-Wigner strings) and for multiplication rules.

Returns

- combined_term – Equivalent to term but with at most one operator per site.
- overall_sign (+1 | -1 | 0) – Comes from the (anti-)commutation relations. When the operators in term are multiplied from left to right, and then multiplied by overall_sign, the result is the same operator as the product of combined_term from left to right.

Module description

Classes to store a collection of operator names and sites they act on, together with prefactors.

This modules collects classes which are not strictly speaking tensor networks but represent “terms” acting on them. Each term is given by a collection of (onsite) operator names and indices of the sites it acts on. Moreover, we associate a strength to each term, which corresponds to the prefactor when specifying e.g. a Hamiltonian.

7.12.5 purification_mps

- full name: tenpy.networks.purification_mps
- parent module: tenpy.networks
- type: module
Classes

MPS

PurificationMPS

PurificationMPS(sites, Bs, SVs[, bc, form, norm]) An MPS representing a finite-temperature ensemble using purification.

Module description

This module contains an MPS class representing an density matrix by purification.

Usually, an MPS represents a pure state, i.e. the density matrix is $\rho = |\psi > < \psi|$, describing observables as $< O > = Tr(O|\psi > < \psi|) = < \psi|O|\psi >$. Clearly, if $|\psi >$ is the ground state of a Hamiltonian, this is the density matrix at $T=0$.

At finite temperatures $T > 0$, we want to describe a non-pure density matrix $\rho = \exp(-H/T)$. This can be achieved by the so-called purification: in addition to the physical space $P$, we introduce a second ‘auxiliar’ space $Q$ and define the density matrix of the physical system as $\rho = Tr_Q(|\phi > < \phi|)$, where $|\phi >$ is a pure state in the combined physical and auxiliar system.

For $T = \infty$, the density matrix $\rho_\infty$ is the identity matrix. In other words, expectation values are sums over all possible states $< O > = Tr_P(\rho_\infty O) = Tr_P(O)$. Saying that each : on top is to be connected with the corresponding : on the bottom, the trace is simply a contraction:

Clearly, we get the same result, if we insert an identity operator, written as MPO, on the top and bottom:

(continues on next page)
We use the following label convention:

```
   q
  ^
 vL --> B --> vR
  |
  |
  p
```

You can view the MPO as an MPS by combining the $p$ and $q$ leg and defining every physical operator to act trivial on the $q$ leg. In expectation values, you would then sum over over the $q$ legs, which is exactly what we need. In other words, the choice $B = \delta_{p,q}$ with trivial (length-1) virtual bonds yields infinite temperature expectation values for operators action only on the $p$ legs!

Now, you go a step further and also apply imaginary time evolution (acting only on $p$ legs) to the initial infinite temperature state. For example, the normalized state $|\psi > \propto \exp(-\beta/2H)|\phi >$ yields expectation values

$$< O > = Tr(\exp(-\beta H)O)/Tr(\exp(-\beta H)) \propto < \phi | \exp(-\beta/2H)O \exp(-\beta/2H) |\phi > .$$

An additional real-time evolution allows to calculate time correlation functions:

$$< A(t)B(0)|\phi > \propto < \phi | \exp(-\beta H/2) \exp(+iHt)A \exp(-iHt)B \exp(-\beta H/2) |\phi >$$

Time evolution algorithms (TEBD and MPO application) are adjusted in the module `purification`.

See also [karrasch2013] for additional tricks! On of their crucial observations is, that one can apply arbitrary unitaries on the auxiliar space (i.e. the $q$) without changing the result. This can actually be used to reduce the necessary virtual bond dimensions: From the definition, it is easy to see that if we apply $\exp(-iHt)$ to the $p$ legs of $|\phi >$, and $\exp(+iHt)$ to the $q$ legs, they just cancel out! (They commute with $\exp(-\beta H/2)$...) If the state is modified (e.g. by applying $A$ or $B$ to calculate correlation functions), this is not true any more. However, we still can find unitaries, which are ‘optimal’ in the sense of reducing the entanglement of the MPS/MPO to the minimal value. For a discussion of Disentanglers (implemented in `disentanglers`), see [hauschild2018].

**Note:** The classes MPSEnvironment and TransferMatrix should also work for the PurificationMPS defined here. For example, you can use `expectation_value()` for the expectation value of operators between different PurificationMPS. However, this makes only sense if the same disentangler was applied to the `bra` and `ket` PurificationMPS.

**Note:** The literature (e.g. section 7.2 of [schollwoeck2011] or [karrasch2013]) suggests to use a singlet as a maximally entangled state. Here, we use instead the identity $\delta_{p,q}$, since it is easier to generalize for $p$ running over more than two indices, and allows a simple use of charge conservation with the above `qconj` convention. Moreover, we don’t split the physical and auxiliar space into separate sites, which makes TEBD as costly as $O(d^6\chi^3)$.

**Todo:** One can also look at the canonical ensembles by defining the conserved quantities differently, see [barthel2016] for details. Idea: usual charges on $p$, trivial charges on $q$; fix total charge to desired value. I think it should suffice to implement another `from_infiniteT`.
7.13 tools

- full name: tenpy.tools
- parent module: tenpy
- type: module

Module description

A collection of tools: mostly short yet quite useful functions.

Some functions are explicitly imported in other parts of the library, others might just be useful when using the library. Common to all tools is that they are not just useful for a single algorithm but fairly general.

Submodules

<table>
<thead>
<tr>
<th>Submodule</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>hdf5_io</td>
<td>Tools to save and load data (from TeNPy) to disk.</td>
</tr>
<tr>
<td>params</td>
<td>Tools to handle config options/parameters for algorithms.</td>
</tr>
<tr>
<td>events</td>
<td>Event handler.</td>
</tr>
<tr>
<td>misc</td>
<td>Miscellaneous tools, somewhat random mix yet often helpful.</td>
</tr>
<tr>
<td>math</td>
<td>Different math functions needed at some point in the library.</td>
</tr>
<tr>
<td>fit</td>
<td>Tools to fit to an algebraic decay.</td>
</tr>
<tr>
<td>string</td>
<td>Tools for handling strings.</td>
</tr>
<tr>
<td>process</td>
<td>Tools to read out total memory usage and get/set the number of threads.</td>
</tr>
<tr>
<td>optimization</td>
<td>Optimization options for this library.</td>
</tr>
</tbody>
</table>

7.13.1 hdf5_io

- full name: tenpy.tools.hdf5_io
- parent module: tenpy.tools
- type: module

Classes

```
Hdf5FormatError  Hdf5Exportable  Hdf5Ignored  Hdf5Loader  Hdf5Saver
Hdf5ExportError  Hdf5ImportError
```
Hdf5Exportable

- full name: tenpy.tools.hdf5_io.Hdf5Exportable
- parent module: tenpy.tools.hdf5_io
- type: class

Inheritance Diagram

Hdf5Exportable

Methods

Hdf5Exportable.__init__() Initialize self.
Hdf5Exportable.from_hdf5(hdf5_loader, h5gr, ...)
Load instance from a HDF5 file.
Hdf5Exportable.save_hdf5(hdf5_saver, h5gr, ...
Export self into a HDF5 file.

class tenpy.tools.hdf5_io.Hdf5Exportable

Bases: object

Interface specification for a class to be exportable to our HDF5 format.

To allow a class to be exported to HDF5 with save_to_hdf5(), it only needs to implement the save_hdf5() method as documented below. To allow import, a class should implement the classmethod from_hdf5(). During the import, the class already needs to be defined; loading can only initialize instances, not define classes.

The implementation given works for sufficiently simple (sub-)classes, for which all data is stored in __dict__. In particular, this works for python-defined classes which simply store data using self.data = data in their methods.

save_hdf5(hdf5_saver, h5gr, subpath)
Export self into a HDF5 file.

This method saves all the data it needs to reconstruct self with from_hdf5().
This implementation saves the content of \_dict\_ with \_save_dict_content\_(), storing the format under the attribute 'format'.

**Parameters**

- \texttt{hdf5\_saver (Hdf5Saver)} – Instance of the saving engine.
- \texttt{h5gr (:class:`Group`) – HDF5 group which is supposed to represent self.}
- \texttt{subpath (str) – The name of h5gr with a '/ ' in the end.}

**classmethod from\_hdf5 (hdf5\_loader, h5gr, subpath)**

Load instance from a HDF5 file.

This method reconstructs a class instance from the data saved with \_save\_hdf5\_().

**Parameters**

- \texttt{hdf5\_loader (Hdf5Loader)} – Instance of the loading engine.
- \texttt{h5gr (Group) – HDF5 group which is represent the object to be constructed.}
- \texttt{subpath (str) – The name of h5gr with a '/ ' in the end.}

**Returns** \texttt{obj} – Newly generated class instance containing the required data.

**Return type** \texttt{cls}

---

**Hdf5Ignored**

- full name: tenpy.tools.hdf5\_io.Hdf5Ignored
- parent module: \texttt{tenpy.tools.hdf5\_io}
- type: class

**Inheritance Diagram**

![Inheritance Diagram](image)

**Methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hdf5Ignored.<strong>init</strong>([name])</td>
<td>Initialize self.</td>
</tr>
</tbody>
</table>

**class tenpy.tools.hdf5\_io.Hdf5Ignored (name='unknown')**

**Bases:** \texttt{object}

Placeholder for a dataset/group to be ignored during both loading and saving.

Objects of this type are not saved. Moreover, if a saved dataset/group has the type attribute matching \texttt{REPR\_IGNORED}, instance of this class are returned instead of loading the data.
Parameters name (str) – The name of the dataset during loading; just for reference.

name
See above.

Type str

Hdf5Loader

- full name: tenpy.tools.hdf5_io.Hdf5Loader
- parent module: tenpy.tools.hdf5_io
- type: class

Inheritance Diagram

![Hdf5Loader]

Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hdf5Loader.<strong>init</strong>(h5group[, ignore_unknown])</td>
<td>Initialize self.</td>
</tr>
<tr>
<td>Hdf5Loader.find_global(module, classname)</td>
<td>Get the class of the qualified classname in a given python module.</td>
</tr>
<tr>
<td>Hdf5Loader.get_attr(h5gr, attr_name)</td>
<td>Return attribute h5gr.attrs[attr_name], if existent.</td>
</tr>
<tr>
<td>Hdf5Loader.load([path])</td>
<td>Load a Python object from the dataset.</td>
</tr>
<tr>
<td>Hdf5Loader.load_dataset(h5gr, type_info, subpath)</td>
<td>Load a h5py Dataset and convert it into the desired type.</td>
</tr>
<tr>
<td>Hdf5Loader.load_dict(h5gr, type_info, subpath)</td>
<td>Load a dictionary in the format according to type_info.</td>
</tr>
<tr>
<td>Hdf5Loader.load_dtype(h5gr, type_info, subpath)</td>
<td>Load a numpy.dtype.</td>
</tr>
<tr>
<td>Hdf5Loader.load_general_dict(h5gr, ...)</td>
<td>Load a dictionary with general keys.</td>
</tr>
<tr>
<td>Hdf5Loader.load_global(h5gr, type_info, subpath)</td>
<td>Load a global object like a class or function from its qualified name and module.</td>
</tr>
<tr>
<td>Hdf5Loader.load_hdf5exportable(h5gr, ...)</td>
<td>Load an instance of a userdefined class.</td>
</tr>
<tr>
<td>Hdf5Loader.load_ignored(h5gr, type_info, subpath)</td>
<td>Ignore the group to be loaded.</td>
</tr>
<tr>
<td>Hdf5Loader.load_list(h5gr, type_info, subpath)</td>
<td>Load a list.</td>
</tr>
<tr>
<td>Hdf5Loader.load_none(h5gr, type_info, subpath)</td>
<td>Load the None object from a dataset.</td>
</tr>
</tbody>
</table>

continues on next page
**Table 161 – continued from previous page**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hdf5Loader.load_range(h5gr, type_info, subpath)</td>
<td>Load a range.</td>
</tr>
<tr>
<td>Hdf5Loader.load_reduce(h5gr, type_info, subpath)</td>
<td>Load an object where the return values of obj.<strong>reduce</strong> has been exported.</td>
</tr>
<tr>
<td>Hdf5Loader.load_set(h5gr, type_info, subpath)</td>
<td>Load a set.</td>
</tr>
<tr>
<td>Hdf5Loader.load_simple_dict(h5gr, type_info, ...)</td>
<td>Load a dictionary with simple keys.</td>
</tr>
<tr>
<td>Hdf5Loader.load_str(h5gr, type_info, subpath)</td>
<td>Load a string from a h5py Dataset.</td>
</tr>
<tr>
<td>Hdf5Loader.load_tuple(h5gr, type_info, subpath)</td>
<td>Load a tuple.</td>
</tr>
<tr>
<td>Hdf5Loader.memorize_load(h5gr, obj)</td>
<td>Store objects already loaded in the memo_load.</td>
</tr>
</tbody>
</table>

**Class Attributes and Properties**

**Hdf5Loader.dispatch_load**

class tenpy.tools.hdf5_io.Hdf5Loader(h5group, ignore_unknown=True)

- **Bases**: object

Class to load and import object from a HDF5 file.

The intended use of this class is through `load_from_hdf5()`, which is simply an alias for `Hdf5Loader(h5group).load(path)`.

It can load data exported with `save_to_hdf5()` or the `Hdf5Saver`, respectively.

The basic structure of this class is similar as the `Unpickler` from `pickle`.

See *Saving to disk: input/output* for a specification of what can be saved and what the resulting datastructure is.

**Parameters**

- **h5group** (Group) – The HDF5 group (or file) where to save the data.

- **ignore_unknown** (bool) – Whether to just warn (True) or raise an Error (False) if a class to be loaded is not found.

**h5group**

The HDF5 group (or HDF5 File) where to save the data.

**Type** Group

**ignore_unknown**

Whether to just warn (True) or raise an Error (False) if a class to be loaded is not found.

**Type** bool

**dispatch_load**

Mapping from one of the global `REPR_*` variables to (unbound) methods `f` of this class. The method is called as `f(self, h5gr, type_info, subpath)`. The call to `f` should load and return an object `obj` from the h5py Group or Dataset `h5gr`; and memorize the loaded `obj` with `memorize_load()`.

`subpath` is just the name of `h5gr` with a guaranteed `'/'` in the end. `type_info` is often the `REPR_*` variable of the type or some other information about the type, which allows to use a single `dispatch_load` function for different datatypes.

**Type** dict
memo_load
A dictionary to remember all the objects which we already loaded from h5group. The dictionary key is a h5py group- or dataset id; the value is the loaded object. See memorize_load().

Type  dict
load (path=None)
Load a Python object from the dataset.
See load_from_hdf5() for more details.

Parameters  path (None | str | Reference) – Path within h5group to be used for loading.
Defaults to the name of h5group itself.

Returns  obj – The Python object loaded from h5group (specified by path).

Return type  object
memorize_load (h5gr, obj)
Store objects already loaded in the memo_load.
This allows to avoid copies, if the same dataset appears multiple times in the hdf5 group of obj. Examples can be shared LegCharge objects or even shared Array.

To handle cyclic references correctly, this function should be called before loading data from subgroups with new calls of load().

static get_attr (h5gr, attr_name)
Return attribute h5gr.attrs[attr_name], if existent.

Raises  Hdf5ImportError – If the attribute does not exist.
static find_global (module, classname)
Get the class of the qualified classname in a given python module.

Imports the module.
load_none (h5gr, type_info, subpath)
Load the None object from a dataset.
load_dataset (h5gr, type_info, subpath)
Load a h5py Dataset and convert it into the desired type.
load_str (h5gr, type_info, subpath)
Load a string from a h5py Dataset.
load_list (h5gr, type_info, subpath)
Load a list.
load_set (h5gr, type_info, subpath)
Load a set.
load_tuple (h5gr, type_info, subpath)
Load a tuple.
load_dict (h5gr, type_info, subpath)
Load a dictionary in the format according to type_info.
load_general_dict (h5gr, type_info, subpath)
Load a dictionary with general keys.
load_simple_dict (h5gr, type_info, subpath)
Load a dictionary with simple keys.
load_range (h5gr, type_info, subpath)
Load a range.

load_dtype (h5gr, type_info, subpath)
Load a numpy.dtype.

load_hdf5exportable (h5gr, type_info, subpath)
Load an instance of a userdefined class.

load_ignored (h5gr, type_info, subpath)
Ignore the group to be loaded.

load_global (h5gr, type_info, subpath)
Load a global object like a class or function from its qualified name and module.

load_reduce (h5gr, type_info, subpath)
Load an object where the return values of obj.__reduce__ has been exported.

Hdf5Saver

- full name: tenpy.tools.hdf5_io.Hdf5Saver
- parent module: tenpy.tools.hdf5_io
- type: class

Inheritance Diagram

Methods

Hdf5Saver.__init__ (h5group[, format_selection])
Initialize self.

Hdf5Saver.create_group_for_obj (path, obj)
Create an HDF5 group self.h5group[path] to store obj.

Hdf5Saver.memorize_save (h5gr, obj)
Store objects already saved in the memo_save.

Hdf5Saver.save (obj[, path])
Save obj in self.h5group[path].

Hdf5Saver.save_dataset (obj, path, type_repr)
Save obj as a hdf5 dataset; in dispatch table.

Hdf5Saver.save_dict (obj, path, type_repr)
Save the dictionary obj; in dispatch table.

Hdf5Saver.save_dict_content (obj, h5gr, subpath)
Save contents of a dictionary obj in the existing h5gr.

Hdf5Saver.save_dtype (obj, path, type_repr)
Save a dtype object; in dispatch table.

Hdf5Saver.save_global (obj, path, type_repr)
Save a global object like a function or class.

Hdf5Saver.save_ignored (obj, path, type_repr)
Don’t save the Hdf5Ignored object; just return None.

continues on next page
### Table 163 – continued from previous page

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>Hdf5Saver.save_iterable(obj, path, type_repr)</code></td>
<td>Save an iterable <code>obj</code> like a list, tuple or set; in dispatch table.</td>
</tr>
<tr>
<td><code>Hdf5Saver.save_iterable_content(obj, h5gr, ...)</code></td>
<td>Save contents of an iterable <code>obj</code> in the existing <code>h5gr</code>.</td>
</tr>
<tr>
<td><code>Hdf5Saver.save_none(obj, path, type_repr)</code></td>
<td>Save the None object as a string (dataset); in dispatch table.</td>
</tr>
<tr>
<td><code>Hdf5Saver.save_range(obj, path, type_repr)</code></td>
<td>Save a range object; in dispatch table.</td>
</tr>
<tr>
<td><code>Hdf5Saver.save_reduce(func, args[, state, ...])</code></td>
<td>Save the return values of <code>obj.__reduce__</code> following the pickle protocol.</td>
</tr>
</tbody>
</table>

### Class Attributes and Properties

#### `Hdf5Saver.dispatch_save`

**class** `tenpy.tools.hdf5_io.Hdf5Saver(h5group, format_selection=None)`

**Bases:** `object`

Class to save simple enough objects into a HDF5 file.

The intended use of this class is through `save_to_hdf5()`, which is simply an alias for `Hdf5Saver(h5group).save(obj, path)`.

It exports python objects to a HDF5 file such that they can be loaded with the `Hdf5Loader`, or a call to `load_from_hdf5()`, respectively.

The basic structure of this class is similar as the `Pickler` from `pickle`.

See *Saving to disk: input/output* for a specification of what can be saved and what the resulting datastructure is.

**Parameters**

- **h5group** *(Group)* – The HDF5 group (or HDF5 `File`) where to save the data.

- **format_selection** *(dict)* – This dictionary allows to set a output format selection for user-defined `Hdf5Exportable.save_hdf5()` implementations. For example, `LegCharge` checks it for the key "LegCharge".

**h5group**

The HDF5 group (or HDF5 `File`) where to save the data.

**Type** `Group`

**dispatch_save**

Mapping from a type `keytype` to methods `f` of this class. The method is called as `f(self, obj, path, type_repr)`. The call to `f` should save the object `obj` in `self.h5group[path]`, call `memorize_save()`, and set `h5gr.attr[ATTR_TYPE] = type_repr` to a string `type_repr` in order to allow loading with the dispatcher in `Hdf5Loader.dispatch_save[type_repr]`.

**Type** `dict`

**memo_save**

A dictionary to remember all the objects which we already stored to `h5group`. The dictionary key is the object id; the value is a two-tuple of the hdf5 group or dataset where an object was stored, and the object itself. See `memorize_save()`.

**Type** `dict`
format_selection
This dictionary allows to set a output format selection for user-defined Hdf5Exportable. save_hdf5() implementations. For example, LegCharge checks it for the key "LegCharge".

Type  dict

save (obj, path='/')
Save obj in self.h5group[path].

Parameters
•  obj (object) – The object (=data) to be saved.
•  path (str) – Path within h5group under which the obj should be saved. To avoid unwanted overwriting of important data, the group/object should not yet exist, except if path is the default '/'.

Returns  h5gr – The h5py group or dataset in which obj was saved.

Return type  Group | Dataset

create_group_for_obj (path, obj)
Create an HDF5 group self.h5group[path] to store obj. Also handle ending of path with '/', and memorize obj in memo_save.

Parameters
•  path (str) – Path within h5group under which the obj should be saved. To avoid unwanted overwriting of important data, the group/object should not yet exist, except if path is the default '/'.
•  obj (object) – The object (=data) to be saved.

Returns
•  h5group (Group) – Newly created h5py (sub)group self.h5group[path], unless path is '/', in which case it is simply the existing self.h5group['/'].
•  subpath (str) – The group.name ending with '/', such that other names can be appended to get the path for subgroups or datasets in the group.

:raises ValueError : if self.h5group[path] already existed and path is not '/'.:

memorize_save (h5gr, obj)
Store objects already saved in the memo_save.

This allows to avoid copies, if the same python object appears multiple times in the data of obj. Examples can be shared LegCharge objects or even shared Array. Using the memo also avoids crashes from cyclic references, e.g., when a list contains a reference to itself.

Parameters
•  h5gr (Group | Dataset) – The h5py group or dataset in which obj was saved.
•  obj (object) – The object saved.

save_reduce (func, args, state=None, listitems=None, dictitems=None, state_setter=None, obj=None, path=None)
Save the return values of obj.__reduce__ following the pickle protocol.

save_none (obj, path, type_repr)
Save the None object as a string (dataset); in dispatch table.

save_dataset (obj, path, type_repr)
Save obj as a hdf5 dataset; in dispatch table.
save_iterable(obj, path, type_repr)
    Save an iterable obj like a list, tuple or set; in dispatch table.

save_iterable_content(obj, h5gr, subpath)
    Save contents of an iterable obj in the existing h5gr.

Parameters
    - obj(dict) – The data to be saved
    - h5gr(Group) – h5py Group under which the keys and values of obj should be saved.
    - subpath(str) – Name of h5gr with '/' in the end.

save_dict(obj, path, type_repr)
    Save the dictionary obj; in dispatch table.

save_dict_content(obj, h5gr, subpath)
    Save contents of a dictionary obj in the existing h5gr.

The format depends on whether the dictionary obj has simple keys valid for hdf5 path components (see valid_hdf5_path_component()) or not. For simple keys: directly use the keys as path. For non-simple keys: save list of keys und 'keys' and list of values und 'values'.

Parameters
    - obj(dict) – The data to be saved
    - h5gr(Group) – h5py Group under which the keys and values of obj should be saved.
    - subpath(str) – Name of h5gr with '/' in the end.

Returns type_repr – Indicates whether the data was saved in the format for a dictionary with simple keys or general keys, see comment above.

Return type REPR_DICT_SIMPLE | REPR_DICT_GENERAL

save_range(obj, path, type_repr)
    Save a range object; in dispatch table.

save_dtype(obj, path, type_repr)
    Save a dtype object; in dispatch table.

save_ignored(obj, path, type_repr)
    Don’t save the Hdf5Ignored object; just return None.

save_global(obj, path, type_repr)
    Save a global object like a function or class.

Exceptions

<table>
<thead>
<tr>
<th>Exception</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hdf5ExportError</td>
<td>This exception is raised when something went wrong during export to hdf5.</td>
</tr>
<tr>
<td>Hdf5FormatError</td>
<td>Common base class for errors regarding our HDF5 format.</td>
</tr>
<tr>
<td>Hdf5ImportError</td>
<td>This exception is raised when something went wrong during import from hdf5.</td>
</tr>
</tbody>
</table>
Hdf5ExportError

- full name: tenpy.tools.hdf5_io.Hdf5ExportError
- parent module: tenpy.tools.hdf5_io
- type: exception

```python
def tenpy.tools.hdf5_io.Hdf5ExportError
    This exception is raised when something went wrong during export to hdf5.
```

Hdf5FormatError

- full name: tenpy.tools.hdf5_io.Hdf5FormatError
- parent module: tenpy.tools.hdf5_io
- type: exception

```python
def tenpy.tools.hdf5_io.Hdf5FormatError
    Common base class for errors regarding our HDF5 format.
```

Hdf5ImportError

- full name: tenpy.tools.hdf5_io.Hdf5ImportError
- parent module: tenpy.tools.hdf5_io
- type: exception

```python
def tenpy.tools.hdf5_io.Hdf5ImportError
    This exception is raised when something went wrong during import from hdf5.
```

Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>load(filename)</code></td>
<td>Load data from file with given filename.</td>
</tr>
<tr>
<td><code>load_from_hdf5(h5group[, path, ignore_unknown])</code></td>
<td>Load an object from hdf5 file or group.</td>
</tr>
<tr>
<td><code>save(data, filename[, mode])</code></td>
<td>Save data to file with given filename.</td>
</tr>
<tr>
<td><code>save_to_hdf5(h5group, obj[, path])</code></td>
<td>Save an object obj into a hdf5 file or group.</td>
</tr>
<tr>
<td><code>valid_hdf5_path_component(name)</code></td>
<td>Determine if name is a valid HDF5 path component.</td>
</tr>
</tbody>
</table>

load

- full name: tenpy.tools.hdf5_io.load
- parent module: tenpy.tools.hdf5_io
- type: function

```python
def tenpy.tools.hdf5_io.load(filename)
    Load data from file with given filename.
```

Guess the type of the file from the filename ending, see `save()` for possible endings.

Parameters:

- `filename (str)` – The name of the file to load.
load_from_hdf5

- **Full name:** tenpy.tools.hdf5_io.load_from_hdf5
- **Parent module:** tenpy.tools.hdf5_io
- **Type:** function

```python
tenpy.tools.hdf5_io.load_from_hdf5(h5group, path=None, ignore_unknown=True)
```

Load an object from hdf5 file or group.

Roughly equivalent to `obj = h5group[path][...]`, but handle more complicated objects saved as hdf5 groups and/or datasets with `save_to_hdf5()`. For example, dictionaries are handled recursively. See *Saving to disk: input/output* for a specification of what can be saved/loaded and what the corresponding datastructure is.

**Parameters**

- **h5group** (Group) – The HDF5 group (or h5py File) to be loaded.
- **path** (None | str | Reference) – Path within h5group to be used for loading. Defaults to the h5group itself specified.
- **ignore_unknown** (bool) – Whether to just warn (True) or raise an Error (False) if a class to be loaded is not found.

**Returns** `obj` – The Python object loaded from h5group (specified by path).

**Return type** `object`

save

- **Full name:** tenpy.tools.hdf5_io.save
- **Parent module:** tenpy.tools.hdf5_io
- **Type:** function

```python
tenpy.tools.hdf5_io.save(data, filename, mode='w')
```

Save data to file with given filename.

This function guesses the type of the file from the filename ending. Supported endings:

<table>
<thead>
<tr>
<th>ending</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>.pkl</td>
<td>Pickle without compression</td>
</tr>
<tr>
<td>.pklz</td>
<td>Pickle with gzip compression.</td>
</tr>
<tr>
<td>.hdf5, .h5</td>
<td>HDF5 file (using h5py).</td>
</tr>
</tbody>
</table>

**Parameters**

- **filename** (str) – The name of the file where to save the data.
- **mode** (str) – File mode for opening the file. 'w' for write (discard existing file), 'a' for append (add data to existing file). See `open()` for more details.
save_to_hdf5

- full name: tenpy.tools.hdf5_io.save_to_hdf5
- parent module: tenpy.tools.hdf5_io
- type: function

```python
tenpy.tools.hdf5_io.save_to_hdf5(h5group, obj, path='')
```

Save an object `obj` into a hdf5 file or group.

Roughly equivalent to `h5group[path] = obj`, but handle different types of `obj`. For example, dictionaries are handled recursively. See Saving to disk: input/output for a specification of what can be saved and what the resulting datastructure is.

**Parameters**

- **h5group** (`Group`) – The HDF5 group (or h5py `File`) to which `obj` should be saved.
- **obj** (`object`) – The object (=data) to be saved.
- **path** (`str`) – Path within `h5group` under which the `obj` should be saved. To avoid unwanted overwriting of important data, the group/object should not yet exist, except if `path` is the default '/'.

**Returns**

- **h5obj** – The h5py group or dataset under which `obj` was saved.

**Return type** `Group`|`Dataset`

valid_hdf5_path_component

- full name: tenpy.tools.hdf5_io.valid_hdf5_path_component
- parent module: tenpy.tools.hdf5_io
- type: function

```python
tenpy.tools.hdf5_io.valid_hdf5_path_component(name)
```

Determine if `name` is a valid HDF5 path component.

**Conditions**

- String, no '/', and overall `name` != '. '.

Module description

Tools to save and load data (from TeNPy) to disk.

**Note:** This module is maintained in the repository [https://github.com/tenpy/hdf5_io.git](https://github.com/tenpy/hdf5_io.git)

See Saving to disk: input/output for a motivation and specification of the HDF5 format implemented below. .. online at [https://tenpy.readthedocs.io/en/latest/intro/input_output.html](https://tenpy.readthedocs.io/en/latest/intro/input_output.html)

The functions `save()` and `load()` are convenience functions for saving and loading quite general python objects (like dictionaries) to/from files, guessing the file type (and hence protocol for reading/writing) from the file ending.

On top of that, this function provides support for saving python objects to [HDF5] files with the `Hdf5Saver` and `Hdf5Loader` classes and the wrapper functions `save_to_hdf5()`, `load_from_hdf5()`.
Note: To use the export/import features to HDF5, you need to install the h5py python package (and hence some version of the HDF5 library).

Warning: Like loading a pickle file, loading data from a manipulated HDF5 file with the functions provided below has the potential to cause arbitrary code execution. Only load data from trusted sources!

Global module constants used for our HDF5 format

Names of HDF5 attributes:

```python
tenpy.tools.hdf5_io.ATTR_TYPE = 'type'
    Attribute name for type of the saved object, should be one of the REPR_*
tenpy.tools.hdf5_io.ATTR_CLASS = 'class'
    Attribute name for the class name of an HDF5Exportable
ntenpy.tools.hdf5_io.ATTR_MODULE = 'module'
    Attribute name for the module where ATTR_CLASS can be retrieved
ntenpy.tools.hdf5_io.ATTR_LEN = 'len'
    Attribute name for the length of iterables, e.g, list, tuple
ntenpy.tools.hdf5_io.ATTR_FORMAT = 'format'
    indicates the ATTR_TYPE format used by Hdf5Exportable
```

Names for the ATTR_TYPE attribute:

```python
tenpy.tools.hdf5_io.REPR_HDF5EXPORTABLE = 'instance'
    saved object is instance of a user-defined class following the Hdf5Exportable style.
tenpy.tools.hdf5_io.REPR_ARRAY = 'array'
    saved object represents a numpy array
ntenpy.tools.hdf5_io.REPR_INT = 'int'
    saved object represents a (python) int
ntenpy.tools.hdf5_io.REPR_FLOAT = 'float'
    saved object represents a (python) float
ntenpy.tools.hdf5_io.REPR_STR = 'str'
    saved object represents a (python unicode) string
ntenpy.tools.hdf5_io.REPR_COMPLEX = 'complex'
    saved object represents a complex number
ntenpy.tools.hdf5_io.REPR_INT64 = 'np.int64'
    saved object represents a np.int64
ntenpy.tools.hdf5_io.REPR_FLOAT64 = 'np.float64'
    saved object represents a np.float64
ntenpy.tools.hdf5_io.REPR_INT32 = 'np.int32'
    saved object represents a np.int32
ntenpy.tools.hdf5_io.REPR_FLOAT32 = 'np.float32'
    saved object represents a np.float32
```
tenpy.tools.hdf5_io.REPR_BOOL = 'bool'
saved object represents a boolean

十nepy.tools.hdf5_io.REPR_NONE = 'None'
saved object is None

tenpy.tools.hdf5_io.REPR_RANGE = 'range'
saved object is a range

tenpy.tools.hdf5_io.REPR_LIST = 'list'
saved object represents a list

tenpy.tools.hdf5_io.REPR_TUPLE = 'tuple'
saved object represents a tuple

tenpy.tools.hdf5_io.REPR_SET = 'set'
saved object represents a set

tenpy.tools.hdf5_io.REPR_DICT_GENERAL = 'dict'
saved object represents a dict with complicated keys

十nepy.tools.hdf5_io.REPR_DICT_SIMPLE = 'simple_dict'
saved object represents a dict with simple keys

tenpy.tools.hdf5_io.REPR_DTYPE = 'dtype'
saved object represents a np.dtype

tenpy.tools.hdf5_io.REPR_IGNORED = 'ignore'
ignore the object/dataset during loading and saving

tenpy.tools.hdf5_io.TYPES_FOR_HDF5 DATASETS = ((<class 'numpy.ndarray'>, 'array'), (<class 'int'>, 'int'), (<class 'float'>, 'float'), ... 'np.float32'), (<class 'numpy.complex64'>, 'np.complex64'), (<class 'numpy.bool_'>, 'bool'), (<class 'bool'>, 'bool'))
tuple of (type, type_repr) which h5py can save as datasets; one entry for each type.

Todo: For memory caching with big MPO environments, we need a Hdf5Cacher clearing the memo’s every now and then (triggered by what?).

7.13.2 params

- full name: tenpy.tools.params
- parent module: tenpy.tools
- type: module
Classes

- **Config**

  Dict-like wrapper class for parameter/configuration dictionaries.

Functions

- **asConfig(config, name)**
  Convert a dict-like `config` to a `Config`.

- **get_parameter(params, key, default, descr[, . . .])**
  Read out a parameter from the dictionary and/or provide default values.

- **unused_parameters(params[, warn])**
  Returns a set of the parameters which have not been read out with `get_parameters`. 
asConfig

- full name: tenpy.tools.params.asConfig
- parent module: tenpy.tools.params
- type: function

tenpy.tools.params.asConfig(config, name)
Convert a dict-like config to a Config.

Parameters

- config (dict | Config) – If this is a Config, just return it. Otherwise, create a Config from it and return that.
- name (str) – Name to be used for the Config.

Returns config – Either directly config or Config(config, name).

Return type Config

get_parameter

- full name: tenpy.tools.params.get_parameter
- parent module: tenpy.tools.params
- type: function

tenpy.tools.params.get_parameter(params, key, default, descr, asarray=False)
Read out a parameter from the dictionary and/or provide default values.

This function provides a similar functionality as params.get(key, default). Unlike dict.get this function writes the default value into the dictionary (i.e. in other words it’s more similar to params.setdefault(key, default)).

This allows the user to save the modified dictionary as meta-data, which gives a concrete record of the actually used parameters and simplifies reproducing the results and restarting simulations.

Moreover, a special entry with the key 'verbose' in the params can trigger this function to also print the used value. A higher verbose level implies more output. If verbose >= 100, it is printed every time it’s used. If verbose >= 2., its printed for the first time time its used. and for verbose >= 1, non-default values are printed the first time they are used. otherwise only for the first use.

Internally, whether a parameter was used is saved in the set params[‘_used_param’]. This is used in unused_parameters() to print a warning if the key wasn’t used at the end of the algorithm, to detect mis-spelled parameters.

Parameters

- params (dict) – A dictionary of the parameters as provided by the user. If key is not a valid key, params[key] is set to default.
- key (string) – The key for the parameter which should be read out from the dictionary.
- default – The default value for the parameter.
- asarray (bool) – If True, convert the result to a numpy array with np.asarray(...) before returning.
**Returns** params[key] if the key is in params, otherwise default. Converted to a numpy array, if `asarray`.

**Return type** value

### Examples

In the algorithm Engine gets a dictionary of parameters. Beside doing other stuff, it calls `tenpy.models.model.NearestNeighborModel.calc_U_bond()` with the dictionary as argument, which looks similar like:

```python
>>> from tenpy.tools.params import get_parameter
>>> def model_calc_U(params):
...     dt = get_parameter(params, 'dt', 0.01, 'TEBD')
...     order = get_parameter(params, 'order', 1, 'TEBD')
...     print("calc U with dt =", dt, "and order =", order)
...     # ... calculate exp(-i * dt* H) ....
```

Then, when you call it without any parameters, it just uses the default value:

```python
>>> model_calc_U(dict())
calc U with dt = 0.01 and order = 1
```

Of course you can also provide the parameter to use a non-default value:

```python
>>> model_calc_U(dict(dt=0.02))
calc U with dt = 0.02 and order = 1
```

Increasing the special keyword 'verbose' generally prints more:

```python
>>> model_calc_U(dict(dt=0.02, verbose=1))
parameter 'dt'=0.02 for TEBD
calc U with dt = 0.02 and order = 1
>>> model_calc_U(dict(dt=0.02, verbose=2))
parameter 'dt'=0.02 for TEBD
parameter 'order'=1 (default) for TEBD
calc U with dt = 0.02 and order = 1
```

### unused_parameters

- **full name**: `tenpy.tools.params.unused_parameters`
- **parent module**: `tenpy.tools.params`
- **type**: function

`tenpy.tools.params.unused_parameters(params, warn=None)`

Returns a set of the parameters which have not been read out with `get_parameters`.

This function might be useful to check for typos in the parameter keys.

**Parameters**

- `params (dict)` – A dictionary of parameters which was given to (functions using) `get_parameter()`
- `warn (None | str)` – If given, print a warning “unused parameter for {warn!s}: {unused_keys!s}”.

---

626 Chapter 7. License
Returns **unused_keys** – The set of keys of the params which was not used

**Return type** set

**Module description**

Tools to handle config options/parameters for algorithms.

See the doc-string of `Config` for details.

### 7.13.3 events

- full name: `tenpy.tools.events`
- parent module: `tenpy.tools`
- type: module

#### Classes

<table>
<thead>
<tr>
<th>Class</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>EventHandler</code></td>
<td>Handler for an event represented by an instance of this class.</td>
</tr>
<tr>
<td><code>Listener</code></td>
<td><code>Listener(listener_id, callback, priority)</code></td>
</tr>
</tbody>
</table>

**EventHandler**

- full name: `tenpy.tools.events.EventHandler`
- parent module: `tenpy.tools.events`
- type: class

**Inheritance Diagram**

```
EventHandler
```

```
Listener
```
Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>EventHandler.__init__((arg_descr))</code></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>EventHandler.connect((callback, priority))</code></td>
<td>Register a callback function as a listener to the event.</td>
</tr>
<tr>
<td><code>EventHandler.disconnect(listener_id)</code></td>
<td>De-register a listener.</td>
</tr>
<tr>
<td><code>EventHandler.emit(*args, **kwargs)</code></td>
<td>Call the callback functions of all listeners.</td>
</tr>
<tr>
<td><code>EventHandler.emit_until_result(*args, **kwargs)</code></td>
<td>Call the listeners callback until one returns not None.</td>
</tr>
</tbody>
</table>

Class Attributes and Properties

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>EventHandler.id_of_last_connected</code></td>
<td></td>
</tr>
</tbody>
</table>

```
class tenpy.tools.events.EventHandler(arg_descr=None)
Bases: object
Handler for an event represented by an instance of this class.

All in all, events provide a flexible extension mechanism for classes to define “checkpoints” in the code where the user of a class might want to run something else, for example doing some measurements or saving intermediate results.

Parameters

arg_descr (str) – An informative description how the callback function is called.
An empty string indicates no arguments.

arg_descr
An informative description how the callback function is called.

Type str

listeners
Entries are tuples (listener_id, callback, priority).

Type list of (int, function, int)
```

Examples

Instances of this class typically get defined during class initialization and define an event. The event “happens” each time `emit()` or `emit_until_result()` is called, typically inside a method of the class defining the event. Example:

```python
>>> class MyAlgorithm:
...     def __init__(self):
...         self.checkpoint = EventHandler("algorithm, iteration")
...         self.data = 0
...     def run(self):
...         for i in range(4):
...             self.data += i  # do some complicated stuff
...             self.checkpoint.emit(self, i)
```

Other code with access to the event can then connect a listener to the event, i.e., give a function to the event that should be called each time the event is `emit()`-ed.

```python
>>> my_alg = MyAlgorithm()
>>> def my_listener(algorithm, iteration):
...     # do something with the event
```
As you can see, the function `my_listener` has been called during the `MyAlgorithm.run()` and had full access to the current status of the algorithm class. This is convenient to e.g. perform measurements of the state so far, print a status message of the progress or save intermediate results.

If the `EventHandler` is already initialized when you define the function, you can also use `connect()` as a function property like this:

```python
>>> @my_alg.checkpoint.connect
... def another_one(algorithm, iteration):
...     print("another_one called: iteration", iteration)
>>> @my_alg.checkpoint.connect(priority=5)
... def high_priority(algorithm, iteration):
...     print("high_priority call: iteration", iteration)
>>> my_alg.run()
high_priority call: iteration 0
my_listener called: iteration 0 with data 0
another_one called: iteration 0
high_priority call: iteration 1
my_listener called: iteration 1 with data 1
another_one called: iteration 1
high_priority call: iteration 2
my_listener called: iteration 2 with data 3
another_one called: iteration 2
high_priority call: iteration 3
my_listener called: iteration 3 with data 6
another_one called: iteration 3
```

``connect(callback=None, priority=0)`

Register a `callback` function as a listener to the event.

You can either call this function directly or use it as a function decorator, see the example in `EventHandler`.

If you ever plan to `disconnect()` again, you can read it out with `id_of_last_connected` right after connecting, i.e., right after calling this method.

**Parameters**

- `callback (callable)` – A function to be called during each `emit()` of the event.
- `priority (int)` – Higher priority indicates that the callback function should be called before other possibly registered callback functions.

**Returns** `callback` – The callback function exactly as given.

**Return type** callable

``disconnect(listener_id)`

De-register a listener.
Parameters **listener_id** (*int*) – The id of the listener returned by `connect()`.

**emit** (*args, **kwargs*)

Call the `callback` functions of all listeners.

**Returns** results – List of results returned by the individual callback functions.

**Return type** list

**emit_until_result** (*args, **kwargs*)

Call the listeners `callback` until one returns not `None`.

**Listener**

- full name: `tenpy.tools.events.Listener`
- parent module: `tenpy.tools.events`
- type: class

**Inheritance Diagram**

![Inheritance Diagram](image)

**Methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Signature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>Listener.__init__()</code></td>
<td></td>
<td>Initialize self.</td>
</tr>
<tr>
<td><code>Listener.count(value, /)</code></td>
<td></td>
<td>Return number of occurrences of value.</td>
</tr>
<tr>
<td><code>Listener.index(value[, start, stop])</code></td>
<td></td>
<td>Return first index of value.</td>
</tr>
</tbody>
</table>

**Class Attributes and Properties**

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>Listener.callback</code></td>
<td>Alias for field number 1</td>
</tr>
<tr>
<td><code>Listener.listener_id</code></td>
<td>Alias for field number 0</td>
</tr>
<tr>
<td><code>Listener.priority</code></td>
<td>Alias for field number 2</td>
</tr>
</tbody>
</table>

**class** `tenpy.tools.events.Listener`(*listener_id, callback, priority*)

**Bases:** `tuple`

**property** `callback`

Alias for field number 1

**count** (*value, /*)

Return number of occurrences of value.

**index** (*value, start=0, stop=9223372036854775807, /*)
Return first index of value.
Raises ValueError if the value is not present.

**property listener_id**
Alias for field number 0

**property priority**
Alias for field number 2

**Module description**

Event handler.
The `EventHandler` is basically just holds a list of functions which can get called once a certain “event” happens. Examples are given in the class doc-string.

**7.13.4 misc**

- full name: tenpy.tools.misc
- parent module: tenpy.tools
- type: module

**Functions**

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>add_with_None_0(a, b)</code></td>
<td>Return <code>a + b</code>, treating <code>None</code> as zero.</td>
</tr>
<tr>
<td><code>any_nonzero(params, keys[, verbose_msg])</code></td>
<td>Check for any non-zero or non-equal entries in some parameters.</td>
</tr>
<tr>
<td><code>anynan(a)</code></td>
<td>check whether any entry of a ndarray <code>a</code> is ‘NaN’.</td>
</tr>
<tr>
<td><code>argsort(a[, sort])</code></td>
<td>wrapper around np.argsort to allow sorting ascending/descending and by magnitude.</td>
</tr>
<tr>
<td><code>atleast_2d_pad(a[, pad_item])</code></td>
<td>Transform <code>a</code> into a 2D array, filling missing places with <code>pad_item</code>.</td>
</tr>
<tr>
<td><code>build_initial_state(size, states, filling[, ....])</code></td>
<td></td>
</tr>
<tr>
<td><code>chi_list(chi_max[, dchi, nsweeps, verbose])</code></td>
<td></td>
</tr>
<tr>
<td><code>group_by_degeneracy(E, *args[, subset, cutoff])</code></td>
<td>Find groups of indices for which (energy) values are degenerate.</td>
</tr>
<tr>
<td><code>inverse_permutation(perm)</code></td>
<td>reverse sorting indices.</td>
</tr>
<tr>
<td><code>lexsort(a[, axis])</code></td>
<td>wrapper around np.lexsort: allow for trivial case a.shape[0] = 0 without sorting</td>
</tr>
<tr>
<td><code>list_to_dict_list(l)</code></td>
<td>Given a list <code>l</code> of objects, construct a lookup table.</td>
</tr>
<tr>
<td><code>pad(a[, w_l, v_l, w_r, v_r, axis])</code></td>
<td>Pad an array along a given <code>axis</code>.</td>
</tr>
<tr>
<td><code>setup_executable(mod, run_defaults[, ....])</code></td>
<td>Read command line arguments and turn into useable dicts.</td>
</tr>
<tr>
<td><code>to_array(a[, shape])</code></td>
<td>Convert <code>a</code> to an numpy array and tile to matching dimension/shape.</td>
</tr>
<tr>
<td><code>to_iterable(a)</code></td>
<td>If <code>a</code> is a not iterable or a string, return <code>[a]</code>, else return <code>a</code>.</td>
</tr>
<tr>
<td><code>to_iterable_of_len(a, L)</code></td>
<td>If <code>a</code> is a non-string iterable of length <code>L</code>, return <code>a</code>, otherwise return <code>[a]**L</code>.</td>
</tr>
</tbody>
</table>

continues on next page
Table 174 – continued from previous page

<table>
<thead>
<tr>
<th>transpose_list_list(D[, pad])</th>
<th>Returns a list of lists $T$, such that $T[i][j] = D[j][i]$.</th>
</tr>
</thead>
<tbody>
<tr>
<td>zero_if_close(a[, tol])</td>
<td>set real and/or imaginary part to 0 if their absolute value is smaller than $tol$.</td>
</tr>
</tbody>
</table>

add_with_None_0

- full name: tenpy.tools.misc.add_with_None_0
- parent module: tenpy.tools.misc
- type: function

```python
tenpy.tools.misc.add_with_None_0(a, b)
Return $a + b$, treating $None$ as zero.
```

Parameters

- **a** – The two things to be added, or $None$.
- **b** – The two things to be added, or $None$.

Returns $a + b$, except if $a$ or $b$ is $None$, in which case the other variable is returned.

Return type sum

any_nonzero

- full name: tenpy.tools.misc.any_nonzero
- parent module: tenpy.tools.misc
- type: function

```python
tenpy.tools.misc.any_nonzero(params, keys, verbose_msg=None)
Check for any non-zero or non-equal entries in some parameters.
```

Parameters

- **params** (dict / Config) – A dictionary of parameters, or a Config instance.
- **keys** (list of {key | tuple of keys}) – For a single key, check params[key] for non-zero entries. For a tuple of keys, all the params[key] have to be equal (as numpy arrays).
- **verbose_msg** (None / str) – If params[‘verbose’] >= 1, we print verbose_msg before checking, and a short notice with the key, if a non-zero entry is found.

Returns **match** – False, if all params[key] are zero or $None$ and True, if any of the params[key] for single key in keys, or if any of the entries for a tuple of keys

Return type bool
anynan

- full name: tenpy.tools.misc.anynan
- parent module: tenpy.tools.misc
- type: function

tenpy.tools.misc.anynan(a)
check whether any entry of a ndarray \( a \) is ‘NaN’.

argsort

- full name: tenpy.tools.misc.argsort
- parent module: tenpy.tools.misc
- type: function

tenpy.tools.misc.argsort(a, sort=None, **kwargs)
wrapper around np.argsort to allow sorting ascending/descending and by magnitude.

Parameters

- \( a \) (array_like) – The array to sort.
- \( \text{sort} \) (‘m>’, ‘m<’, ‘>’, ‘<’, None) – Specify how the arguments should be sorted.

<table>
<thead>
<tr>
<th>sort</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>‘m&gt;’, ‘LM’</td>
<td>Largest magnitude first</td>
</tr>
<tr>
<td>‘m&lt;’, ‘SM’</td>
<td>Smallest magnitude first</td>
</tr>
<tr>
<td>‘&gt;’, ‘LR’, ‘LA’</td>
<td>Largest real part first</td>
</tr>
<tr>
<td>‘&lt;’, ‘SR’, ‘SA’</td>
<td>Smallest real part first</td>
</tr>
<tr>
<td>‘LI’</td>
<td>Largest imaginary part first</td>
</tr>
<tr>
<td>‘SI’</td>
<td>Smallest imaginary part first</td>
</tr>
<tr>
<td>None</td>
<td>numpy default: same as ‘&lt;’</td>
</tr>
</tbody>
</table>

- **kwargs – Further keyword arguments given directly to numpy.argsort().

Returns index_array – Same shape as \( a \), such that \( a[index_array] \) is sorted in the specified way.

Return type ndarray, int

atleast_2d_pad

- full name: tenpy.tools.misc.atleast_2d_pad
- parent module: tenpy.tools.misc
- type: function

tenpy.tools.misc.atleast_2d_pad(a, pad_item=0)
Transform a into a 2D array, filling missing places with pad_item.

Given a list of lists, turn it to a 2D array (pad with 0), or turn a 1D list to 2D.

Parameters a (list of lists) – to be converted into ad 2D array.
Returns a 2D – a converted into a numpy array.

Return type 2D ndarray

Examples

```python
>>> atleast_2d_pad([3, 4, 0])
array([[3, 4, 0]])

>>> atleast_2d_pad([[3, 4], [1, 6, 7]])
array([[3., 4., 0.],
       [1., 6., 7.]])
```

---

**build_initial_state**

- full name: tenpy.tools.misc.build_initial_state
- parent module: tenpy.tools.misc
- type: function

```python
tenpy.tools.misc.build_initial_state(size, states, filling, mode='random', seed=None)
```

---

**chi_list**

- full name: tenpy.tools.misc.chi_list
- parent module: tenpy.tools.misc
- type: function

```python
tenpy.tools.misc.chi_list(chi_max, dchi=20, nsweeps=20, verbose=0)
```

---

**group_by_degeneracy**

- full name: tenpy.tools.misc.group_by_degeneracy
- parent module: tenpy.tools.misc
- type: function

```python
tenpy.tools.misc.group_by_degeneracy(E, *args, subset=None, cutoff=1e-12)
```

Find groups of indices for which (energy) values are degenerate.

**Parameters**

- `values (1D array)` – Values (e.g. energies) which need to be close to count as degenerate.
- `*args (1D array)` – Additional vectors (with same length as `values`), which also need to be close (up to `cutoff`) to count as degenerate.
- `subset (1D array)` – Optionally selects a subset of the indices
- `cutoff (float)` – Precision up to which values still count as degenerate.

**Returns**
• **idx_groups** *(list of tuple of int)* – Each tuple group contains indices i, j, k, ... for which the values are closer than cutoff, i.e., |E[j, k, ...] - E[i]| <= cutoff. Each index appears exactly once (if it is contained in subset).

• .. *testsetup* :: – from tenpy.tools.misc import *

• >>> E = [2., 2.4, 1.9999, 1.8, 2.3999, 5, 1.8]
  ... # -> 0 1 2 3 4 5 6
  • >>> k = [0, 1, 2, 2, 1, 2, 1]
  • >>> group_by_degeneracy(E, cutoff=0.001)
  • [(0, 2), (1, 4), (3, 6), (5,)]
  • >>> group_by_degeneracy(E, k, cutoff=0.001) # k and E need to be close
  • [(0,), (1, 4), (2,), (3,), (5,), (6,)]

### inverse_permutation

- full name: tenpy.tools.misc.inverse_permutation
- parent module: tenpy.tools.misc
- type: function

\[
\text{tenpy.tools.misc.} \text{inverse_permutation}(\text{perm}) \\
\text{reverse sorting indices.}
\]

Sort functions (as LegCharge.sort()) return a (1D) permutation perm array, such that sorted_array = old_array[perm]. This function inverts the permutation perm, such that old_array = sorted_array[inverse_permutation(perm)].

**Parameters** perm *(1D array_like)* – The permutation to be reversed. Assumes that it is a permutation with unique indices. If it is, \(\text{inverse_permutation(} \text{inverse_permutation(perm)}\) == perm.

**Returns** inv_perm – The inverse permutation of perm such that inv_perm[perm[j]] = j = perm[inv_perm[j]].

**Return type** 1D array (int)

### lexsort

- full name: tenpy.tools.misc.lexsort
- parent module: tenpy.tools.misc
- type: function

\[
\text{tenpy.tools.misc.} \text{lexsort}(a, axis=-1) \\
\text{wrapper around np.lexsort: allow for trivial case a.shape[0] = 0 without sorting}
\]
list_to_dict_list

- full name: tenpy.tools.misc.list_to_dict_list
- parent module: tenpy.tools.misc
- type: function

`tenpy.tools.misc.list_to_dict_list(l)`

Given a list `l` of objects, construct a lookup table.

This function will handle duplicate entries in `l`.

**Parameters**

`l` *(iterable of iterable of immutable)* – A list of objects that can be converted to tuples to be used as keys for a dictionary.

**Returns**

`lookup` – A dictionary with (key, value) pairs `key:[i1,i2,...]` where `i1, i2, ...` are the indices where `key` is found in `l`: i.e. `key == tuple(l[i1]) == tuple(l[i2]) == ...`

**Return type** dict

pad

- full name: tenpy.tools.misc.pad
- parent module: tenpy.tools.misc
- type: function

`tenpy.tools.misc.pad(a, w_l=0, v_l=0, w_r=0, v_r=0, axis=0)`

Pad an array along a given `axis`.

**Parameters**

- `a` *(ndarray)* – the array to be padded
- `w_l` *(int)* – the width to be padded in the front
- `v_l` *(dtype)* – the value to be inserted before `a`
- `w_r` *(int)* – the width to be padded after the last index
- `v_r` *(dtype)* – the value to be inserted after `a`
- `axis` *(int)* – the axis along which to pad

**Returns**

`padded` – a copy of `a` with enlarged `axis`, padded with the given values.

**Return type** ndarray

setup_executable

- full name: tenpy.tools.misc.setup_executable
- parent module: tenpy.tools.misc
- type: function

`tenpy.tools.misc.setup_executable(mod, run_defaults, identifier_list=None)`

Read command line arguments and turn into useable dicts.

Uses default values defined at: - model class for model_par - here for sim_par - executable file for run_par

Alternatively, a model_defaults dictionary and identifier_list can be supplied without the model
NB: for setup_executable to work with a model class, the model class needs to define two things:

- defaults, a static (class level) dictionary with (key, value) pairs that have the name of the parameter (as string) as key, and the default value as value.
- identifier, a static (class level) list or other iterable with the names of the parameters to be used in filename identifiers.

**Parameters**

- **mod** *(model | dict)* – Model class (or instance) OR a dictionary containing model defaults
- **run_defaults** *(dict)* – default values for executable file parameters
- **identifier_list** *(iterable, optional)* – variables

**Returns** containing all parameters. args | namespace with raw arguments for some backwards compatibility with executables.

**Return type** model_par, sim_par, run_par (dicts)

### to_array

- full name: tenpy.tools.misc.to_array
- parent module: tenpy.tools.misc
- type: function

`tenpy.tools.misc.to_array(a, shape=(None))`

Convert `a` to an numpy array and tile to matching dimension/shape.

This function provides similar functionality as numpy's broadcast, but not quite the same: Only scalars are broadcasted to higher dimensions, for a non-scalar, we require the number of dimension to match. If the shape does not match, we repeat periodically, e.g. we tile `(3, 4) -> (6, 16)` but `(4, 4) -> (6, 16)` will raise an error.

**Parameters**

- **a** *(scalar | array_like)* – The input to be converted to an array. A scalar is reshaped to the desired dimension.
- **shape** *(tuple of (None | int))* – The desired shape of the array. An entry `None` indicates arbitrary len >1. For int entries, tile the array periodically to fit the len.

**Returns** `a_array` – A copy of `a` converted to a numpy ndarray of desired dimension and shape.

**Return type** ndarray

### to_iterable

- full name: tenpy.tools.misc.to_iterable
- parent module: tenpy.tools.misc
- type: function

`tenpy.tools.misc.to_iterable(a)`

If `a` is a not iterable or a string, return `[a]`, else return `a`. 
to_iterable_of_len

- full name: tenpy.tools.misc.to_iterable_of_len
- parent module: tenpy.tools.misc
- type: function

```
import tenpy.tools.misc as tpm

tpm.to_iterable_of_len(a, L)
```

If `a` is a non-string iterable of length `L`, return `a`, otherwise return `[a] * L`.

Raises ValueError if `a` is already an iterable of different length.

transpose_list_list

- full name: tenpy.tools.misc.transpose_list_list
- parent module: tenpy.tools.misc
- type: function

```
import tenpy.tools.misc as tpm

tpm.transpose_list_list(D, pad=None)
```

Returns a list of lists `T`, such that `T[i][j] = D[j][i]`.

Parameters

- `D (list of list)` – to be transposed
- `pad` – Used to fill missing places, if `D` is not rectangular.

Returns `T` – transposed, rectangular version of `D`, constructed such that `T[i][j] = D[j][i]` if `i < len(D[j])` else `pad`

Return type list of lists

zero_if_close

- full name: tenpy.tools.misc.zero_if_close
- parent module: tenpy.tools.misc
- type: function

```
import tenpy.tools.misc as tpm

tpm.zero_if_close(a, tol=1e-15)
```

set real and/or imaginary part to 0 if their absolute value is smaller than `tol`.

Parameters

- `a (ndarray)` – numpy array to be rounded
- `tol (float)` – the threshold which values to consider as ‘0’.
Module description

Miscellaneous tools, somewhat random mix yet often helpful.

7.13.5 math

- full name: tenpy.tools.math
- parent module: tenpy.tools
- type: module

Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>entropy(p[, n])</td>
<td>Calculate the entropy of a distribution.</td>
</tr>
<tr>
<td>gcd(a, b)</td>
<td>Computes the greatest common divisor (GCD) of two numbers.</td>
</tr>
<tr>
<td>gcd_array(a)</td>
<td>Return the greatest common divisor of all of entries in a</td>
</tr>
<tr>
<td>lcm(a, b)</td>
<td>Returns the least common multiple (LCM) of two positive numbers.</td>
</tr>
<tr>
<td>matvec_to_array(H)</td>
<td>transform an linear operator with a matvec method into a dense numpy array.</td>
</tr>
<tr>
<td>perm_sign(p)</td>
<td>Given a permutation p of numbers, returns its sign.</td>
</tr>
<tr>
<td>qr_li(A[, cutoff])</td>
<td>QR decomposition with cutoff to discard nearly linear dependent columns in Q.</td>
</tr>
<tr>
<td>rq_li(A[, cutoff])</td>
<td>RQ decomposition with cutoff to discard nearly linear dependent columns in Q.</td>
</tr>
<tr>
<td>speigs(A, k, *args, **kwargs)</td>
<td>Wrapper around scipy.sparse.linalg.eigs(), lifting the restriction k &lt; rank(A)−1.</td>
</tr>
<tr>
<td>speigsh(A, k, *args, **kwargs)</td>
<td>Wrapper around scipy.sparse.linalg.eigsh(), lifting the restriction k &lt; rank(A)−1.</td>
</tr>
</tbody>
</table>

entropy

- full name: tenpy.tools.math.entropy
- parent module: tenpy.tools.math
- type: function

```python
import numpy as np

tenpy.tools.math.entropy(p, n=1)
```

Calculate the entropy of a distribution. Assumes that p is a normalized distribution (np.sum(p) == 1.).

Parameters

- **p** (1D array) – A normalized distribution.
- **n** (1 | float | np.inf) – Selects the entropy, see below.

Returns entropy – Shannon-entropy \(-\sum_i p_i \log(p_i)\) (n=1) or Renyi-entropy \(\frac{1}{1-n} \log(\sum_i p_i^n)\) (n != 1) of the distribution p.

Return type float
gcd

- full name: tenpy.tools.math.gcd
- parent module: tenpy.tools.math
- type: function

tenpy.tools.math.gcd(a, b)
Computes the greatest common divisor (GCD) of two numbers.
Return 0 if both a, b are zero, otherwise always return a non-negative number.

gcd_array

- full name: tenpy.tools.math.gcd_array
- parent module: tenpy.tools.math
- type: function

tenpy.tools.math.gcd_array(a)
Return the greatest common divisor of all of entries in a

lcm

- full name: tenpy.tools.math.lcm
- parent module: tenpy.tools.math
- type: function

tenpy.tools.math.lcm(a, b)
Returns the least common multiple (LCM) of two positive numbers.

matvec_to_array

- full name: tenpy.tools.math.matvec_to_array
- parent module: tenpy.tools.math
- type: function

matvec_to_array(H)
transform an linear operator with a matvec method into a dense numpy array.

Parameters
- H (linear operator) – should have shape, dtype attributes and a matvec method.

Returns
- H_dense – a dense array version of H.

Return type
- ndarray, shape (H.dim, H.dim)
perm_sign

- full name: tenpy.tools.math.perm_sign
- parent module: tenpy.tools.math
- type: function

\[
\text{tenpy.tools.math.perm_sign}(p)
\]

Given a permutation \( p \) of numbers, returns its sign. (+1 or -1)

Assumes that all the elements are distinct, if not, you get crap.

Examples

```python
>>> import itertools
>>> for p in itertools.permutations(range(3)):
    ...    print('({p!s}): {sign!s}'.format(p=p, sign=tenpy.tools.math.perm_sign(p)))
(0, 1, 2): 1
(0, 2, 1): -1
(1, 0, 2): -1
(1, 2, 0): 1
(2, 0, 1): 1
(2, 1, 0): -1
```

qr_li

- full name: tenpy.tools.math.qr_li
- parent module: tenpy.tools.math
- type: function

\[
\text{tenpy.tools.math.qr_li}(A, \text{cutoff}=1e-15)
\]

QR decomposition with cutoff to discard nearly linear dependent columns in \( Q \).

Perform a QR decomposition with pivoting, discard columns where \( R[i,i] < \text{cutoff} \), reverse the permutation from pivoting and perform another QR decomposition to ensure that \( R \) is upper right.

Parameters

- \( A \) (numpy.ndarray) – Matrix to be decomposed as \( A = Q.R \)

Returns \( Q, R \) – Decomposition of \( A \) into isometry \( Q^d Q = I \) and upper right \( R \) with diagonal entries larger than \( \text{cutoff} \).

Return type

numpy.ndarray

rq_li

- full name: tenpy.tools.math.rq_li
- parent module: tenpy.tools.math
- type: function

\[
\text{tenpy.tools.math.rq_li}(A, \text{cutoff}=1e-15)
\]

RQ decomposition with cutoff to discard nearly linear dependent columns in \( Q \).

Uses \( qr_li() \) on tranpose of \( A \). Note that \( R \) is nonzero in the lowest left corner; \( R \) has entries below the diagonal for non-square \( R \).
Parameters `A` *(numpy.ndarray)* – Matrix to be decomposed as \( A = Q.R \)

Returns `R, Q` – Decomposition of `A` into isometry \( Q.Q^d = 1 \) and upper right \( R \) with diagonal entries larger than `cutoff`. If \( M, N = A.shape \), then `R.shape = M, K` and `Q.shape = K, N` with \( K <= \text{min}(M, N) \).

Return type `numpy.ndarray`

---

**speigs**

- full name: `tenpy.tools.math.speigs`
- parent module: `tenpy.tools.math`
- type: function

`tenpy.tools.math.speigs(A, k, *args, **kwargs)`

Wrapper around `scipy.sparse.linalg.eigs()`, lifting the restriction \( k < \text{rank}(A)-1 \).

Parameters

- `A` *(MxM ndarray or like scipy.sparse.linalg.LinearOperator)* – The (square) linear operator for which the eigenvalues should be computed.
- `k` *(int)* – The number of eigenvalues to be computed.
- `*args` – Further arguments directly given to `scipy.sparse.linalg.eigs()`.
- `**kwargs` – Further keyword arguments directly given to `scipy.sparse.linalg.eigs()`.

Returns

- `w` *(ndarray)* – Array of \( \min(k, A.shape[0]) \) eigenvalues.
- `v` *(ndarray)* – Array of \( \min(k, A.shape[0]) \) eigenvectors, \( v[:, i] \) is the \( i \)-th eigenvector. Only returned if `kwargs['return_eigenvectors'] == True`.

**speigsh**

- full name: `tenpy.tools.math.speigsh`
- parent module: `tenpy.tools.math`
- type: function

`tenpy.tools.math.speigsh(A, k, *args, **kwargs)`

Wrapper around `scipy.sparse.linalg.eigsh()`, lifting the restriction \( k < \text{rank}(A)-1 \).

Parameters

- `A` *(MxM ndarray or like scipy.sparse.linalg.LinearOperator)* – The (square) hermitian linear operator for which the eigenvalues should be computed.
- `k` *(int)* – The number of eigenvalues to be computed.
- `*args` – Further arguments directly given to `scipy.sparse.linalg.eigsh()`.
- `**kwargs` – Further keyword arguments directly given to `scipy.sparse.linalg.eigsh()`.

Returns

- `w` *(ndarray)* – Array of \( \min(k, A.shape[0]) \) eigenvalues.
• v (ndarray) – Array of \(\min(k, A.shape[0])\) eigenvectors, \(v[:, i]\) is the \(i\)-th eigenvector. Only returned if \(\text{kwargs['return_eigenvectors']} == \text{True}\).

### Module description

Different math functions needed at some point in the library.

```python
tenpy.tools.math.LeviCivita3 = array([[ 0, 0, 0], [ 0, 0, 1], [ 0, -1, 0]], [[ 0, 0, -1], [ 0, 0, 0], [ 1, 0, 0]], [[ 0, 1, 0], [-1, 0, 0], [ 0, 0, 0]])
```

**Levi-Civita Symbol of int type**

#### 7.13.6 fit

- full name: tenpy.tools.fit
- parent module: tenpy.tools
- type: module

### Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>alg_decay(x, a, b, c)</code></td>
<td>define the algebraic decay.</td>
</tr>
<tr>
<td><code>alg_decay_fit(x, y[, npts, power_range, ...])</code></td>
<td>Fit (y) to the form (a*\exp(-b) + c).</td>
</tr>
<tr>
<td><code>alg_decay_fit_res(log_b, x, y)</code></td>
<td>Returns the residue of an algebraic decay fit of the form (x**(-\exp(log_b))).</td>
</tr>
<tr>
<td><code>alg_decay_fits(x, ys[, npts, power_range, ...])</code></td>
<td>Fit arrays of (y)'s to the form (a * x**(-b) + c).</td>
</tr>
<tr>
<td><code>central_charge_from_S_profile(psi[, exclude])</code></td>
<td>Fit the entanglement entropy of a finite MPS to the expected profile for critical models.</td>
</tr>
<tr>
<td><code>entropy_profile_from_CFT(size_A, l, ...)</code></td>
<td>Expected profile for the entanglement entropy at a critical point.</td>
</tr>
<tr>
<td><code>fit_with_sum_of_exp(f, n[, N])</code></td>
<td>Approximate a decaying function (f) with a sum of exponentials.</td>
</tr>
<tr>
<td><code>lin_fit_res(x, y)</code></td>
<td>Returns the least-square residue of a linear fit (y) vs (x).</td>
</tr>
<tr>
<td><code>linear_fit(x, y)</code></td>
<td>Perform a linear fit of (y) to (ax + b).</td>
</tr>
<tr>
<td><code>plot_alg_decay_fit(plot_module, x, y, fit_par)</code></td>
<td>Given (x, y,) and (fit_par) (output from (\text{alg}_decay_fit)), produces a plot of the algebraic decay fit.</td>
</tr>
<tr>
<td><code>sum_of_exp(lambdas, prefactors, x)</code></td>
<td>Evaluate (\sum_{i} \text{prefactor}[i] * \text{lambda}[i]**x) for different (x).</td>
</tr>
</tbody>
</table>

#### alg_decay

- full name: tenpy.tools.fit.alg_decay
- parent module: tenpy.tools.fit
- type: function

```python
tenpy.tools.fit.alg_decay(x, a, b, c)
```

define the algebraic decay.
alg_decay_fit

- full name: tenpy.tools.fit.alg_decay_fit
- parent module: tenpy.tools.fit
- type: function

`tenpy.tools.fit.alg_decay_fit(x, y, npts=5, power_range=(0.01, 4.0), power_mesh=[60, 10])`

Fit y to the form \(a \cdot x^{-b} + c\).

Returns a triplet \([a, b, c]\).

npts specifies the maximum number of points to fit. If npts < len(x), then alg_decay_fit() will only fit to the last npts points. power_range is a tuple that gives that restricts the possible ranges for b. power_mesh is a list of numbers, which specifies how fine to search for the optimal b. E.g., if power_mesh = [60,10], then it’ll first divide the power_range into 60 intervals, and then divide those intervals by 10.

alg_decay_fit_res

- full name: tenpy.tools.fit.alg_decay_fit_res
- parent module: tenpy.tools.fit
- type: function

`tenpy.tools.fit.alg_decay_fit_res(log_b, x, y)`

Returns the residue of an algebraic decay fit of the form \(x**(-np.exp(log_b))\).

alg_decay_fits

- full name: tenpy.tools.fit.alg_decay_fits
- parent module: tenpy.tools.fit
- type: function

`tenpy.tools.fit.alg_decay_fits(x, ys, npts=5, power_range=(0.01, 4.0), power_mesh=[60, 10])`

Fit arrays of y’s to the form \(a \cdot x^{**(-b)} + c\).

Returns arrays of \([a, b, c]\).

central_charge_from_S_profile

- full name: tenpy.tools.fit.central_charge_from_S_profile
- parent module: tenpy.tools.fit
- type: function

`tenpy.tools.fit.central_charge_from_S_profile(psi, exclude=None)`

Fit the entanglement entropy of a finite MPS to the expected profile for critical models. See `entropy_profile_from_CFT()` for the function we fit to.

Parameters

- `psi` (MPS) – Ground state of a finite system at a critical point (i.e. gapless!). The bond dimension should be large enough to be converged!
• **exclude** (*int*) – How many sites at the left (and at the right) boundary to exclude from the fit (to avoid boundary effects). Defaults to \(\psi.L // 4\)

**Returns**

• **central_charge**, **const** (*float*) – Central charge and constant offset as in `entropy_profile_from_CFT()`.
• **res** (*float*) – Residuum of the error.

**entropy_profile_from_CFT**

- full name: tenpy.tools.fit.entropy_profile_from_CFT
- parent module: tenpy.tools.fit
- type: function

```python
tenpy.tools.fit.entropy_profile_from_CFT(size_A, L, central_charge, const)
```

Expected profile for the entanglement entropy at a critical point.

Conformal field theory predicts the entanglement entropy for cutting a ground state of a finite, critical (i.e. gapless) system of length \(L\) into the left \(l\) and right \(L-l\) sites to be (eq. 2 of [calabrese2004]):

\[
S(l, L) = \frac{c}{6} \log \left( \frac{2L}{\pi a} \sin \left( \frac{\pi l}{L} \right) \right) + \text{const}
\]

Here, \(c\) is the central charge of the system, and \(a\) is the lattice spacing, which we set to 1, and \(\text{const}\) is a non-universal constant.

Returns exactly that formula.

**fit_with_sum_of_exp**

- full name: tenpy.tools.fit.fit_with_sum_of_exp
- parent module: tenpy.tools.fit
- type: function

```python
tenpy.tools.fit.fit_with_sum_of_exp(f, n, N=50)
```

Approximate a decaying function \(f\) with a sum of exponentials.

MPOs can naturally represent long-range interactions with an exponential decay. A common technique for other (e.g. powerlaw) long-range interactions is to approximate them by sums of exponentials and to include them into the MPOs. This function allows to do that.

The algorithm/implementation follows the appendix of [murg2010].

**Parameters**

- **f** (*function*) – Decaying function to be approximated. Needs to accept a 1D numpy array \(x\)
- **n** (*int*) – Number of exponentials to be used.
- **N** (*int*) – Number of points at which to evaluate/fit \(f\); we evaluate and fit \(f\) at the points \(x = \text{np.linspace}(1, N+1)\).

**Returns**

- **lambdas**, **prefactors** – Such that \(f(k) \approx \sum_i x_i \lambda_i^k\) for (integer) \(1 \leq k \leq N\). The function `sum_of_exp()` evaluates this for given \(x\).

**Return type** 1D arrays
lin_fit_res

- full name: tenpy.tools.fit.lin_fit_res
- parent module: tenpy.tools.fit
- type: function

tenpy.tools.fit.lin_fit_res(x, y)
Returns the least-square residue of a linear fit y vs x.

linear_fit

- full name: tenpy.tools.fit.linear_fit
- parent module: tenpy.tools.fit
- type: function

tenpy.tools.fit.linear_fit(x, y)
Perform a linear fit of y to ax + b.
Returns a, b, res.

plot_alg_decay_fit

- full name: tenpy.tools.fit.plot_alg_decay_fit
- parent module: tenpy.tools.fit
- type: function

tenpy.tools.fit.plot_alg_decay_fit(plot_module, x, y, fit_par, xfunc=None, kwargs={}, plot_fit_args={})
Given x, y, and fit_par (output from alg_decay_fit), produces a plot of the algebraic decay fit.
plot_module is matplotlib.pyplot, or a subplot. x, y are the data (real, 1-dimensional np.ndarray) fit_par is a triplet of numbers [a, b, c] that describes and algebraic decay (see alg_decay()). xfunc is an optional parameter that scales the x-axis in the resulting plot. kwargs is a dictionary, whose key/items are passed to the plot function. plot_fit_args is a dictionary that controls how the fit is shown.

sum_of_exp

- full name: tenpy.tools.fit.sum_of_exp
- parent module: tenpy.tools.fit
- type: function

tenpy.tools.fit.sum_of_exp(lambdas, prefactors, x)
Evaluate \sum_i \text{prefactor}[i] \times \text{lambda}[i]**x for different x.
See fit_sum_of_exp() for more details.
Module description

tools to fit to an algebraic decay.

7.13.7 string

- full name: tenpy.tools.string
- parent module: tenpy.tools
- type: module

Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>is_non_string_iterable(x)</td>
<td>Check if x is a non-string iterable, (e.g., list, tuple, dictionary, np.ndarray)</td>
</tr>
<tr>
<td>to_mathematica_lists(a)</td>
<td>convert nested a to string readable by mathematica using curly brackets ‘[…]’</td>
</tr>
<tr>
<td>vert_join(strlist[, valign, halign, delim])</td>
<td>Join strings with multilines vertically such that they appear next to each other.</td>
</tr>
</tbody>
</table>

is_non_string_iterable

- full name: tenpy.tools.string.is_non_string_iterable
- parent module: tenpy.tools.string
- type: function

tenpy.tools.string.is_non_string_iterable(x)
Check if x is a non-string iterable, (e.g., list, tuple, dictionary, np.ndarray)

to_mathematica_lists

- full name: tenpy.tools.string.to_mathematica_lists
- parent module: tenpy.tools.string
- type: function

tenpy.tools.string.to_mathematica_lists(a)
convert nested a to string readable by mathematica using curly brackets ‘[…]’.

vert_join

- full name: tenpy.tools.string.vert_join
- parent module: tenpy.tools.string
- type: function

tenpy.tools.string.vert_join(strlist[, valign, halign, delim])
Join strings with multilines vertically such that they appear next to each other.

Parameters
**strlist** (*list of str*) – the strings to be joined vertically

**valing** ('t', 'c', 'b') – vertical alignment of the strings: top, center, or bottom

**halign** ('l', 'c', 'r') – horizontal alignment of the strings: left, center, or right

**delim** (*str*) – field separator between the strings

Returns **joined** – a string where the strings of strlist are aligned vertically

Return type **str**

**Examples**

```python
>>> from tenpy.tools.string import vert_join
>>> print(vert_join(['a
sample
multiline
string', str(np.arange(9).reshape(3,3))],
                  delim=' | '))
a | [[0 1 2]
sample | [3 4 5]
multiline | [6 7 8]
string | 
```

**Module description**

Tools for handling strings.

**7.13.8 process**

- full name: tenpy.tools.process
- parent module: tenpy.tools
- type: module

**Functions**

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>load_omp_library(libs, verbose)</code></td>
<td>Tries to load openMP library.</td>
</tr>
<tr>
<td><code>memory_usage()</code></td>
<td>Return memory usage of the running python process.</td>
</tr>
<tr>
<td><code>mkl_get_nthreads()</code></td>
<td>wrapper around MKL <code>get_max_threads</code>.</td>
</tr>
<tr>
<td><code>mkl_set_nthreads(n)</code></td>
<td>wrapper around MKL <code>set_num_threads</code>.</td>
</tr>
<tr>
<td><code>omp_get_nthreads()</code></td>
<td>wrapper around OpenMP <code>get_max_threads</code>.</td>
</tr>
<tr>
<td><code>omp_set_nthreads(n)</code></td>
<td>wrapper around OpenMP <code>set_num_threads</code>.</td>
</tr>
</tbody>
</table>
### load_omp_library

- **full name:** `tenpy.tools.process.load_omp_library`
- **parent module:** `tenpy.tools.process`
- **type:** function

```python
tenpy.tools.process.load_omp_library(libs=['libiomp5.so', None, 'libgomp.so.1'], verbose=True)
```

Tries to load openMP library.

**Parameters**
- `libs` – list of possible library names we should try to load (with ctypes.CDLL).
- `verbose` (bool) – whether to print the name of the loaded library.

**Returns**
- `omp` – OpenMP shared library if found, otherwise None. Once it was successfully imported, no re-imports are tried.

**Return type** `CDLL | None`

### memory_usage

- **full name:** `tenpy.tools.process.memory_usage`
- **parent module:** `tenpy.tools.process`
- **type:** function

```python
tenpy.tools.process.memory_usage()
```

Return memory usage of the running python process.

You can `pip install psutil` if you get only `-1`.

**Returns**
- `mem` – Currently used memory in megabytes. `-1` if no way to read out.

**Return type** `float`

### mkl_get_nthreads

- **full name:** `tenpy.tools.process.mkl_get_nthreads`
- **parent module:** `tenpy.tools.process`
- **type:** function

```python
tenpy.tools.process.mkl_get_nthreads()
```

Wrapper around MKL `get_max_threads`.

**Returns**
- `max_threads` – The maximum number of threads used by MKL. `-1` if unable to read out.

**Return type** `int`
mkl_set_nthreads

- full name: tenpy.tools.process.mkl_set_nthreads
- parent module: tenpy.tools.process
- type: function

```python
tenpy.tools.process.mkl_set_nthreads(n)
```

wrapper around MKL set_num_threads.

**Parameters**
- `n (int)` – the number of threads to use

**Returns**
- `success` – whether the shared library was found and set.

**Return type**
- `bool`

omp_get_nthreads

- full name: tenpy.tools.process.omp_get_nthreads
- parent module: tenpy.tools.process
- type: function

```python
tenpy.tools.process.omp_get_nthreads()
```

wrapper around OpenMP get_max_threads.

**Returns**
- `max_threads` – The maximum number of threads used by OpenMP (and thus MKL). -1 if unable to read out.

**Return type**
- `int`

omp_set_nthreads

- full name: tenpy.tools.process.omp_set_nthreads
- parent module: tenpy.tools.process
- type: function

```python
tenpy.tools.process.omp_set_nthreads(n)
```

wrapper around OpenMP set_nthreads.

**Parameters**
- `n (int)` – the number of threads to use

**Returns**
- `success` – whether the shared library was found and set.

**Return type**
- `bool`

**Module description**

Tools to read out total memory usage and get/set the number of threads.

If your python is compiled against MKL (e.g. if you use anaconda as recommended in INSTALL), it will by default use as many threads as CPU cores are available. If you run a job on a cluster, you should limit this to the number of cores you reserved – otherwise your colleagues might get angry... A simple way to achieve this is to set a suitable environment variable before calling your python program, e.g. on the linux bash `export OMP_NUM_THREADS=4` for 4 threads. (MKL used OpenMP and thus respects its settings.)
Alternatively, this module provides `omp_get_nthreads()` and `omp_set_nthreads()`, which give their best to get and set the number of threads at runtime, while still being fail-safe if the shared OpenMP library is not found. In the latter case, you might also try the equivalent `mkl_get_nthreads()` and `mkl_set_nthreads()`.

### 7.13.9 optimization

- full name: `tenpy.tools.optimization`
- parent module: `tenpy.tools`
- type: module

#### Classes

- **Enum**
- **IntEnum**
- **OptimizationFlag**
- **temporary_level**

<table>
<thead>
<tr>
<th>OptimizationFlag(value)</th>
<th>Options for the global ‘optimization level’ used for dynamical optimizations.</th>
</tr>
</thead>
<tbody>
<tr>
<td>temporary_level(temporary_level)</td>
<td>Context manager to temporarily set the optimization level to a different value.</td>
</tr>
</tbody>
</table>

#### OptimizationFlag

- full name: `tenpy.tools.optimization.OptimizationFlag`
- parent module: `tenpy.tools.optimization`
- type: class
Inheritance Diagram

![Inheritance Diagram]

Class Attributes and Properties

<table>
<thead>
<tr>
<th>OptimizationFlag.default</th>
<th>OptimizationFlag.none</th>
<th>OptimizationFlag.safe</th>
<th>OptimizationFlag.skip_arg_checks</th>
</tr>
</thead>
</table>

\begin{code}
\begin{verbatim}
class tenpy.tools.optimization.optimizationFlag (value)
    Bases: enum.IntEnum

    Options for the global ‘optimization level’ used for dynamical optimizations.
    
    Whether we optimize dynamically is decided by comparison of the global “optimization level” with one of the following flags. A higher level includes all the previous optimizations.

    | Level | Flag         | Description                                                                 |
    |-------|--------------|------------------------------------------------------------------------------|
    | 0     | none         | Don’t do any optimizations, i.e., run many sanity checks. Used for testing.  |
    | 1     | default      | Skip really unnecessary sanity checks, but also don’t try any optional optimizations if they might give an overhead. |
    | 2     | safe         | Activate safe optimizations in algorithms, even if they might give a small overhead. Example: Try to compress the MPO representing the hamiltonian. |
    | 3     | skip_arg_checks | safe! Skip (some) class sanity tests and (function) argument checks.         |
\end{verbatim}
\end{code}

\textbf{Warning}: When unsafe optimizations are enabled, errors will not be detected that easily, debugging is much harder, and you might even get segmentation faults in the compiled parts. Use this kind of optimization only for code which you succesfully ran before with (very) similar parameters and disabled optimizations! Enable this optimization only during the parts of the code where it is really necessary. Check whether it actually helps - if it doesn’t, keep the optimization disabled!
temporary_level

- full name: tenpy.tools.optimization.temporary_level
- parent module: tenpy.tools.optimization
- type: class

Inheritance Diagram

```
temporary_level
```

Methods

```
temporary_level.__init__(temporary_level) Initialize self.
```

class tenpy.tools.optimization.temporary_level(temporary_level)

Bases: object

Context manager to temporarily set the optimization level to a different value.

Parameters temporary_level (int | OptimizationFlag | str | None) – The optimization level to be set during the context. None defaults to the current value of the optimization level.

temporary_level
The optimization level to be set during the context.

Type None | OptimizationFlag

_old_level
Optimization level to be restored at the end of the context manager.

Type OptimizationFlag

Examples

It is recommended to use this context manager in a with statement:

```
# optimization level default
with temporary_level(OptimizationFlag.safe):
    do_some_stuff()  # temporarily have Optimization level `safe`
    # you can even change the optimization level to something else:
    set_level(OptimizationFlag.skip_args_check)
    do_some_really_heavy_stuff()
# here we are back to the optimization level as before the `with ...` statement
```
### Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>get_level()</code></td>
<td>Return the global optimization level.</td>
</tr>
<tr>
<td><code>optimize([level_compare])</code></td>
<td>Called by algorithms to check whether it should (try to) do some optimizations.</td>
</tr>
<tr>
<td><code>set_level([level])</code></td>
<td>Set the global optimization level.</td>
</tr>
<tr>
<td><code>to_OptimizationFlag(level)</code></td>
<td>Convert strings and int to a valid OptimizationFlag.</td>
</tr>
<tr>
<td><code>use_cython([func, replacement, check_doc])</code></td>
<td>Decorator to replace a function with a Cython-equivalent from _npc_helper.pyx.</td>
</tr>
</tbody>
</table>

#### get_level

- full name: `tenpy.tools.optimization.get_level`
- parent module: `tenpy.tools.optimization`
- type: function

```python
tenpy.tools.optimization.get_level()
```

Return the global optimization level.

#### optimize

- full name: `tenpy.tools.optimization.optimize`
- parent module: `tenpy.tools.optimization`
- type: function

```python
tenpy.tools.optimization.optimize(level_compare=<OptimizationFlag.default: 1>)
```

Called by algorithms to check whether it should (try to) do some optimizations.

**Parameters**
- **level_compare** (`OptimizationFlag`) – At which level to start optimization, i.e., how safe the suggested optimization is.

**Returns**
- **optimize** – True if the algorithms should try to optimize, i.e., whether the global “optimization level” is equal or higher than the level to compare to.

**Return type**
- `bool`

#### set_level

- full name: `tenpy.tools.optimization.set_level`
- parent module: `tenpy.tools.optimization`
- type: function

```python
tenpy.tools.optimization.set_level(level=1)
```

Set the global optimization level.

**Parameters**
- **level** (`int | OptimizationFlag | str | None`) – The new global optimization level to be set. `None` defaults to keeping the current level.
to_OptimizationFlag

- full name: tenpy.tools.optimization.to_OptimizationFlag
- parent module: tenpy.tools.optimization
- type: function

```
tenpy.tools.optimization.to_OptimizationFlag(level)
```

Convert strings and int to a valid OptimizationFlag.

None defaults to the current level.

use_cython

- full name: tenpy.tools.optimization.use_cython
- parent module: tenpy.tools.optimization
- type: function

```
tenpy.tools.optimization.use_cython(func=None, replacement=None, check_doc=True)
```

Decorator to replace a function with a Cython-equivalent from _npc_helper.pyx.

This is a decorator, which is supposed to be used in front of function definitions with an @ sign, for example:

```
@use_cython
def my_slow_function(a):
    "some example function with slow python loops"
    result = 0.
    for i in range(a.shape[0]):
        for j in range(a.shape[1]):
            #... heavy calculations ...
            result += np.cos(a[i, j]**2) * (i + j)
    return result
```

This decorator indicates that there is a Cython implementation in the file tenpy/linalg/_npc_helper.pyx, which should have the same signature (i.e. same arguments and return values) as the decorated function, and can be used as a replacement for the decorated function. However, if the cython code could not be compiled on your system (or if the environment variable TENPY_OPTIMIZE is set to negative values, or the environment variable TENPY_NO_CYTHON is “true”), we just pass the previous function.

**Note:** In case that the decorator is used for a class method, the corresponding Cython version needs to have an @cython.binding(True).

**Parameters**

- **func** *(function)* – The defined function
- **replacement** *(string / None)* – The name of the function defined in tenpy/linalg/_npc_helper.pyx which should replace the decorated function. None defaults to the name of the decorated function, e.g., in the above example my_slow_function.
- **check_doc** *(bool)* – If True, we check that the cython version of the function has the exact same doc string (up to a possible first line containing the function signature) to exclude typos and inconsistent versions.

**Returns** **replacement_func** – The function replacing the decorated function func. If the cython code can not be loaded, this is just func, otherwise it’s the cython version specified by replacement.
Return type function

Module description

Optimization options for this library.

Let me start with a quote of “Micheal Jackson” (a programmer, not the musician):

| First rule of optimization: "Don’t do it." |
| Second rule of optimization (for experts only): "Don’t do it yet." |
| Third rule of optimization: "Profile before optimizing." |

Luckily, following the third optimization rule, namely profiling code, is fairly simple in python, see the documentation. If you have a python skript running your code, you can simply call it with python -m "cProfile" -s "tottime" your_skript.py. Alternatively, save the profiling statistics with python -m "cProfile" -o "profile_data.stat" your_skript.py and run these few lines of python code:

```python
import pstats
p = pstats.Pstats("profile_data.stat")
p.sort_stats('cumtime')  # sort by 'cumtime' column
p.print_stats(30)  # prints first 30 entries
```

That being said, I actually did profile and optimize (parts of) the library; and there are a few knobs you can turn to tweak the most out of this library, explained in the following.

1) Simply install the ‘bottleneck’ python package, which allows to optimize slow parts of numpy, most notably ‘NaN’ checking.

2) Figure out which numpy/scipy/python you are using. As explained in Installation instructions, we recommend to use the Python distributed provided by Intel or Anaconda. They ship with numpy and scipy which use Intels MKL library, such that e.g. np.tensordot is parallelized to use multiple cores.

3) In case you didn’t do that yet: some parts of the library are written in both python and Cython with the same interface, so you can simply compile the Cython code, as explained in Installation instructions. Then everything should work the same way from a user perspective, while internally the faster, pre-compiled cython code from tenpy/linalg/_npc_helper.pyx is used. This should also be a safe thing to do. The replacement of the optimized functions is done by the decorator use_cython().

4) One of the great things about python is its dynamical nature - anything can be done at runtime. In that spirit, this module allows to set a global “optimization level” which can be changed dynamically (i.e., during runtime) with set_level(). The library will then try some extra optimization, most notably skip sanity checks of arguments. The possible choices for this global level are given by the OptimizationFlag. The default initial value for the global optimization level can be adjusted by the environment variable TENPY_OPTIMIZE.

**Warning:** When this optimizing is enabled, we skip (some) sanity checks. Thus, errors will not be detected that easily, and debugging is much harder! We recommend to use this kind of optimization only for code which you succesfully have run before with (very) similar parameters! Enable this optimization only during the parts of the code where it is really necessary. The context manager temporary_level can help with that. Check whether it actually helps - if it doesn’t, keep the optimization disabled! Some parts of the library already do that as well (e.g. DMRG after the first sweep).

5) You might want to try some different compile time options for the cython code, set in the setup.py in the top directory of the repository. Since the setup.py reads out the TENPY_OPTIMIZE environment variable, you can simple use an export TENPY_OPTIMIZE=3 (in your bash/terminal) right before compilation. An export TENPY_OPTIMIZE=0 activates profiling hooks instead.
Warning: This increases the probability of getting segmentation faults and anyway might not help that much; in the crucial parts of the cython code, these optimizations are already applied. We do not recommend using this!

```python
tenpy.tools.optimization.bottleneck = None
ntenpy.tools.optimization.have_cython_functions = False

bool whether the import of the cython file tenpy/linalg/_npc_helper.pyx succeeded.
The value is set in the first call of use_cython().
```

## 7.14 version

- **full name**: tenpy.version
- **parent module**: tenpy
- **type**: module

### Module description

Access to version of this library.

The version is provided in the standard python format major.minor.revision as string. Use pkg_resources.parse_version before comparing versions.

```python
tenpy.version.version = '0.7.2'
current release version as a string
tenpy.version.released = False
whether this is a released version or modified
tenpy.version.short_version = 'v0.7.2'
same as version, but with ‘v’ in front
tenpy.version.git_revision = '68eae2c1194f4f4f0d032b92bb0d42ba65e5e504b34'
the hash of the last git commit (if available)
tenpy.version.full_version = '0.7.2.dev55+68eae2c'
if not released additional info with part of git revision
tenpy.version.version_summary = 'tenpy 0.7.2.dev55+68eae2c (not compiled),
git revision 68eae2c1194f4f4f0d032b92bb0d42ba65e5e504b34
summary of the tenpy, python, numpy and scipy versions used'
```
CHAPTER
EIGHT

INDICES AND TABLES

• genindex
• modindex
• cfg-config-index
• cfg-option-index
• search
BIBLIOGRAPHY


[TeNPySource] https://github.com/tenpy/tenpy


[TeNPyForum] Community forum for discussions, FAQ and announcements, https://tenpy.johannes-hauschild.de

[git] “git version control system”, https://git-scm.com A software which we use to keep track of changes in the source code.

[conda] “conda package manger”, https://docs.conda.io/en/latest/ A package and environment management system that allows to easily install (multiple version of) various software, and in particular python packages like TeNPy.


[jupyter] Jupyter notebooks, https://jupyter.org/ An amazing interface for (python) notebooks which can contain both source code, text and outputs in a single file. They provide a good way to get started with python, we use them for examples.


tenpy, 152
  tenpy.algorithms, 153
  tenpy.algorithms.dmrq, 191
  tenpy.algorithms.exact_diag, 218
  tenpy.algorithms.mpo_evolution, 212
  tenpy.algorithms.mps_common, 166
  tenpy.algorithms.network_contractor, 214
  tenpy.algorithms.purification, 211
  tenpy.algorithms.tdvp, 195
  tenpy.algorithms.tebd, 158
  tenpy.algorithms.truncation, 157
  tenpy.linalg, 218
  tenpy.linalg.charges, 273
  tenpy.linalg.lanczos, 300
  tenpy.linalg.np_conserved, 251
  tenpy.linalg.random_matrix, 278
  tenpy.linalg.sparse, 297
  tenpy.linalg.svd_robust, 275
  tenpy.models, 300
  tenpy.models.fermions_spinless, 486
  tenpy.models.haldane, 516
  tenpy.models.hofstadter, 515
  tenpy.models.hubbard, 513
  tenpy.models.lattice, 400
  tenpy.models.model, 429
  tenpy.models.spins, 471
  tenpy.models.spins_nnn, 472
  tenpy.models.tf_ising, 443
  tenpy.models.toric_code, 527
  tenpy.models.xxz_chain, 457
  tenpy.networks, 527
  tenpy.networks.mpo, 587
  tenpy.networks.mps, 576
  tenpy.networks.purification_mps, 607
  tenpy.networks.site, 566
  tenpy.networks.terms, 606
  tenpy.tools, 609
  tenpy.tools.events, 631
  tenpy.tools.fit, 647
  tenpy.tools.hdf5_io, 621
  tenpy.tools.math, 643
  tenpy.tools.misc, 639
  tenpy.tools.optimization, 656
  tenpy.tools.params, 627
  tenpy.tools.process, 650
  tenpy.tools.string, 648
  tenpy.version, 657
**CONFIG INDEX**

A
ApplyMPO, ??

B
BoseHubbardModel, ??
BosonicHaldaneModel, ??

C
Config, ??
CouplingMPOModel, ??

D
DMRG, ??
DMRGEngine, ??

E
ExpMPOEvolution, ??

F
FermiHubbardModel, ??
FermionicHaldaneModel, ??
FermionModel, ??

H
HofstadterBosons, ??
HofstadterFermions, ??

L
Lanczos, ??
LanczosEvolution, ??

M
Mixer, ??
MPS_compress (master), ??
MPS_compress, ??
MPS_compress, ??

R
RandomUnitaryEvolution, ??

S
SingleSiteDMRGEngine, ??

SpinChainNNN, ??
SpinChainNNN2, ??
SpinModel, ??
Sweep, ??

T
TDVP, ??
TEBD, ??
TFIModel, ??
ToricCode, ??
truncation, ??
TwoSiteDMRGEngine, ??

V
VariationalApplyMPO, ??
VariationalCompression, ??

X
XXZChain, ??

Z
ZipUpApplyMPO, ??
ApplyMPO
combine (Sweep), ??
compression_method (MPO.apply), ??
init_env_data (multiple definitions), ??
init_env_data (DMRGEEngine.init_env), ??
init_env_data (EngineCombine.init_env), 174
init_env_data (EngineFracture.init_env), 182
init_env_data (SingleSiteDMRGEEngine.init_env), ??
init_env_data (TwoSiteDMRGEEngine.init_env), ??
lanczos_params (Sweep), ??
m_temp (MPO.apply_zipup), ??
N_sweeps (VariationalCompression), ??
_orthogonal_to (multiple definitions), ??
_orthogonal_to (DMRGEEngine.init_env), ??
_orthogonal_to (EngineCombine.init_env), 174
_orthogonal_to (EngineFracture.init_env), 182
_orthogonal_to (SingleSiteDMRGEEngine.init_env), ??
_orthogonal_to (TwoSiteDMRGEEngine.init_env), ??
start_env (multiple definitions), ??
start_env (DMRGEEngine.init_env), ??
start_env (EngineCombine.init_env), 174
start_env (EngineFracture.init_env), 182
start_env (SingleSiteDMRGEEngine.init_env), ??
start_env (TwoSiteDMRGEEngine.init_env), ??
sweep_0 (multiple definitions), ??
sweep_0 (Sweep.reset_stats), ??
sweep_0 (VariationalApplyMPO.reset_stats), ??
sweep_0 (VariationalCompression.reset_stats), ??
sweep_0 (PurificationApplyMPO.reset_stats), 199
trunc_params (multiple definitions), ??
trunc_params (MPO.apply), ??
trunc_params (MPO.apply_zipup), ??
trunc_params (VariationalCompression), ??
trunc_params (Sweep), ??
trunc_weight (MPO.apply_zipup), ??
verbose (multiple definitions), ??
verbose (Sweep), ??

BoseHubbardModel
bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIChain.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionChain.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
bc_x (BosonicHaldaneModel.init_lattice), ??
bc_x (FermionicHaldaneModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (CouplingMPOModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChainNNN.init_lattice), ??
bc_x (SpinChainNNN2.init_lattice), ??
bc_x (TFIChain.init_lattice), 442
bc_x (TFIModel.init_lattice), ??
bc_x (ToricCode.init_lattice), ??
bc_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionChain.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (BosonicHaldaneModel.init_lattice), ??
bc_y (FermionicHaldaneModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (FermiHubbardChain.init_lattice), 512
bc_y (FermiHubbardModel.init_lattice), ??
bc_y (CouplingMPOModel.init_lattice), ??
bc_y (SpinModel.init_lattice), 470
bc_y (SpinModelNNN.init_lattice), ??
bc_y (SpinModelNNN2.init_lattice), ??
bc_y (TFICModel.init_lattice), ??
bc_y (TFIModel.init_lattice), ??
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
conserve (BosonicHubbardModel), ??
explicit_plus_hc (CouplingMPOModel), ??
filling (BosonicHubbardModel), ??
L (multiple definitions), 485
L (FermionChain.init_lattice), 485
L (FermionModel.init_lattice), ??
L (BosonicHaldaneModel.init_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinModel.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinModelNNN.init_lattice), ??
L (SpinModelNNN2.init_lattice), ??
L (TFICModel.init_lattice), ??
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionModel.init_lattice), ??
lattice (BosonicHaldaneModel.init_lattice), ??
lattice (FermionicHaldaneModel.init_lattice), ??
lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardChain.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ??
lattice (FermiHubbardChain.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOModel.init_lattice), ??
lattice (SpinModel.init_lattice), ??
lattice (SpinModelNNN.init_lattice), ??
lattice (SpinModelNNN2.init_lattice), ??
lattice (TFICModel.init_lattice), ??
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
Lx (multiple definitions), 485
Lx (FermionChain.init_lattice), 485
Lx (FermionModel.init_lattice), ??
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Lx (SpinModel.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinModelNNN.init_lattice), ??
Lx (SpinModelNNN2.init_lattice), ??
Lx (TFICModel.init_lattice), 442
Lx (TFIModel.init_lattice), ??
Lx (ToricCode.init_lattice), ??
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (HofstadterFermions.init_lattice), ??
Ly (BoseHubbardChain.init_lattice), 499
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), 512
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinModel.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinModelNNN.init_lattice), ??
Ly (SpinModelNNN2.init_lattice), ??
Ly (TFICModel.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
lattice (BoseHubbardModel), ??
n_max (BoseHubbardModel), ??
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??  
order (BosonicHaldaneModel.init_lattice), ??  
order (FermionicHaldaneModel.init_lattice), ??  
order (HofstadterBosons.init_lattice), ??  
order (HofstadterFermions.init_lattice), ??  
order (BoseHubbardChain.init_lattice), 499  
order (BoseHubbardModel.init_lattice), ??  
order (FermiHubbardChain.init_lattice), 512  
order (FermiHubbardModel.init_lattice), ??  
order (CouplingMPOModel.init_lattice), ??  
order (SpinChain.init_lattice), 470  
order (SpinModel.init_lattice), ??  
order (SpinChainNNN.init_lattice), ??  
order (SpinChainNNN2.init_lattice), ??  
order (TFIClassifier.init_lattice), ??  
order (ToricCode.init_lattice), ??  
order (XXZChain2.init_lattice), 456  
sort_mpo_legs (CouplingMPOModel), ??  
t (BoseHubbardModel), ??  
U (BoseHubbardModel), ??  
V (BoseHubbardModel), ??  
verbose (Config), ??  

BosonicHaldaneModel  
bc_MPS (multiple definitions), 485  
bc_MPS (FermionChain.init_lattice), 485  
bc_MPS (FermionModel.init_lattice), ??  
bc_MPS (BosonicHaldaneModel.init_lattice), ??  
bc_MPS (FermionicHaldaneModel.init_lattice), ??  
bc_MPS (HofstadterBosons.init_lattice), ??  
bc_MPS (HofstadterFermions.init_lattice), ??  
bc_MPS (BoseHubbardChain.init_lattice), 499  
bc_MPS (BoseHubbardModel.init_lattice), ??  
bc_MPS (FermiHubbardChain.init_lattice), 512  
bc_MPS (FermiHubbardModel.init_lattice), ??  
bc_MPS (CouplingMPOModel.init_lattice), ??  
bc_MPS (SpinChain.init_lattice), 470  
bc_MPS (SpinModel.init_lattice), ??  
bc_MPS (SpinChainNNN.init_lattice), ??  
bc_MPS (SpinChainNNN2.init_lattice), ??  
bc_MPS (TFIClassifier.init_lattice), 442  
bc_MPS (ToricCode.init_lattice), ??  
bc_MPS (XXZChain2.init_lattice), 456  
bc_x (multiple definitions), 485  
bc_x (FermionChain.init_lattice), 485  
bc_x (FermionModel.init_lattice), ??  
bc_x (BosonicHaldaneModel.init_lattice), ??  
bc_x (FermionicHaldaneModel.init_lattice), ??  
bc_x (HofstadterBosons.init_lattice), ??  
bc_x (HofstadterFermions.init_lattice), ??  
bc_x (BoseHubbardChain.init_lattice), 499  
bc_x (BoseHubbardModel.init_lattice), ??  

bc_y (multiple definitions), 485  
bc_y (FermionChain.init_lattice), 485  
bc_y (FermionModel.init_lattice), ??  
bc_y (BosonicHaldaneModel.init_lattice), ??  
bc_y (FermionicHaldaneModel.init_lattice), ??  
bc_y (HofstadterBosons.init_lattice), ??  
bc_y (HofstadterFermions.init_lattice), ??  
bc_y (BoseHubbardChain.init_lattice), 499  
bc_y (BoseHubbardModel.init_lattice), ??  
bc_y (FermiHubbardChain.init_lattice), 512  
bc_y (FermiHubbardModel.init_lattice), ??  
bc_y (CouplingMPOModel.init_lattice), ??  
bc_y (SpinChain.init_lattice), 470  
bc_y (SpinModel.init_lattice), ??  
bc_y (SpinChainNNN.init_lattice), ??  
bc_y (SpinChainNNN2.init_lattice), ??  
bc_y (TFIClassifier.init_lattice), 442  
bc_y (ToricCode.init_lattice), ??  
bc_y (XXZChain2.init_lattice), 456  
conserve (BosonicHaldaneModel), ??  
extricital_plus_hc (CouplingMPOModel), ??  
L (multiple definitions), 485  
L (FermionChain.init_lattice), 485  
L (FermionModel.init_lattice), ??  
L (BosonicHaldaneModel.init_lattice), ??  
L (FermionicHaldaneModel.init_lattice), ??  
L (HofstadterBosons.init_lattice), ??  
L (HofstadterFermions.init_lattice), ??  
L (BoseHubbardChain.init_lattice), 499  
L (BoseHubbardModel.init_lattice), ??  
L (FermiHubbardChain.init_lattice), 512  
L (FermiHubbardModel.init_lattice), ??  
L (CouplingMPOModel.init_lattice), ??  
L (SpinChain.init_lattice), 470  
L (SpinModel.init_lattice), ??  
L (SpinChainNNN.init_lattice), ??  
L (SpinChainNNN2.init_lattice), ??  
L (TFIClassifier.init_lattice), 442  
L (ToricCode.init_lattice), ??  
L (XXZChain2.init_lattice), 456  
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionModel.init_lattice), ??
lattice (BosonicHaldaneModel.init_lattice), ??
lattice (FermionicHaldaneModel.init_lattice), ??
lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardChain.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ??
lattice (FermiHubbardModel.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOModel.init_lattice), ??
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice), ??
lattice (SpinChainNNN.init_lattice), ??
lattice (SpinChainNNN2.init_lattice), ??
lattice (TFIChaın.init_lattice), 442
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
Lx (multiple definitions), 485
Lx (FermionChain.init_lattice), 485
Lx (FermionModel.init_lattice), ??
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Lx (SpinChain.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinChainNNN.init_lattice), ??
Lx (SpinChainNNN2.init_lattice), ??
Lx (TFIChaın.init_lattice), 442
Lx (TFIModel.init_lattice), ??
Lx (ToricCode.init_lattice), ??
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (HofstadterFermions.init_lattice), ??
Ly (BoseHubbardChain.init_lattice), 499
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), 512
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNNN.init_lattice), ??
Ly (SpinChainNNN2.init_lattice), ??
Ly (TFIChaın.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
mu (BosonicHaldaneModel), ??
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardChain.init_lattice), 499
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardModel.init_lattice), 512
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (SpinChainNNN2.init_lattice), ??
order (TFIChaın.init_lattice), 442
order (TFIModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), ??
sort_mpo_legs (CouplingMPOModel), ??
t1 (BosonicHaldaneModel), ??
t2 (BosonicHaldaneModel), ??
V (BosonicHaldaneModel), ??
verbose (Config), ??

Config
verbose (Config), ??

CouplingMPOModel
bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIChaın.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
b erot (XXXChain2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionChain.init_lattice), 485
bc_x (FermiHubbardModel.init_lattice), ??
b_c_x (BosonicHaldaneModel.init_lattice), ??
b_c_x (FermionicHaldaneModel.init_lattice), ??
b c_x (HofstadterBosons.init_lattice), ??
b c_x (HofstadterFermions.init_lattice), ??
b c_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
b c_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
b c_x (CouplingMPOModel.init_lattice), ??
b c_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
b_c_x (SpinChainNN.init_lattice), ??
b c_x (SpinChainNN2.init_lattice), ??
b c_x (TFIChain.init_lattice), 442
bc_x (TFIModel.init_lattice), ??
b c_x (ToricCode.init_lattice), ??
b c_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionChain.init_lattice), 485
bc_y (FermiHubbardModel.init_lattice), ??
b c_y (BosonicHaldaneModel.init_lattice), ??
b c_y (FermionicHaldaneModel.init_lattice), ??
b c_y (HofstadterBosons.init_lattice), ??
b c_y (HofstadterFermions.init_lattice), ??
b c_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
b c_y (BosonicHubbardModel.init_lattice), ??
b c_y (FermiHubbardChain.init_lattice), 499
bc_y (FermiHubbardModel.init_lattice), ??
b c_y (SpinChainNN2.init_lattice), ??
b c_y (SpinChainNN2.init_lattice), ??
b c_y (TFIChain.init_lattice), 442
bc_y (TFIModel.init_lattice), ??
b c_y (ToricCode.init_lattice), ??
b c_y (XXZChain2.init_lattice), 456
explicit_plus_hc (CouplingMPOModel.init_lattice), ??
L (multiple definitions), 485
L (FermionChain.init_lattice), 485
L (FermionModel.init_lattice), ??
L (BosonicHaldaneModel.init_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNN.init_lattice), ??
L (SpinChainNN2.init_lattice), ??
L (TFIChain.init_lattice), 442
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermiHubbardModel.init_lattice), ??
lattice (BosonicHaldaneModel.init_lattice), ??
lattice (FermionicHaldaneModel.init_lattice), ??
lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardChain.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ??
lattice (FermiHubbardChain.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOModel.init_lattice), ??
lattice (SpinModel.init_lattice), 470
lattice (SpinChain.init_lattice), ??
lattice (SpinChainNN.init_lattice), ??
lattice (SpinChainNN2.init_lattice), ??
lattice (TFIChain.init_lattice), 442
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
Lx (multiple definitions), 485
Lx (FermionChain.init_lattice), 485
Lx (FermiHubbardModel.init_lattice), ??
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Lx (SpinChain.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinChainNN.init_lattice), ??
Lx (SpinChainNN2.init_lattice), ??
Lx (TFIChain.init_lattice), 442
Lx (TFIModel.init_lattice), ??
Lx (ToricCode.init_lattice), ??
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionChain.init_lattice), 485
Ly (FermiHubbardModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (HofstadterFermions.init_lattice), ??
Ly (BoseHubbardChain.init_lattice), 499
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), 512
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNNN.init_lattice), ??
Ly (SpinChainNNN2.init_lattice), ??
Ly (TFCIChain.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardChain.init_lattice), 499
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardChain.init_lattice), 512
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (SpinChainNNN2.init_lattice), ??
order (TFCIChain.init_lattice), 442
order (TFIModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
sort_mpo_legs (CouplingMPOModel), ??
verbose (Config), ??

diag_method (SingleSiteDMRGEngine.diag), ??
diag_method (SingleSiteDMRGEngine.run), ??
diag_method (TwoSiteDMRGEngine.diag), ??
diag_method (TwoSiteDMRGEngine.run), ??
E_tol_max (multiple definitions), ??
E_tol_max (DMRGEngine.run), ??
E_tol_max (EngineCombine.run), 176
E_tol_max (EngineFracture.run), 184
E_tol_max (SingleSiteDMRGEngine.run), ??
E_tol_max (TwoSiteDMRGEngine.run), ??
E_tol_min (multiple definitions), ??
E_tol_min (DMRGEngine.run), ??
E_tol_min (EngineCombine.run), 176
E_tol_min (EngineFracture.run), 184
E_tol_min (SingleSiteDMRGEngine.run), ??
E_tol_min (TwoSiteDMRGEngine.run), ??
init_env_data (multiple definitions), ??
init_env_data (DMRGEngine.init_env), ??
init_env_data (EngineCombine.init_env), 174
init_env_data (EngineFracture.init_env), 182
init_env_data (SingleSiteDMRGEngine.init_env), ??
init_env_data (TwoSiteDMRGEngine.init_env), ??
init_env_data (Sweep.init_env), ??
lanczos_params (Sweep), ??
max_E_err (multiple definitions), ??
max_E_err (DMRGEngine.run), ??
max_E_err (EngineCombine.run), 176
max_E_err (EngineFracture.run), 184
max_E_err (SingleSiteDMRGEngine.run), ??
max_E_err (TwoSiteDMRGEngine.run), ??
max_hours (multiple definitions), ??
max_hours (DMRGEngine.run), ??
max_hours (EngineCombine.run), 176
max_hours (EngineFracture.run), 184
max_hours (SingleSiteDMRGEngine.run), ??
max_hours (TwoSiteDMRGEngine.run), ??
max_N_for_ED (multiple definitions), ??
max_N_for_ED (DMRGEngine.diag), ??
max_N_for_ED (EngineCombine.diag), 172
max_N_for_ED (EngineFracture.diag), 180
max_N_for_ED (SingleSiteDMRGEngine.diag), ??
max_N_for_ED (TwoSiteDMRGEngine.diag), ??
max_S_err (multiple definitions), ??
max_S_err (DMRGEngine.run), ??
max_S_err (EngineCombine.run), 177
max_S_err (EngineFracture.run), 184
max_S_err (SingleSiteDMRGEngine.run), ??

DMRG
active_sites (run), ??
chi_list (multiple definitions), ??
chi_list (DMRGEngine.reset_stats), ??
chi_list (EngineCombine.reset_stats), 176
chi_list (EngineFracture.reset_stats), 184
chi_list (SingleSiteDMRGEngine.reset_stats), ??
chi_list (TwoSiteDMRGEngine.reset_stats), ??
combine (Sweep), ??
diag_method (multiple definitions), ??
diag_method (DMRGEngine.run), ??
diag_method (DMRGEngine.diag), ??
diag_method (EngineCombine.diag), 173
diag_method (EngineCombine.run), 176
diag_method (EngineFracture.diag), 180
diag_method (EngineFracture.run), 184
max_S_err (TwoSiteDMRGEngine.run), ??
max_sweeps (multiple definitions), ??
max_sweeps (DMRGEngine.run), ??
max_sweeps (EngineCombine.run), 177
max_sweeps (EngineFracture.run), 184
max_sweeps (SingleSiteDMRGEngine.run), ??
max_sweeps (TwoSiteDMRGEngine.run), ??
min_sweeps (multiple definitions), ??
min_sweeps (DMRGEngine.run), ??
min_sweeps (EngineCombine.run), 177
min_sweeps (EngineFracture.run), 185
min_sweeps (SingleSiteDMRGEngine.run), ??
min_sweeps (TwoSiteDMRGEngine.run), ??
mixer (multiple definitions), ??
mixer (DMRGEngine.mixer_activate), ??
mixer (EngineCombine.mixer_activate), 174
mixer (EngineFracture.mixer_activate), 182
mixer (SingleSiteDMRGEngine.mixer_activate), ??
mixer (TwoSiteDMRGEngine.mixer_activate), ??
mixer_params (multiple definitions), ??
mixer_params (DMRGEngine.mixer_activate), ??
mixer_params (EngineCombine.mixer_activate), ??
mixer_params (EngineFracture.mixer_activate), 182
mixer_params (SingleSiteDMRGEngine.mixer_activate), ??
mixer_params (TwoSiteDMRGEngine.mixer_activate), ??
N_sweeps_check (multiple definitions), ??
N_sweeps_check (DMRGEngine.run), ??
N_sweeps_check (EngineCombine.run), 177
N_sweeps_check (EngineFracture.run), 185
N_sweeps_check (SingleSiteDMRGEngine.run), ??
N_sweeps_check (TwoSiteDMRGEngine.run), ??
norm_tol (multiple definitions), ??
norm_tol (DMRGEngine.run), ??
norm_tol (EngineCombine.run), 177
norm_tol (EngineFracture.run), 185
norm_tol (SingleSiteDMRGEngine.run), ??
norm_tol (TwoSiteDMRGEngine.run), ??
norm_tol_iter (multiple definitions), ??
norm_tol_iter (DMRGEngine.run), ??
norm_tol_iter (EngineCombine.run), 177
norm_tol_iter (EngineFracture.run), 185
norm_tol_iter (SingleSiteDMRGEngine.run), ??
norm_tol_iter (TwoSiteDMRGEngine.run), ??
orthogonal_to (multiple definitions), ??
orthogonal_to (DMRGEngine.init_env), ??
orthogonal_to (EngineCombine.init_env), 174
orthogonal_to (EngineFracture.init_env), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
P_tol_max (multiple definitions), ??
P_tol_max (DMRGEngine.run), ??
P_tol_max (EngineCombine.run), 177
P_tol_max (EngineFracture.run), 185
P_tol_max (SingleSiteDMRGEngine.run), ??
P_tol_max (TwoSiteDMRGEngine.run), ??
P_tol_min (multiple definitions), ??
P_tol_min (DMRGEngine.run), ??
P_tol_min (EngineCombine.run), 177
P_tol_min (EngineFracture.run), 185
P_tol_min (SingleSiteDMRGEngine.run), ??
P_tol_min (TwoSiteDMRGEngine.run), ??
P_tol_to_trunc (multiple definitions), ??
P_tol_to_trunc (DMRGEngine.run), ??
P_tol_to_trunc (EngineCombine.run), 177
P_tol_to_trunc (EngineFracture.run), 185
P_tol_to_trunc (SingleSiteDMRGEngine.run), ??
P_tol_to_trunc (TwoSiteDMRGEngine.run), ??
start_env (multiple definitions), ??
start_env (DMRGEngine.init_env), ??
start_env (EngineCombine.init_env), 174
start_env (EngineFracture.init_env), 182
start_env (SingleSiteDMRGEngine.init_env), ??
start_env (TwoSiteDMRGEngine.init_env), ??
start_env (Sweep.init_env), ??
sweep_0 (multiple definitions), ??
sweep_0 (DMRGEngine.reset_stats), ??
sweep_0 (EngineCombine.reset_stats), 176
sweep_0 (EngineFracture.reset_stats), 184
sweep_0 (SingleSiteDMRGEngine.reset_stats), ??
sweep_0 (TwoSiteDMRGEngine.reset_stats), ??
sweep_0 (Sweep.reset_stats), ??
sweep_0 (VariationalApplyMPO.reset_stats), ??
sweep_0 (VariationalCompression.reset_stats), ??
sweep_0 (PurificationApplyMPO.reset_stats), 199
trunc_params (Sweep), ??
update_env (multiple definitions), ??
update_env (DMRGEngine.run), ??
update_env (EngineCombine.run), 177
update_env (EngineFracture.run), 185
update_env (SingleSiteDMRGEngine.run), ??
update_env (TwoSiteDMRGEngine.run), ??
verbose (multiple definitions), ??
verbose (Sweep), ??
verbose (Config), ??

DMRGEngine
chi_list (multiple definitions), ??
chi_list (DMRGEngine.reset_stats), ??
chi_list (EngineCombine.reset_stats), 176
chi_list (EngineFracture.reset_stats), 184
chi_list (SingleSiteDMRGEngine.reset_stats), ??
chi_list (TwoSiteDMRGEngine.reset_stats), ??
combine (Sweep), ??
diag_method (multiple definitions), ??
diag_method (DMRGEngine.run), ??
diag_method (DMRGEngine.diag), ??
diag_method (EngineCombine.diag), 173
diag_method (EngineCombine.run), 176
diag_method (EngineFracture.diag), 180
diag_method (EngineFracture.run), 184
diag_method (SingleSiteDMRGEngine.diag), ??
diag_method (SingleSiteDMRGEngine.run), ??
diag_method (TwoSiteDMRGEngine.diag), ??
diag_method (TwoSiteDMRGEngine.run), ??
E_tol_max (multiple definitions), ??
E_tol_max (DMRGEngine.run), ??
E_tol_max (EngineCombine.run), 176
E_tol_max (EngineFracture.run), 184
E_tol_max (SingleSiteDMRGEngine.run), ??
E_tol_max (TwoSiteDMRGEngine.run), ??
E_tol_min (multiple definitions), ??
E_tol_min (DMRGEngine.run), ??
E_tol_min (EngineCombine.run), 176
E_tol_min (EngineFracture.run), 184
E_tol_min (SingleSiteDMRGEngine.run), ??
E_tol_min (TwoSiteDMRGEngine.run), ??
E_tol_to_trunc (multiple definitions), ??
E_tol_to_trunc (DMRGEngine.run), ??
E_tol_to_trunc (EngineCombine.run), 176
E_tol_to_trunc (EngineFracture.run), 184
E_tol_to_trunc (SingleSiteDMRGEngine.run), ??
E_tol_to_trunc (TwoSiteDMRGEngine.run), ??
ininit_env_data (multiple definitions), ??
ininit_env_data (DMRGEngine.init_env), ??
ininit_env_data (EngineCombine.init_env), 174
ininit_env_data (EngineFracture.init_env), 182
ininit_env_data (SingleSiteDMRGEngine.init_env), ??
ininit_env_data (TwoSiteDMRGEngine.init_env), ??
lanczos_params (Sweep), ??
max_E_err (multiple definitions), ??
max_E_err (DMRGEngine.run), ??
max_E_err (EngineCombine.run), 176
max_E_err (EngineFracture.run), 184
max_E_err (SingleSiteDMRGEngine.run), ??
max_E_err (TwoSiteDMRGEngine.run), ??
max_hours (multiple definitions), ??
max_hours (DMRGEngine.run), ??
max_hours (EngineCombine.run), 176
max_hours (EngineFracture.run), 184
max_hours (SingleSiteDMRGEngine.run), ??
max_hours (TwoSiteDMRGEngine.run), ??
max_N_for_ED (multiple definitions), ??
max_N_for_ED (DMRGEngine.diag), ??
max_N_for_ED (EngineCombine.diag), 172
max_N_for_ED (EngineFracture.diag), 180
max_N_for_ED (SingleSiteDMRGEngine.diag), ??
max_N_for_ED (TwoSiteDMRGEngine.diag), ??
max_s_err (multiple definitions), ??
max_s_err (DMRGEngine.run), ??
max_s_err (EngineCombine.run), 177
max_s_err (EngineFracture.run), 184
max_s_err (SingleSiteDMRGEngine.run), ??
max_s_err (TwoSiteDMRGEngine.run), ??
max_sweeps (multiple definitions), ??
max_sweeps (DMRGEngine.run), ??
max_sweeps (EngineCombine.run), 177
max_sweeps (EngineFracture.run), 184
max_sweeps (SingleSiteDMRGEngine.run), ??
max_sweeps (TwoSiteDMRGEngine.run), ??
min_sweeps (multiple definitions), ??
min_sweeps (DMRGEngine.run), ??
min_sweeps (EngineCombine.run), 177
min_sweeps (EngineFracture.run), 185
min_sweeps (SingleSiteDMRGEngine.run), ??
min_sweeps (TwoSiteDMRGEngine.run), ??
N_sweeps_check (multiple definitions), ??
N_sweeps_check (DMRGEngine.run), ??
N_sweeps_check (EngineCombine.run), 177
N_sweeps_check (EngineFracture.run), 185
N_sweeps_check (SingleSiteDMRGEngine.run), ??
N_sweeps_check (TwoSiteDMRGEngine.run), ??
norm_tol (multiple definitions), ??
norm_tol (DMRGEngine.run), ??
norm_tol (EngineCombine.run), 177
norm_tol (EngineFracture.run), 185
norm_tol (SingleSiteDMRGEngine.run), ??
norm_tol (TwoSiteDMRGEngine.run), ??
norm_tol_iter (multiple definitions), ??
norm_tol_iter (DMRGEngine.run), ??
norm_tol_iter (EngineCombine.run), 177
norm_tol_iter (EngineFracture.run), 185
norm_tol_iter (SingleSiteDMRGEngine.run), ??
norm_tol_iter (TwoSiteDMRGEngine.run), ??
orthogonal_to (multiple definitions), ??
orthogonal_to (DMRGEngine.init_env), ??
orthogonal_to (EngineCombine.init_env), 174
orthogonal_to (EngineFracture.init_env), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
orthogonal_to (Sweep.init_env), ??
P_tol_max (multiple definitions), ??
P_tol_max (DMRGEngine.run), ??
P_tol_max (EngineCombine.run), 177
P_tol_max (EngineFracture.run), 185
P_tol_max (SingleSiteDMRGEngine.run), ??
P_tol_max (TwoSiteDMRGEngine.run), ??
P_tol_min (multiple definitions), ??
P_tol_min (DMRGEngine.run), ??
P_tol_min (EngineCombine.run), 177
P_tol_min (EngineFracture.run), 184
P_tol_min (SingleSiteDMRGEngine.run), ??
P_tol_min (TwoSiteDMRGEngine.run), ??

P_tol_min (EngineFracture.run), 185
P_tol_min (SingleSiteDMRGEngine.run), ??
P_tol_min (TwoSiteDMRGEngine.run), ??
P_tol_to_trunc (multiple definitions), ??
P_tol_to_trunc (DMRGEngine.run), ??
P_tol_to_trunc (EngineCombine.run), 177
P_tol_to_trunc (EngineFracture.run), 185
P_tol_to_trunc (SingleSiteDMRGEngine.run), ??
P_tol_to_trunc (TwoSiteDMRGEngine.run), ??
start_env (multiple definitions), ??
start_env (DMRGEngine_init_env), ??
start_env (EngineCombine_init_env), 174
start_env (EngineFracture_init_env), 182
start_env (SingleSiteDMRGEngine_init_env), ??
start_env (TwoSiteDMRGEngine_init_env), ??
start_env (Sweep.init_env), ??
sweep_0 (multiple definitions), ??
sweep_0 (DMRGEngine.reset_stats), ??
sweep_0 (EngineCombine.reset_stats), 176
sweep_0 (EngineFracture.reset_stats), 184
sweep_0 (SingleSiteDMRGEngine.reset_stats), ??
sweep_0 (TwoSiteDMRGEngine.reset_stats), ??
sweep_0 (Sweep.reset_stats), ??
sweep_0 (VariationalApplyMPO.reset_stats), ??
sweep_0 (VariationalCompression.reset_stats), ??
sweep_0 (PurificationApplyMPO.reset_stats), 199
trunc_params (Sweep), ??
update_env (multiple definitions), ??
update_env (DMRGEngine.run), ??
update_env (EngineCombine.run), 177
update_env (EngineFracture.run), 185
update_env (SingleSiteDMRGEngine.run), ??
update_env (TwoSiteDMRGEngine.run), ??
verbose (multiple definitions), ??
verbose (Sweep), ??
verbose (Config), ??

ExpMPOEvolution

approximation (ExpMPOEvolution.run), ??
combine (Sweep), ??
compression_method (MPO.apply), ??
dt (ExpMPOEvolution.run), ??
init_env_data (multiple definitions), ??
init_env_data (DMRGEngine.init_env), ??
init_env_data (EngineCombine.init_env), 174
init_env_data (EngineFracture.init_env), 182
init_env_data (SingleSiteDMRGEngine.init_env), ??
init_env_data (TwoSiteDMRGEngine.init_env), ??
lanczos_params (Sweep), ??
m_temp (MPO.apply_zipup), ??
N_steps (ExpMPOEvolution.run), ??
N_sweeps (VariationalCompression), ??

FermiHubbardModel

bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFICinit_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
FermionicHaldaneModel

bc_MPS (CouplingMPOModel.init_lattice), 472
bc_MPS (SpinMPOModel.init_lattice), 470
bc_MPS (SpinMPOModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFCModel.init_lattice), 442
bc_MPS (TFCModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionChain.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
b_c_x (FermionModel.init_lattice), ??
b_c_x (FermionicHaldaneModel.init_lattice), ??
b_c_x (HofstadterBosons.init_lattice), ??
b_c_x (SpinChainNNN2.init_lattice), ??
b_c_x (TFIModel.init_lattice), 442
bc_x (TFIModel.init_lattice), ??
b_c_x (ToricCode.init_lattice), ??
b_c_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionModel.init_lattice), 485
bc_y (FermionicHaldaneModel.init_lattice), ??
b_c_y (FermionicHaldaneModel.init_lattice), ??
b_c_y (HofstadterBosons.init_lattice), ??
b_c_y (HofstadterFermions.init_lattice), ??
b_c_y (SpinChainNNN.init_lattice), ??
b_c_y (SpinChainNNN2.init_lattice), ??
b_c_y (TFIModel.init_lattice), 442
bc_y (TFIModel.init_lattice), ??
b_c_y (ToricCode.init_lattice), ??
b_c_y (XXZChain2.init_lattice), 456

bc_mps (multiple definitions), 485
bc_mps (FermionModel.init_lattice), 485
bc_mps (FermionicHaldaneModel.init_lattice), ??
bc_mps (HofstadterBosons.init_lattice), ??
b_c_mps (HofstadterFermions.init_lattice), ??
b_c_mps (HofstadterBosons.init_lattice), ??
b_c_mps (HofstadterFermions.init_lattice), ??
b_c_mps (BosonicHaldaneModel.init_lattice), ??
b_c_mps (FermionicHaldaneModel.init_lattice), ??
b_c_mps (FermionicHaldaneModel.init_lattice), ??
b_c_mps (FermionicHaldaneModel.init_lattice), ??
b_c_mps (FermionicHaldaneModel.init_lattice), ??

TeNPy, Release 0.7.2.dev55+68eae2c

Config Option Index 679
L (BosonicHaldaneModel.init_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNNN.init_lattice), ??
L (SpinChainNNN2.init_lattice), ??
L (TFICModel.init_lattice), 442
L (TFICModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionicHaldaneModel.init_lattice), ??
lattice (BosonicHaldaneModel.init_lattice), ??
lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardModel.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ??
lattice (FermiHubbardChain.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOModel.init_lattice), ??
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice), ??
lattice (SpinChainNNN.init_lattice), ??
lattice (SpinChainNNN2.init_lattice), ??
lattice (TFIChain.init_lattice), 442
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice), ??
lattice (SpinChainNNN.init_lattice), ??
lattice (SpinChainNNN2.init_lattice), ??
lattice (TFICModel.init_lattice), 442
lattice (TFICModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
mu (FermionicHaldaneModel), ??
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionicHaldaneModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardModel.init_lattice), 499
order (BoseHubbardChain.init_lattice), ??
order (FermiHubbardChain.init_lattice), 512
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (SpinChainNNN2.init_lattice), ??
order (TFIModel.init_lattice), 442
order (TFIModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
sort_mpo_legs (CouplingMPOModel), ??
t1 (FermionicHaldaneModel), ??
t2 (FermionicHaldaneModel), ??
V (FermionicHaldaneModel), ??
verbose (Config), ??

FermionModel
bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardModel.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOM.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNN.init_lattice), ??
bc_MPS (SpinChainNN2.init_lattice), ??
bc_MPS (TFIModel.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
cbc_x (multiple definitions), 485
cbc_x (FermionChain.init_lattice), 485
cbc_x (FermionModel.init_lattice), ??
cbc_x (BosonicHaldaneModel.init_lattice), ??
cbc_x (HofstadterBosons.init_lattice), ??
cbc_x (HofstadterFermions.init_lattice), ??
cbc_x (BoseHubbardChain.init_lattice), 499
cbc_x (BoseHubbardModel.init_lattice), ??
cbc_x (BoseHubbardModel.init_lattice), 512
cbc_x (FermiHubbardChain.init_lattice), ??
cbc_x (FermiHubbardModel.init_lattice), ??
cbc_x (CouplingMPOM.init_lattice), ??
cbc_x (SpinChain.init_lattice), 470
cbc_x (SpinModel.init_lattice), ??
cbc_x (SpinChainNN.init_lattice), ??
cbc_x (SpinChainNN2.init_lattice), ??
cbc_x (TFIChain.init_lattice), 442
cbc_x (TFIModel.init_lattice), ??
cbc_x (ToricCode.init_lattice), ??
cbc_x (XXZChain2.init_lattice), 456
cbc_y (multiple definitions), 485
cbc_y (FermionChain.init_lattice), 485
cbc_y (FermionModel.init_lattice), ??
cbc_y (BosonicHaldaneModel.init_lattice), ??
cbc_y (FermionicHaldaneModel.init_lattice), ??
cbc_y (HofstadterBosons.init_lattice), ??
cbc_y (HofstadterFermions.init_lattice), ??
cbc_y (BoseHubbardChain.init_lattice), 499
cbc_y (BoseHubbardModel.init_lattice), ??
cbc_y (FermiHubbardChain.init_lattice), 512
cbc_y (FermiHubbardModel.init_lattice), ??
cbc_y (CouplingMPOM.init_lattice), ??
cbc_y (SpinChain.init_lattice), 470
cbc_y (SpinModel.init_lattice), ??
cbc_y (SpinChainNN.init_lattice), ??
cbc_y (SpinChainNN2.init_lattice), ??
cbc_y (TFIChain.init_lattice), 442
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
conserve (FermionModel), ??
explicit_plus_hc (CouplingMPOM.init_lattice), ??
J (FermionModel), ??
L (multiple definitions), 485
L (FermionChain.init_lattice), 485
L (FermionModel.init_lattice), ??
L (BosonicHaldaneModel.init_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOM.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNN.init_lattice), ??
L (SpinChainNN2.init_lattice), ??
L (TFIChain.init_lattice), 442
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionModel.init_lattice), ??
lattice (BosonicHaldaneModel.init_lattice), ??
lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardChain.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ??
lattice (FermiHubbardChain.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOM.init_lattice), ??
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice), ??
lattice (SpinChainNN.init_lattice), ??
lattice (SpinChainNN2.init_lattice), ??
lattice (TFIChain.init_lattice), 442
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
Lx (multiple definitions), 485
Lx (FermionChain.init_lattice), 485
Lx (FermionModel.init_lattice), ??
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499

Config Option Index 681
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Lx (SpinChain.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinChainNN.init_lattice), ??
Lx (SpinChainNN2.init_lattice), ??
Lx (TFICinit_lattice), 442
Lx (TFModel.init_lattice), ??
Lx (ToricCode.init_lattice), ??
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (HofstadterFermions.init_lattice), ??
Ly (BoseHubbardChain.init_lattice), 499
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), 512
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNN.init_lattice), ??
Ly (SpinChainNN2.init_lattice), ??
Ly (TFICinit_lattice), 442
Ly (TFModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionModel), ??
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardChain.init_lattice), 499
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardChain.init_lattice), 512
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNN.init_lattice), ??
order (SpinChainNN2.init_lattice), ??
order (TFICinit_lattice), 442
order (TFModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
sort_mpo_legs (CouplingMPOModel), ??
v (FermionModel), ??
verbose (Config), ??

HofstadterBosons
bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNN.init_lattice), ??
bc_MPS (SpinChainNN2.init_lattice), ??
bc_MPS (TFICinit_lattice), 442
bc_MPS (TFModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionModel.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (CouplingMPOModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChainNN.init_lattice), ??
bc_x (SpinChainNN2.init_lattice), ??
bc_x (TFICinit_lattice), 442
bc_x (TFModel.init_lattice), ??
bc_x (ToricCode.init_lattice), ??
bc_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionModel.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (BosonicHaldaneModel.init_lattice), ??
bc_y (FermionicHaldaneModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (FermiHubbardChain.init_lattice), 512
bc_y (FermiHubbardModel.init_lattice), ??
bc_y (CouplingMPOModel.init_lattice), ??
bc_y (SpinModel.init_lattice, 470)
bc_y (SpinChain.init_lattice, ??
bc_y (SpinChainNN.init_lattice, ??
bc_y (SpinChainNN2.init_lattice, ??
bc_y (TFIChain.init_lattice, 442)
bc_y (TFIModel.init_lattice, ??
bc_y (ToricCode.init_lattice, ??
bc_y (XXZChain2.init_lattice, 456)
conserve (HofstadterBosons), ?? explicit_plus_hc (CouplingMPOModel, ??
filling (HofstadterBosons), ??
gauge (HofstadterBosons), ??
Jx (HofstadterBosons), ??
Jy (HofstadterBosons), ??
L (multiple definitions), 485
L (FermionChain.init_lattice), 485
L (FermionModel.init_lattice, ??
L (BosonicHaldaneModel.init_lattice, ??
L (FermionicHaldaneModel.init_lattice, ??
L (HofstadterBosons.init_lattice, ??
L (HofstadterFermions.init_lattice, ??
L (BoseHubbardChain.init_lattice, 499
L (BoseHubbardModel.init_lattice, ??
L (FermiHubbardChain.init_lattice, ??
L (FermiHubbardModel.init_lattice, ??
L (CouplingMPOModel.init_lattice, ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice, ??
L (SpinChainNN.init_lattice, ??
L (SpinChainNN2.init_lattice, ??
L (TFIChain.init_lattice, 442
L (TFIModel.init_lattice, ??
L (ToricCode.init_lattice, ??
L (XXZChain2.init_lattice, 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionModel.init_lattice, ??
 latticelattice (BosonicHaldaneModel.init_lattice, ??
lattice (FermionicHaldaneModel.init_lattice, ??
lattice (HofstadterBosons.init_lattice, ??
lattice (HofstadterFermions.init_lattice, ??
lattice (BoseHubbardChain.init_lattice, ??
lattice (BoseHubbardModel.init_lattice, ??
lattice (FermiHubbardChain.init_lattice, 512
lattice (FermiHubbardModel.init_lattice, ??
lattice (CouplingMPOModel.init_lattice, ??
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice, ??
lattice (SpinChainNN.init_lattice, ??
lattice (SpinChainNN2.init_lattice, ??
lattice (TFIChain.init_lattice), 442
lattice (TFIModel.init_lattice), ??

lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice, ??
lattice (XXZChain2.init_lattice, 456
Lx (multiple definitions), ??
Lx (HofstadterBosons), ??
Lx (FermionChain.init_lattice), 485
Lx (FermionModel.init_lattice, ??
Lx (BosonicHaldaneModel.init_lattice, ??
Lx (FermionicHaldaneModel.init_lattice, ??
Lx (HofstadterBosons.init_lattice, ??
Lx (HofstadterFermions.init_lattice, ??
Lx (BoseHubbardChain.init_lattice, 499
Lx (BoseHubbardModel.init_lattice, ??
Lx (FermiHubbardChain.init_lattice, 512
Lx (FermiHubbardModel.init_lattice, ??
Lx (CouplingMPOModel.init_lattice, ??
Lx (SpinChainNN.init_lattice, ??
Ly (multiple definitions), ??
Ly (HofstadterBosons), ??
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice, ??
Ly (BosonicHaldaneModel.init_lattice, ??
Ly (FermionicHaldaneModel.init_lattice, ??
Ly (HofstadterBosons.init_lattice, ??
Ly (HofstadterFermions.init_lattice, ??
Ly (BoseHubbardChain.init_lattice, 499
Ly (BoseHubbardModel.init_lattice, ??
Ly (FermiHubbardChain.init_lattice, ??
Ly (FermiHubbardModel.init_lattice, ??
Ly (CouplingMPOModel.init_lattice, ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice, ??
Ly (SpinChainNN.init_lattice, ??
Ly (SpinChainNN2.init_lattice, ??
Ly (TFIChain.init_lattice, 442
Ly (TFIModel.init_lattice, ??
Ly (ToricCode.init_lattice, ??
Ly (XXZChain2.init_lattice, 456
mu (HofstadterBosons), ??
mx (HofstadterBosons), ??
my (HofstadterBosons), ??
Nmax (HofstadterBosons), ??

order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice, ??
order (BosonicHaldaneModel.init_lattice, ??
order (FermionicHaldaneModel.init_lattice, ??
order (HofstadterBosons.init_lattice, ??

Config Option Index 683
HofstadterFermions

bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionicModel.init_lattice), ?
bc_MPS (BosonicHaldaneModel.init_lattice), ?
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), ??
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), ??
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIChain.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionChain.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (FermionicModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN2.init_lattice), ??
bc_y (TFIChain.init_lattice), 442
bc_y (TFIModel.init_lattice), ??
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
conserve (HofstadterFermions), ??
explicit_plus_hc (CouplingMPOModel), ??
filling (HofstadterFermions), ??
gauge (HofstadterFermions), ??
Jx (HofstadterFermions), ??
Jy (HofstadterFermions), ??
L (multiple definitions), 485
L (FermionModel.init_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNNN.init_lattice), ??
L (SpinChainNNN2.init_lattice), ??
L (TFIChain.init_lattice), 442
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionModel.init_lattice), ??
lattice (BosonicHaldaneModel.init_lattice), ??
lattice (FermionicHaldaneModel.init_lattice), ??
lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardChain.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ?
lattice (FermiHubbardChain.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOModel.init_lattice), ??
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice), ??
lattice (SpinChainNNN.init_lattice), ??
lattice (SpinChainNN2.init_lattice), ??
lattice (TFIChain.init_lattice), 442
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
Lx (multiple definitions), ??
Lx (HofstadterFermions), ??
Lx (FermionChain.init_lattice), 485
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNNN.init_lattice), ??
Ly (SpinChainNN2.init_lattice), ??
Ly (TFIChain.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
mu (HofstadterFermions), ??
mx (HofstadterFermions), ??
my (HofstadterFermions), ??
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardChain.init_lattice), 499
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardChain.init_lattice), 512
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (SpinChainNN2.init_lattice), ??
order (TFIChain.init_lattice), 442
order (TFIModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
phi (HofstadterFermions), ??
phi_ext (HofstadterFermions), ??
sort_mpo_legs (CouplingMPOModel), ??
v (HofstadterFermions), ??
verbose (Config), ??

Lanczos

cutoff (LanczosGroundState), ??
E_shift (LanczosGroundState), ??
E_tol (LanczosGroundState), ??
min_gap (LanczosGroundState), ??
N_cache (LanczosGroundState), ??
N_max (LanczosGroundState), ??
N_min (LanczosGroundState), ??
P_tol (LanczosGroundState), ??
reortho (LanczosGroundState), ??
verbose (Config), ??

LanczosEvolution

cutoff (LanczosGroundState), ??
E_shift (LanczosGroundState), ??
E_tol (multiple definitions), ??
E_tol (LanczosEvolution), ??
E_tol (LanczosGroundState), ??
min_gap (multiple definitions), ??
min_gap (LanczosEvolution), ??
min_gap (LanczosGroundState), ??
N_cache (LanczosGroundState), ??
N_max (LanczosGroundState), ??
N_min (LanczosGroundState), ??
P_tol (LanczosGroundState), ??
reortho (LanczosGroundState), ??
verbose (Config), ??

Mixer
amplitude (Mixer), ??
decay (Mixer), ??
disable_after (Mixer), ??
verbose (multiple definitions), ??
verbose (Mixer), ??
verbose (Config), ??

MPS_compress
combine (Sweep), ??
compression_method (multiple definitions), ??
compression_method (MPS.compress), ??
compression_method (PurificationMPS.compress), ??
init_env_data (multiple definitions), ??
init_env_data (DMRGEngine.init_env), ??
init_env_data (EngineCombine.init_env), 174
init_env_data (EngineFracture.init_env), 182
init_env_data (SingleSiteDMRGEngine.init_env), ??
init_env_data (TwoSiteDMRGEngine.init_env), ??
init_env_data (Sweep.init_env), ??
lanczos_params (Sweep), ??

N_sweeps (VariationalCompression), ??

orthogonal_to (multiple definitions), ??
orthogonal_to (DMRGEngine.init_env), ??
orthogonal_to (EngineCombine.init_env), 174
orthogonal_to (EngineFracture.init_env), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??

start_env (multiple definitions), ??
start_env (Config), ??

RandomUnitaryEvolution
delta_tau_list (multiple definitions), 203
delta_tau_list (PurificationTEBD.run_GS), 203
delta_tau_list (PurificationTEBD2.run_GS), 208
delta_tau_list (Engine.run_GS), ??
delta_tau_list (RandomUnitaryEvolution.run_GS), ??
dt (multiple definitions), 203
dt (PurificationTEBD.run), 203
dt (PurificationTEBD2.run), 207
dt (Engine.run), ??
N_steps (multiple definitions), ??
N_steps (RandomUnitaryEvolution), ??
N_steps (PurificationTEBD.run), 203
N_steps (PurificationTEBD.run_GS), 203
N_steps (PurificationTEBD2.run), 207
N_steps (PurificationTEBD2.run_GS), 208
N_steps (Engine.run), ??
N_steps (Engine.run_GS), ??
N_steps (RandomUnitaryEvolution.run_GS), ??
order (multiple definitions), 203
order (PurificationTEBD.run), 203
order (PurificationTEBD.run_GS), 203
order (PurificationTEBD2.run), 207
order (PurificationTEBD2.run_GS), 208
order (Engine.run), ??
order (Engine.run_GS), ??
order (RandomUnitaryEvolution.run_GS), ??
start_time (Engine), ??
start_trunc_err (Engine), ??
trunc_params (multiple definitions), ??
trunc_params (RandomUnitaryEvolution), ??
trunc_params (Engine), ??
verbose (Config), ??

SingleSiteDMRGEngine
chi_list (multiple definitions), ??
chi_list (DMRGEngine.reset_stats), ??
chi_list (EngineCombine.reset_stats), 176
chi_list (EngineFracture.reset_stats), 184
chi_list (SingleSiteDMRGEngine.reset_stats), ??
chi_list (TwoSiteDMRGEngine.reset_stats), ??
combine (Sweep), ??
diag_method (multiple definitions), ??
diag_method (DMRGEngine.run), ??
diag_method (DMRGEngine.diag), ??
diag_method (EngineCombine.diag), 173
diag_method (EngineCombine.run), 176
diag_method (EngineFracture.diag), 180
diag_method (EngineFracture.run), 184
diag_method (SingleSiteDMRGEngine.diag), ??
diag_method (SingleSiteDMRGEngine.run), ??
diag_method (TwoSiteDMRGEngine.diag), ??
diag_method (TwoSiteDMRGEngine.run), ??
E_tol_max (multiple definitions), ??
E_tol_max (DMRGEngine.run), ??
E_tol_max (EngineCombine.run), 177
E_tol_max (EngineFracture.run), 184
E_tol_max (SingleSiteDMRGEngine.run), ??
E_tol_max (TwoSiteDMRGEngine.run), ??
max_s_err (multiple definitions), ??
max_s_err (DMRGEngine.run), ??
max_s_err (EngineCombine.run), 177
max_s_err (EngineFracture.run), 184
max_s_err (SingleSiteDMRGEngine.run), ??
max_s_err (TwoSiteDMRGEngine.run), ??
max_sweeps (multiple definitions), ??
max_sweeps (DMRGEngine.run), ??
max_sweeps (EngineCombine.run), 177
max_sweeps (EngineFracture.run), 184
max_sweeps (SingleSiteDMRGEngine.run), ??
max_sweeps (TwoSiteDMRGEngine.run), ??
min_sweeps (multiple definitions), ??
min_sweeps (DMRGEngine.run), ??
min_sweeps (EngineCombine.run), 177
min_sweeps (EngineFracture.run), 185
min_sweeps (SingleSiteDMRGEngine.run), ??
N_sweeps_check (multiple definitions), ??
N_sweeps_check (DMRGEngine.run), ??
N_sweeps_check (EngineCombine.run), 177
N_sweeps_check (EngineFracture.run), 185
N_sweeps_check (SingleSiteDMRGEngine.run), ??
N_sweeps_check (TwoSiteDMRGEngine.run), ??
norm_tol (multiple definitions), ??
norm_tol (DMRGEngine.run), ??
norm_tol (EngineCombine.run), 177
norm_tol (EngineFracture.run), 185
norm_tol (SingleSiteDMRGEngine.run), ??
norm_tol (TwoSiteDMRGEngine.run), ??
norm_tol_iter (multiple definitions), ??
norm_tol_iter (DMRGEngine.run), ??
norm_tol_iter (EngineCombine.run), 177
norm_tol_iter (EngineFracture.run), 185
norm_tol_iter (SingleSiteDMRGEngine.run), ??
norm_tol_iter (TwoSiteDMRGEngine.run), ??
max_S_err (multiple definitions), ??
max_S_err (DMRGEngine.run), ??
max_S_err (EngineCombine.run), 177
max_S_err (EngineFracture.run), 184
orthogonal_to (multiple definitions), ??
orthogonal_to (DMRGEngine.init_env), ??
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
lanczos_params (Sweep), ??
max_E_err (multiple definitions), ??
max_E_err (DMRGEngine.run), ??
max_E_err (EngineCombine.run), 176
max_E_err (EngineFracture.run), 184
max_E_err (SingleSiteDMRGEngine.run), ??
max_E_err (TwoSiteDMRGEngine.run), ??
norm_tol (multiple definitions), ??
norm_tol (DMRGEngine.run), ??
norm_tol (EngineCombine.run), 176
norm_tol (EngineFracture.run), 184
norm_tol (SingleSiteDMRGEngine.run), ??
norm_tol (TwoSiteDMRGEngine.run), ??
norm_tol_iter (multiple definitions), ??
norm_tol_iter (DMRGEngine.run), ??
norm_tol_iter (EngineCombine.run), 177
norm_tol_iter (EngineFracture.run), 185
norm_tol_iter (SingleSiteDMRGEngine.run), ??
norm_tol_iter (TwoSiteDMRGEngine.run), ??
max_N_for_ED (multiple definitions), ??
max_N_for_ED (DMRGEngine.diag), ??
max_N_for_ED (EngineCombine.diag), 172
max_N_for_ED (EngineFracture.diag), 180
max_N_for_ED (SingleSiteDMRGEngine.diag), ??
max_N_for_ED (TwoSiteDMRGEngine.diag), ??
max_hours (multiple definitions), ??
max_hours (DMRGEngine.run), ??
max_hours (EngineCombine.run), 176
max_hours (EngineFracture.run), 184
max_hours (SingleSiteDMRGEngine.run), ??
max_hours (TwoSiteDMRGEngine.run), ??
min_sweeps (multiple definitions), ??
min_sweeps (EngineCombine.run), 177
min_sweeps (EngineFracture.run), 184
min_sweeps (SingleSiteDMRGEngine.run), ??
min_sweeps (TwoSiteDMRGEngine.run), ??
multipe definitions
orthogonal_to (EngineCombine.run), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
orthogonal_to (Sweep.init_env), ??
lanczos_params (Sweep), ??
max_E_err (multiple definitions), ??
max_E_err (DMRGEngine.run), ??
max_E_err (EngineCombine.run), 176
max_E_err (EngineFracture.run), 184
max_E_err (SingleSiteDMRGEngine.run), ??
max_E_err (TwoSiteDMRGEngine.run), ??
multipe definitions
orthogonal_to (EngineCombine.run), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
orthogonal_to (Sweep.init_env), ??
P_tol_max (multiple definitions), ??
P_tol_max (DMRGEngine.run), ??
P_tol_max (EngineCombine.run), 177
P_tol_max (EngineFracture.run), 185
P_tol_max (SingleSiteDMRGEngine.run), ??
P_tol_max (TwoSiteDMRGEngine.run), ??
SpinChainNNN

bc_MPS (mulitple definitions), ??
bc_MPS (SpinChainNNN), ??
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIChain.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionChain.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
bc_x (BosonicHaldaneModel.init_lattice), ??
bc_x (FermionicHaldaneModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (CouplingMPOModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChainNNN.init_lattice), ??
bc_x (FermionicHaldaneModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (CouplingMPOModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChainNNN.init_lattice), ??
bc_x (SpinChainNNN2.init_lattice), ??
bc_x (TFIChain.init_lattice), 442
bc_x (TFIModel.init_lattice), ??
bc_x (ToricCode.init_lattice), ??
bc_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionChain.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (BosonicHaldaneModel.init_lattice), ??
bc_y (FermionicHaldaneModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (FermiHubbardChain.init_lattice), 512
bc_y (FermiHubbardModel.init_lattice), ??
bc_y (CouplingMPOModel.init_lattice), ??
bc_y (SpinChain.init_lattice), 470
bc_y (SpinModel.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN2.init_lattice), ??
bc_y (TFIChain.init_lattice), 442
bc_y (TFIModel.init_lattice), ??
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
conserve (SpinChainNNN), ??
explicit_plus_hc (CouplingMPOModel), ??
hx (SpinChainNNN), ??
hy (SpinChainNNN), ??
hz (SpinChainNNN), ??
Jx (SpinChainNNN), ??
Jxp (SpinChainNNN), ??
Jy (SpinChainNNN), ??
Jyp (SpinChainNNN), ??
Jz (SpinChainNNN), ??
L (multiple definitions), 485
L (FermionChain.init_lattice), 485
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (FermiHubbardChain.init_lattice), ??
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNNN.init_lattice), ??
L (SpinChainNNN2.init_lattice), ??
L (TFIClass.init_lattice), 442
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
Lx (SpinChain.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinChainNNN.init_lattice), ??
Lx (SpinChainNNN2.init_lattice), ??
Lx (TFIClass.init_lattice), 442
Lx (TFIModel.init_lattice), ??
Lx (ToricCode.init_lattice), ??
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), ??
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNNN.init_lattice), ??
Ly (SpinChainNNN2.init_lattice), ??
Ly (TFIClass.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (FermiHubbardChain.init_lattice), ??
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (SpinChainNNN2.init_lattice), ??
order (TFIClass.init_lattice), 442
order (TFIModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
S (SpinChainNNN), ??
sort_mpo_legs (CouplingMPOModel), ??
verbose (Config), ??

SpinChainNNN2

bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIChiain.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), 485
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIChiain.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionChain.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
bc_x (BosonicHaldaneModel.init_lattice), ??
bc_x (FermionicHaldaneModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), ??
bc_x (FermiHubbardModel.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (CouplingMPOModel.init_lattice), ??
bc_x (SpinModel.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChainNNN.init_lattice), ??
bc_x (SpinChainNNN2.init_lattice), ??
bc_x (TFIChiain.init_lattice), 442
bc_x (TFIModel.init_lattice), ??
bc_x (ToricCode.init_lattice), ??
bc_x (XXZChain2.init_lattice), 456
bc_x (XXZChain2.init_lattice), 465
bc_x (XXZChain2.init_lattice), 456
bc_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionChain.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (BosonicHaldaneModel.init_lattice), ??
bc_y (FermionicHaldaneModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (FermiHubbardChain.init_lattice), ??
bc_y (FermiHubbardModel.init_lattice), ??
bc_y (CouplingMPOModel.init_lattice), ??
bc_y (SpinChain.init_lattice), 470
bc_y (SpinModel.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN2.init_lattice), ??
bc_y (TFIChiain.init_lattice), 442
bc_y (TFIModel.init_lattice), ??
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
conserve (SpinChainNNN2), ??
explicit_plus_hc (CouplingMPOModel), ??
hx (SpinChainNNN2), ??
hy (SpinChainNNN2), ??
hz (SpinChainNNN2), ??
Jx (SpinChainNNN2), ??
Jxp (SpinChainNNN2), ??
Jyp (SpinChainNNN2), ??
Jz (SpinChainNNN2), ??
Jzp (SpinChainNNN2), ??
L (multiple definitions), 485
L (SpinModel.init_lattice), 485
L (FermionModel.init_lattice), ??
L (BosonicHaldaneModel.init_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNNN.init_lattice), ??
L (SpinChainNNN2.init_lattice), ??
L (TFIChiain.init_lattice), 442
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionModel.init_lattice), ??
lattice (BosonicHaldaneModel.init_lattice), ??
lattice (FermionicHaldaneModel.init_lattice), ??
lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardChain.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ??
lattice (FermiHubbardChain.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOModel.init_lattice), ??
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice), ??
lattice (SpinChainNNN.init_lattice), ??
lattice (SpinChainNNN2.init_lattice), ??
lattice (TFIChiain.init_lattice), 442
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
Lx (multiple definitions), 485
Lx (FermionChain.init_lattice), 485
Lx (FermionModel.init_lattice), ??
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Lx (SpinChain.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinChainNNN.init_lattice), ??
Lx (SpinChainNNN2.init_lattice), ??
Lx (TFIClass.init_lattice), 442
Lx (TFIModel.init_lattice), ??
Lx (ToricCode.init_lattice), ??
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (HofstadterFermions.init_lattice), ??
Ly (BoseHubbardChain.init_lattice), 499
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), 512
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNNN.init_lattice), ??
Ly (SpinChainNNN2.init_lattice), ??
Ly (TFIClass.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardChain.init_lattice), 499
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardChain.init_lattice), 512
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (SpinChainNNN2.init_lattice), ??
order (TFIClass.init_lattice), 442
order (TFIModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
S (SpinChainNNN2), ??
sort_mpo_legs (CouplingMPOModel), ??
verbose (Config), ??

SpinModel

bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIClass.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionChain.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
bc_x (BosonicHaldaneModel.init_lattice), ??
bc_x (FermionicHaldaneModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (CouplingMPOModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_y (SpinModel.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN2.init_lattice), ??
bc_y (TFIClass.init_lattice), 442
bc_y (TFIModel.init_lattice), ??
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
TeNPy, Release 0.7.2.dev55+68eae2c

bc_y (FermionChain.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (BosonicHaldaneModel.init_lattice), ??
bc_y (FermionicHaldaneModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (FermiHubbardChain.init_lattice), 512
bc_y (FermiHubbardModel.init_lattice), ??
bc_y (CouplingMPOModel.init_lattice), ??
bc_y (SpinChain.init_lattice), 470
bc_y (SpinModel.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN2.init_lattice), ??
bc_y (TFIModel.init_lattice), 442
bc_y (TFIModel.init_lattice), 442
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
bc_y (XXZChain2.init_lattice), 456
conserve (SpinModel), ??
D (SpinModel), ??
E (SpinModel), ??

explicit_plus hc (CouplingMPOModel), ??

hx (SpinModel), ??
hy (SpinModel), ??
hz (SpinModel), ??
Jx (SpinModel), ??
Jy (SpinModel), ??
Jz (SpinModel), ??

L (multiple definitions), 485
L (FermionChain.init_lattice), 485
L (FermionModel.init_lattice), ??
L (BosonicHaldaneModel.init_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNNN.init_lattice), ??
L (SpinChainNNN2.init_lattice), ??
L (TFIClattice.init_lattice), 442
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionModel.init_lattice), 485
lattice (FermionicHaldaneModel.init_lattice), ??

lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardChain.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ??
lattice (FermiHubbardChain.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOModel.init_lattice), ??
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice), ??
lattice (SpinChainNNN.init_lattice), ??
lattice (SpinChainNNN2.init_lattice), ??
lattice (TFIClattice.init_lattice), 442
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
Lx (multiple definitions), 485
Lx (FermionChain.init_lattice), 485
Lx (FermionModel.init_lattice), ??
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Lx (SpinChain.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinChainNNN.init_lattice), ??
Lx (SpinChainNNN2.init_lattice), ??
Lx (TFIClattice.init_lattice), 442
Lx (TFIModel.init_lattice), ??
Lx (ToricCode.init_lattice), ??
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (HofstadterFermions.init_lattice), ??
Ly (BoseHubbardChain.init_lattice), 499
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), 512
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNNN.init_lattice), ??
Ly (SpinChainNNN2.init_lattice), ??
Ly (TFIClattice.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
muJ (SpinModel), ??
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardChain.init_lattice), 499
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardChain.init_lattice), 512
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (TFIChain.init_lattice), 442
order (TFIModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
S (SpinModel), ??
sort_mpo_legs (CouplingMPOModel), ??
verbose (Config), ??

Sweep
combine (Sweep), ??
init_env_data (multiple definitions), ??
init_env_data (DMRGEngine.init_env), ??
init_env_data (EngineCombine.init_env), 174
init_env_data (EngineFracture.init_env), 182
init_env_data (SingleSiteDMRGEngine.init_env), ??
init_env_data (TwoSiteDMRGEngine.init_env), ??
init_env_data (Sweep.init_env), ??
lanczos_params (Sweep), ??
orthogonal_to (multiple definitions), ??
orthogonal_to (DMRGEngine.init_env), ??
orthogonal_to (EngineCombine.init_env), 174
orthogonal_to (EngineFracture.init_env), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
orthogonal_to (Sweep.init_env), ??
start_env (multiple definitions), ??
start_env (DMRGEngine.init_env), ??
start_env (EngineCombine.init_env), 174
start_env (EngineFracture.init_env), 182
start_env (SingleSiteDMRGEngine.init_env), ??
start_env (TwoSiteDMRGEngine.init_env), ??
start_env (Sweep.init_env), ??
sweep_0 (multiple definitions), ??
sweep_0 (Sweep.reset_stats), ??
sweep_0 (VariationalApplyMPO.reset_stats), ??
sweep_0 (VariationalCompression.reset_stats), ??
sweep_0 (PurificationApplyMPO.reset_stats), 199
trupecraps (Sweep), ??
verbose (multiple definitions), ??
verbose (Sweep), ??
verbose (Config), ??

TDVP
active_sites (Engine), ??
dt (Engine), ??
Lanczos (Engine), ??
N_steps (Engine), ??
start_time (Engine), ??
trunc_params (Engine), ??
verbose (Config), ??

TEBD
delta_tau_list (multiple definitions), 203
delta_tau_list (PurificationTEBD.run_GS), 203
delta_tau_list (PurificationTEBD2.run_GS), 208
delta_tau_list (Engine.run_GS), ??
delta_tau_list (RandomUnitaryEvolution.run_GS), ??
dt (multiple definitions), 203
dt (PurificationTEBD.run), 203
dt (PurificationTEBD2.run), 207
dt (Engine.run), ??
N_steps (multiple definitions), 203
N_steps (PurificationTEBD.run), 203
N_steps (PurificationTEBD.run_GS), 203
N_steps (PurificationTEBD2.run), 207
N_steps (PurificationTEBD2.run_GS), 208
N_steps (Engine.run), ??
N_steps (Engine.run_GS), ??
N_steps (RandomUnitaryEvolution.run_GS), ??
order (multiple definitions), 203
order (PurificationTEBD.run), 203
order (PurificationTEBD.run_GS), 203
order (PurificationTEBD2.run), 207
order (PurificationTEBD2.run_GS), 208
order (Engine.run), ??
order (Engine.run_GS), ??
order (RandomUnitaryEvolution.run_GS), ??
start_time (Engine), ??
start trunc_err (Engine), ??
trunc_params (Engine), ??
verbose (Config), ??

TFIModel
bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIChain.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionChain.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
bc_x (BosonicHaldaneModel.init_lattice), ??
bc_x (FermionicHaldaneModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (CouplingMPOModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChainNNN.init_lattice), ??
bc_x (SpinChainNNN2.init_lattice), ??
bc_x (TFIModel.init_lattice), 442
bc_x (ToricCode.init_lattice), ??
bc_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionChain.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (BosonicHaldaneModel.init_lattice), ??
bc_y (FermionicHaldaneModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (FermiHubbardChain.init_lattice), 512
bc_y (FermiHubbardModel.init_lattice), ??
bc_y (CouplingMPOModel.init_lattice), ??
bc_y (SpinChain.init_lattice), 470
bc_y (SpinModel.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN2.init_lattice), ??
bc_y (TFIModel.init_lattice), 442
bc_y (TFIModel.init_lattice), ??
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
bc_y (Conserve(TFModel), ??
explicit_plus_hc (CouplingMPOModel), ??
g (TFIModel), ??
J (TFIModel), ??
L (multiple definitions), 485
L (FermionChain.init_lattice), 485
L (FermionModel.init_lattice), ??
L (BosonicHaldaneModelinit_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardModel.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNNN.init_lattice), ??
L (SpinChainNNN2.init_lattice), ??
L (TFIChain.init_lattice), 442
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), ??
L (XXZChain2.init_lattice), 456
lattice (multiple definitions), 485
lattice (FermionChain.init_lattice), 485
lattice (FermionModel.init_lattice), ??
lattice (BosonicHaldaneModel.init_lattice), ??
lattice (FermionicHaldaneModel.init_lattice), ??
lattice (HofstadterBosons.init_lattice), ??
lattice (HofstadterFermions.init_lattice), ??
lattice (BoseHubbardChain.init_lattice), 499
lattice (BoseHubbardModel.init_lattice), ??
lattice (FermiHubbardChain.init_lattice), 512
lattice (FermiHubbardModel.init_lattice), ??
lattice (CouplingMPOModel.init_lattice), ??
lattice (SpinChain.init_lattice), 470
lattice (SpinModel.init_lattice), ??
lattice (SpinChainNNN.init_lattice), ??
lattice (SpinChainNNN2.init_lattice), ??
lattice (TFIChain.init_lattice), 442
lattice (TFIModel.init_lattice), ??
lattice (ToricCode.init_lattice), ??
lattice (XXZChain2.init_lattice), 456
Lx (multiple definitions), 485
Lx (FermionChain.init_lattice), 485
Lx (FermionModel.init_lattice), ??
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499

TeNPy, Release 0.7.2.dev55+68eae2c
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Lx (SpinChain.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinChainNN.init_lattice), ??
Lx (SpinChainNN2.init_lattice), ??
Lx (TFICHain.init_lattice), 442
Lx (TFIModel.init_lattice), ??
Lx (ToricCode.init_lattice), ??
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), 485
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (HofstadterFermions.init_lattice), ??
Ly (BoseHubbardChain.init_lattice), 499
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), 512
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNN.init_lattice), ??
Ly (SpinChainNN2.init_lattice), ??
Ly (TFICHain.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), ??
Ly (XXZChain2.init_lattice), 456
order (multiple definitions), 485
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardChain.init_lattice), 499
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardChain.init_lattice), 512
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNN.init_lattice), ??
order (SpinChainNN2.init_lattice), ??
order (TFICHain.init_lattice), 442
order (TFIModel.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
sort_mpo_legs (CouplingMPOModel), ??
verbose (Config), ??

ToricCode
bc_MPS (multiple definitions), 485
bc_MPS (FermionChain.init_lattice), 485
bc_MPS (FermionModel.init_lattice), ??
bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNN.init_lattice), ??
bc_MPS (SpinChainNN2.init_lattice), ??
bc_MPS (TFICHain.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_x (multiple definitions), ??
bc_x (ToricCode), ??
bc_x (FermionChain.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
bc_x (BosonicHaldaneModel.init_lattice), ??
bc_x (FermionicHaldaneModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChainNN.init_lattice), ??
bc_x (SpinChainNN2.init_lattice), ??
bc_x (TFICHain.init_lattice), 442
bc_x (TFIModel.init_lattice), ??
bc_x (ToricCode.init_lattice), ??
bc_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), ??
bc_y (ToricCode), ??
bc_y (FermionChain.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (BosonicHaldaneModel.init_lattice), ??
bc_y (FermionicHaldaneModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (FermiHubbardChain.init_lattice), 512
bc_y (FermiHubbardModel.init_lattice), ??

TeNPy, Release 0.7.2.dev55+68eae2c
bc_y (CouplingMPOModel.init_lattice), ??
bc_y (SpinChain.init_lattice), 470
bc_y (SpinModel.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN2.init_lattice), ??
bc_y (TFIChain.init_lattice), 442
bc_y (TFIModel.init_lattice), ??
bc_y (ToricCode.init_lattice), ??
bc_y (XXZChain2.init_lattice), 456
conserve (ToricCode), ??
explicit_plus_HC (CouplingMPOModel), ??
Jc (ToricCode), ??
Jp (ToricCode), ??
L (multiple definitions), 485
L (FermionChain.init_lattice), 485
L (FermionModel.init_lattice), ??
L (BosonicHaldaneModel.init_lattice), ??
L (FermionicHaldaneModel.init_lattice), ??
L (HofstadterBosons.init_lattice), ??
L (HofstadterFermions.init_lattice), ??
L (BoseHubbardChain.init_lattice), 499
L (BoseHubbardModel.init_lattice), ??
L (FermiHubbardChain.init_lattice), 512
L (FermiHubbardModel.init_lattice), ??
L (CouplingMPOModel.init_lattice), ??
L (SpinChain.init_lattice), 470
L (SpinModel.init_lattice), ??
L (SpinChainNNN.init_lattice), ??
L (SpinChainNNN2.init_lattice), ??
L (TFIChain.init_lattice), 442
L (TFIModel.init_lattice), ??
L (ToricCode.init_lattice), 456
Lx (multiple definitions), ??
Lx (ToricCode), ??
Lx (FermionChain.init_lattice), 485
Lx (FermionModel.init_lattice), ??
Lx (BosonicHaldaneModel.init_lattice), ??
Lx (FermionicHaldaneModel.init_lattice), ??
Lx (HofstadterBosons.init_lattice), ??
Lx (HofstadterFermions.init_lattice), ??
Lx (BoseHubbardChain.init_lattice), 499
Lx (BoseHubbardModel.init_lattice), ??
Lx (FermiHubbardChain.init_lattice), 512
Lx (FermiHubbardModel.init_lattice), ??
Lx (CouplingMPOModel.init_lattice), ??
Lx (SpinChain.init_lattice), 470
Lx (SpinModel.init_lattice), ??
Lx (SpinChainNNN.init_lattice), ??
Lx (SpinChainNNN2.init_lattice), ??
Lx (TFIChain.init_lattice), 442
Lx (TFIModel.init_lattice), ??
Lx (ToricCode.init_lattice), 456
Lx (XXZChain2.init_lattice), 456
Ly (multiple definitions), ??
Ly (ToricCode), ??
Ly (FermionChain.init_lattice), 485
Ly (FermionModel.init_lattice), ??
Ly (BosonicHaldaneModel.init_lattice), ??
Ly (FermionicHaldaneModel.init_lattice), ??
Ly (HofstadterBosons.init_lattice), ??
Ly (HofstadterFermions.init_lattice), ??
Ly (BoseHubbardChain.init_lattice), 499
Ly (BoseHubbardModel.init_lattice), ??
Ly (FermiHubbardChain.init_lattice), 512
Ly (FermiHubbardModel.init_lattice), ??
Ly (CouplingMPOModel.init_lattice), ??
Ly (SpinChain.init_lattice), 470
Ly (SpinModel.init_lattice), ??
Ly (SpinChainNNN.init_lattice), ??
Ly (SpinChainNNN2.init_lattice), ??
Ly (TFIChain.init_lattice), 442
Ly (TFIModel.init_lattice), ??
Ly (ToricCode.init_lattice), 456
Ly (XXZChain2.init_lattice), 456
order (multiple definitions), ??
order (ToricCode), ??
order (FermionChain.init_lattice), 485
order (FermionModel.init_lattice), ??
order (BosonicHaldaneModel.init_lattice), ??
order (FermionicHaldaneModel.init_lattice), ??
order (HofstadterBosons.init_lattice), ??
order (HofstadterFermions.init_lattice), ??
order (BoseHubbardChain.init_lattice), 499
order (BoseHubbardModel.init_lattice), ??
order (FermiHubbardChain.init_lattice), 512
order (FermiHubbardModel.init_lattice), ??
order (CouplingMPOModel.init_lattice), ??
order (SpinChain.init_lattice), 470
order (SpinModel.init_lattice), ??
order (SpinChainNNN.init_lattice), ??
order (SpinChainNNN2.init_lattice), ??
order (TF1Chain.init_lattice), 442
order (TF1Model.init_lattice), ??
order (ToricCode.init_lattice), ??
order (XXZChain2.init_lattice), 456
sort_mpo_legs (CouplingMPOModel), ??
verbose (Config), ??

truncation
chi_max (truncate), ??
chi_min (truncate), ??
degeneracy_tol (truncate), ??
svd_min (truncate), ??
trunc_cut (truncate), ??
verbose (Config), ??

TwoSiteDMRGEngine
chi_list (mulitple definitions), ??
chi_list (DMRGEngine.reset_stats), ??
chi_list (EngineCombine.reset_stats), 176
chi_list (EngineFracture.reset_stats), 184
chi_list (SingleSiteDMRGEngine.reset_stats), ??
chi_list (TwoSiteDMRGEngine.reset_stats), ??
combine (Sweep), ??
diag_method (multiple definitions), ??
diag_method (DMRGEngine.run), ??
diag_method (DMRGEngine.diag), ??
diag_method (EngineCombine.diag), 173
diag_method (EngineCombine.run), 176
diag_method (EngineFracture.diag), 180
diag_method (EngineFracture.run), 184
diag_method (SingleSiteDMRGEngine.diag), ??
diag_method (SingleSiteDMRGEngine.run), ??
diag_method (TwoSiteDMRGEngine.diag), ??
diag_method (TwoSiteDMRGEngine.run), ??
E_tol_max (multiple definitions), ??
E_tol_max (DMRGEngine.run), ??
E_tol_max (EngineCombine.run), 176
E_tol_max (EngineFracture.run), 184
E_tol_max (SingleSiteDMRGEngine.run), ??
E_tol_max (TwoSiteDMRGEngine.run), ??
E_tol_min (multiple definitions), ??
E_tol_min (DMRGEngine.run), ??
E_tol_min (EngineCombine.run), 176
E_tol_min (EngineFracture.run), 184
E_tol_min (SingleSiteDMRGEngine.run), ??
E_tol_min (TwoSiteDMRGEngine.run), ??
E_tol_to_trunc (multiple definitions), ??
E_tol_to_trunc (DMRGEngine.run), ??
E_tol_to_trunc (EngineCombine.run), 176
E_tol_to_trunc (EngineFracture.run), 184
E_tol_to_trunc (SingleSiteDMRGEngine.run), ??
E_tol_to_trunc (TwoSiteDMRGEngine.run), ??
init_env_data (multiple definitions), ??
init_env_data (DMRGEngine.init_env), ??
init_env_data (EngineCombine.init_env), 174
init_env_data (EngineFracture.init_env), 182
init_env_data (SingleSiteDMRGEngine.init_env), ??
init_env_data (TwoSiteDMRGEngine.init_env), ??
lanczos_params (Sweep), ??
max_E_err (multiple definitions), ??
max_E_err (DMRGEngine.run), ??
max_E_err (EngineCombine.run), 176
max_E_err (EngineFracture.run), 184
max_E_err (SingleSiteDMRGEngine.run), ??
max_E_err (TwoSiteDMRGEngine.run), ??
max_hours (multiple definitions), ??
max_hours (DMRGEngine.run), ??
max_hours (EngineCombine.run), 176
max_hours (EngineFracture.run), 184
max_hours (TwoSiteDMRGEngine.run), ??
max_N_for_ED (multiple definitions), ??
max_N_for_ED (DMRGEngine.diag), ??
max_N_for_ED (EngineCombine.diag), 172
max_N_for_ED (EngineFracture.diag), 180
max_N_for_ED (SingleSiteDMRGEngine.diag), ??
max_N_for_ED (TwoSiteDMRGEngine.diag), ??
max_S_err (multiple definitions), ??
max_S_err (DMRGEngine.run), ??
max_S_err (EngineCombine.run), 177
max_S_err (EngineFracture.run), 184
max_S_err (SingleSiteDMRGEngine.run), ??
max_S_err (TwoSiteDMRGEngine.run), ??
max_sweeps (multiple definitions), ??
max_sweeps (DMRGEngine.run), ??
max_sweeps (EngineCombine.run), 177
max_sweeps (EngineFracture.run), 184
max_sweeps (Sweep), ??
max_sweeps (SingleSiteDMRGEngine.run), ??
max_sweeps (TwoSiteDMRGEngine.run), ??
min_sweeps (multiple definitions), ??
min_sweeps (DMRGEngine.run), ??
min_sweeps (EngineCombine.run), 177
min_sweeps (EngineFracture.run), 185
min_sweeps (SingleSiteDMRGEngine.run), ??
min_sweeps (TwoSiteDMRGEngine.run), ??
mixer (multiple definitions), ??
mixer (DMRGEngine.mixer_activate), ??
mixer (EngineCombine.mixer_activate), 174
mixer (EngineFracture.mixer_activate), 182
mixer (SingleSiteDMRGEngine.mixer_activate), ??
mixer (TwoSiteDMRGEngine.mixer_activate), ??
mixer_params (multiple definitions), ??
mixin_params (DMRGEngine.mixer_activate), ??
mixin_params (EngineCombine.mixer_activate), 175
mixin_params (EngineFracture.mixer_activate), 182
mixin_params (SingleSiteDMRGEngine.mixer_activate), ??
mixin_params (TwoSiteDMRGEngine.mixer_activate), ??
N_sweeps_check (multiple definitions), ??
N_sweeps_check (DMRGEngine.run), ??
N_sweeps_check (EngineCombine.run), 177
N_sweeps_check (EngineFracture.run), 185
N_sweeps_check (SingleSiteDMRGEngine.run), ??
N_sweeps_check (TwoSiteDMRGEngine.run), ??
norm_tol (multiple definitions), ??
norm_tol (DMRGEngine.run), ??
norm_tol (EngineCombine.run), 177
norm_tol (EngineFracture.run), 185
norm_tol (SingleSiteDMRGEngine.run), ??
norm_tol (TwoSiteDMRGEngine.run), ??
norm_tol_iter (multiple definitions), ??
norm_tol_iter (DMRGEngine.run), ??
norm_tol_iter (EngineCombine.run), 177
norm_tol_iter (EngineFracture.run), 185
norm_tol_iter (SingleSiteDMRGEngine.run), ??
norm_tol_iter (TwoSiteDMRGEngine.run), ??
orthogonal_to (multiple definitions), ??
orthogonal_to (DMRGEngine.init_env), ??
orthogonal_to (EngineCombine.init_env), 174
orthogonal_to (EngineFracture.init_env), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
P_tol_max (multiple definitions), ??
P_tol_max (DMRGEngine.run), ??
P_tol_max (EngineCombine.run), 177
P_tol_max (EngineFracture.run), 185
P_tol_max (SingleSiteDMRGEngine.run), ??
P_tol_max (TwoSiteDMRGEngine.run), ??
P_tol_min (multiple definitions), ??
P_tol_min (DMRGEngine.run), ??
P_tol_min (EngineCombine.run), 177
P_tol_min (EngineFracture.run), 185
P_tol_min (SingleSiteDMRGEngine.run), ??
P_tol_min (TwoSiteDMRGEngine.run), ??
P_tol_to_trunc (multiple definitions), ??
P_tol_to_trunc (DMRGEngine.run), ??
P_tol_to_trunc (EngineCombine.run), 177
P_tol_to_trunc (EngineFracture.run), 185
P_tol_to_trunc (SingleSiteDMRGEngine.run), ??
P_tol_to_trunc (TwoSiteDMRGEngine.run), ??
start_env (multiple definitions), ??
start_env (DMRGEngine.init_env), ??
start_env (EngineCombine.init_env), 174
start_env (EngineFracture.init_env), 182
start_env (SingleSiteDMRGEngine.init_env), ??
start_env (TwoSiteDMRGEngine.init_env), ??
start_env (Sweep.init_env), ??
sweep_0 (multiple definitions), ??
sweep_0 (DMRGEngine.reset_stats), ??
sweep_0 (EngineCombine.reset_stats), 176
sweep_0 (EngineFracture.reset_stats), 184
sweep_0 (SingleSiteDMRGEngine.reset_stats), ??
sweep_0 (TwoSiteDMRGEngine.reset_stats), ??
sweep_0 (Sweep.reset_stats), ??
sweep_0 (VariationalApplyMPO.reset_stats), ??
sweep_0 (VariationalCompression.reset_stats), ??
sweep_0 (PurificationApplyMPO.reset_stats), 199
trunc_params (Sweep), ??
update_env (multiple definitions), ??
update_env (DMRGEngine.run), ??
update_env (EngineCombine.run), 177
update_env (EngineFracture.run), 185
update_env (SingleSiteDMRGEngine.run), ??
update_env (TwoSiteDMRGEngine.run), ??
verbose (multiple definitions), ??
verbose (Sweep), ??
verbose (Config), ??

**VariationalApplyMPO**

combine (Sweep), ??
init_env_data (multiple definitions), ??
init_env_data (DMRGEngine.init_env), ??
init_env_data (EngineCombine.init_env), 174
init_env_data (EngineFracture.init_env), 182
init_env_data (SingleSiteDMRGEngine.init_env), ??
init_env_data (TwoSiteDMRGEngine.init_env), ??
init_env_data (Sweep.init_env), ??
lanczos_params (Sweep), ??
N_sweeps (VariationalCompression), ??
orthogonal_to (multiple definitions), ??
orthogonal_to (DMRGEngine.init_env), ??
orthogonal_to (EngineCombine.init_env), 174
orthogonal_to (EngineFracture.init_env), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
orthogonal_to (Sweep.init_env), ??
start_env (multiple definitions), ??
start_env (DMRGEngine.init_env), ??
start_env (EngineCombine.init_env), 174
start_env (EngineFracture.init_env), 184
start_env (SingleSiteDMRGEngine.init_env), 182
start_env (TwoSiteDMRGEngine.init_env), ??
start_env (Sweep.init_env), ??
sweep_0 (multiple definitions), ??
sweep_0 (Sweep.reset_stats), ??
sweep_0 (VariationalApplyMPO.reset_stats), ??
sweep_0 (VariationalCompression.reset_stats), ??
sweep_0 (PurificationApplyMPO.reset_stats), ??
trunc_params (multiple definitions), ??
trunc_params (VariationalCompression), ??
trunc_params (Sweep), ??
verbose (multiple definitions), ??
verbose (Sweep), ??
verbose (Config), ??

VariationalCompression

combine (Sweep), ??
init_env_data (DMRGEngine.init_env), ??
init_env_data (EngineCombine.init_env), 174
init_env_data (EngineFracture.init_env), 182
init_env_data (SingleSiteDMRGEngine.init_env), ??
init_env_data (TwoSiteDMRGEngine.init_env), ??
lanczos_params (Sweep), ??
N_sweeps (VariationalCompression), ??
orthogonal_to (multiple definitions), ??
orthogonal_to (DMRGEngine.init_env), ??
orthogonal_to (EngineCombine.init_env), 174
orthogonal_to (EngineFracture.init_env), 182
orthogonal_to (SingleSiteDMRGEngine.init_env), ??
orthogonal_to (TwoSiteDMRGEngine.init_env), ??
start_env (Sweep.init_env), ??
start_env (DMRGEngine.init_env), ??
start_env (EngineCombine.init_env), 174
start_env (EngineFracture.init_env), 182
start_env (SingleSiteDMRGEngine.init_env), ??
start_env (TwoSiteDMRGEngine.init_env), ??
start_env (Sweep.init_env), ??
sweep_0 (multiple definitions), ??
sweep_0 (Sweep.reset_stats), ??
sweep_0 (VariationalApplyMPO.reset_stats), ??
sweep_0 (VariationalCompression.reset_stats), ??
sweep_0 (PurificationApplyMPO.reset_stats), ??
trunc_params (multiple definitions), ??
trunc_params (VariationalCompression), ??
trunc_params (Sweep), ??
verbose (multiple definitions), ??
verbose (Sweep), ??
verbose (Config), ??

XXZChain

bc_MPS (BosonicHaldaneModel.init_lattice), ??
bc_MPS (FermionicHaldaneModel.init_lattice), ??
bc_MPS (HofstadterBosons.init_lattice), ??
bc_MPS (HofstadterFermions.init_lattice), ??
bc_MPS (BoseHubbardChain.init_lattice), 499
bc_MPS (BoseHubbardModel.init_lattice), ??
bc_MPS (FermiHubbardChain.init_lattice), 512
bc_MPS (FermiHubbardModel.init_lattice), ??
bc_MPS (CouplingMPOModel.init_lattice), ??
bc_MPS (SpinChain.init_lattice), 470
bc_MPS (SpinModel.init_lattice), ??
bc_MPS (SpinChainNNN.init_lattice), ??
bc_MPS (SpinChainNNN2.init_lattice), ??
bc_MPS (TFIChain.init_lattice), 442
bc_MPS (TFIModel.init_lattice), ??
bc_MPS (ToricCode.init_lattice), ??
bc_MPS (XXZChain2.init_lattice), 456
bc_x (multiple definitions), 485
bc_x (FermionChain.init_lattice), 485
bc_x (FermionModel.init_lattice), ??
bc_x (BosonicHaldaneModel.init_lattice), ??
bc_x (HofstadterBosons.init_lattice), ??
bc_x (HofstadterFermions.init_lattice), ??
bc_x (BoseHubbardChain.init_lattice), 499
bc_x (BoseHubbardModel.init_lattice), ??
bc_x (FermiHubbardChain.init_lattice), 512
bc_x (FermiHubbardModel.init_lattice), ??
bc_x (CouplingMPOModel.init_lattice), ??
bc_x (SpinChain.init_lattice), 470
bc_x (SpinModel.init_lattice), ??
bc_x (SpinChainNNN.init_lattice), ??
bc_x (SpinChainNNN2.init_lattice), ??
bc_x (TFIChain.init_lattice), 442
bc_x (TFIModel.init_lattice), ??
bc_x (ToricCode.init_lattice), ??
bc_x (XXZChain2.init_lattice), 456
bc_y (multiple definitions), 485
bc_y (FermionChain.init_lattice), 485
bc_y (FermionModel.init_lattice), ??
bc_y (BosonicHaldaneModel.init_lattice), ??
bc_y (FermionicHaldaneModel.init_lattice), ??
bc_y (HofstadterBosons.init_lattice), ??
bc_y (HofstadterFermions.init_lattice), ??
bc_y (BoseHubbardChain.init_lattice), 499
bc_y (BoseHubbardModel.init_lattice), ??
bc_y (FermiHubbardChain.init_lattice), 512
bc_y (FermiHubbardModel.init_lattice), ??
bc_y (CouplingMPOModel.init_lattice), ??
bc_y (SpinChain.init_lattice), 470
bc_y (SpinModel.init_lattice), ??
bc_y (SpinChainNNN.init_lattice), ??
bc_y (SpinChainNNN2.init_lattice), ??
bc_y (TFIChain.init_lattice), 442

Config Option Index 699
sort_mpo_legs (CouplingMPOModel), ??
verbose (Config), ??

ZipUpApplyMPO
m_temp (MPO.apply_zipup), ??
trunc_params (MPO.apply_zipup), ??
trunc_weight (MPO.apply_zipup), ??
verbose (Config), ??
INDEX

Symbols

_\text{LP} \quad \text{(tenpy.networks.mps.MPSEnvironment attribute), 569}
_\text{LP\_age} \quad \text{(tenpy.networks.mps.MPSEnvironment attribute), 569}
_\text{RP} \quad \text{(tenpy.networks.mps.MPSEnvironment attribute), 569}
_\text{RP\_age} \quad \text{(tenpy.networks.mps.MPSEnvironment attribute), 569}
_\text{full\_version\_} \quad \text{(in module tenpy), 152}
_\text{version\_} \quad \text{(in module tenpy), 152}
_\text{bra\_N} \quad \text{(tenpy.networks.mps.TransferMatrix attribute), 574}
_\text{data} \quad \text{(tenpy.linalg.np_conserved.Array attribute), 222}
_\text{disent\_iterations} \quad \text{(tenpy.algorithms.purification.PurificationTEBD attribute), 201}
_\text{finite} \quad \text{(tenpy.networks.mps.MPSEnvironment attribute), 569}
_\text{grid\_legs} \quad \text{(tenpy.networks.mpo.MPOGraph attribute), 584}
_\text{guess\_U\_disent} \quad \text{(tenpy.algorithms.purification.PurificationTEBD attribute), 201}
_\text{ket\_M} \quad \text{(tenpy.networks.mps.TransferMatrix attribute), 574}
_\text{labels} \quad \text{(tenpy.linalg.np_conserved.Array attribute), 222}
_\text{labels\_p} \quad \text{(tenpy.algorithms.exact\_diag.ExactDiag attribute), 216}
_\text{labels\_pconj} \quad \text{(tenpy.algorithms.exact\_diag.ExactDiag attribute), 216}
_\text{labels\_split} \quad \text{(tenpy.linalg.sparse.FlatLinearOperator attribute), 287}
_\text{mask} \quad \text{(tenpy.algorithms.exact\_diag.ExactDiag attribute), 216}
_\text{mask} \quad \text{(tenpy.linalg.charges.ChargeInfo attribute), 254}
_\text{mod\_masked} \quad \text{(tenpy.linalg.charges.ChargeInfo attribute), 287}
_\text{mps2lat\_vals\_idx\_fix\_u} \quad \text{(tenpy.models.lattice.Lattice attribute), 352}
_\text{mps\_fix\_u} \quad \text{(tenpy.models.lattice.Lattice attribute), 352}
_\text{npc\_matvec\_multileg} \quad \text{(tenpy.linalg.sparse.FlatLinearOperator attribute), 287}
_\text{old\_level} \quad \text{(tenpy.tools.optimization.temporary\_level attribute), 653}
_\text{order} \quad \text{(tenpy.models.lattice.Lattice attribute), 352}
_\text{perm} \quad \text{(tenpy.linalg.charges.LegPipe attribute), 267}
_\text{perm} \quad \text{(tenpy.models.lattice.Lattice attribute), 352}
_\text{pipe} \quad \text{(tenpy.algorithms.exact\_diag.ExactDiag attribute), 216}
_\text{pipe\_conj} \quad \text{(tenpy.algorithms.exact\_diag.ExactDiag attribute), 216}
_\text{qdata} \quad \text{(tenpy.linalg.np_conserved.Array attribute), 222}
_\text{qdata\_sorted} \quad \text{(tenpy.linalg.np_conserved.Array attribute), 222}
_\text{sites} \quad \text{(tenpy.algorithms.exact\_diag.ExactDiag attribute), 216}
_\text{strides} \quad \text{(tenpy.linalg.charges.LegPipe attribute), 267}
_\text{strides} \quad \text{(tenpy.models.lattice.Lattice attribute), 352}

A

acts\_on \quad \text{(tenpy.algorithms.mps\_common.EffectiveH attribute), 161}
acts\_on \quad \text{(tenpy.algorithms.mps\_common.OneSiteH attribute), 163}
acts\_on \quad \text{(tenpy.algorithms.mps\_common.TwoSiteH attribute), 165}
acts\_on \quad \text{(tenpy.linalg.sparse.NpcLinearOperator attribute), 292}
add() \quad \text{(tenpy.linalg.charges.ChargeInfo class method), 255}
add() \quad \text{(tenpy.networks.mpo.MPOGraph method), 584}
add\_charge() \quad \text{(tenpy.linalg.np\_conserved.Array method), 229}
add\_coupling() \quad \text{(tenpy.models.fermions\_spinless.FermionChain method), 475}
add\_coupling() \quad \text{(tenpy.models.hubbard.BoseHubbardChain method), 703}
add_coupling() (tenpy.models.hubbard.FermiHubbardChain method), 502
add_coupling() (tenpy.models.model.CouplingModel method), 404
add_coupling() (tenpy.models.model.MultiCouplingModel method), 417
add_coupling() (tenpy.models.spins.SpinsChain method), 463
add_coupling() (tenpy.models.tf_ising.TFIChain method), 435
add_coupling() (tenpy.models.xxz_chain.XXZChain2 method), 449
add_coupling_term() (tenpy.models.fermions_spinless.FermionChain method), 477
add_coupling_term() (tenpy.models.hubbard.BoseHubbardChain method), 491
add_coupling_term() (tenpy.models.hubbard.FermiHubbardChain method), 504
add_coupling_term() (tenpy.models.model.CouplingModel method), 406
add_coupling_term() (tenpy.models.model.MultiCouplingModel method), 419
add_coupling_term() (tenpy.models.spins.SpinsChain method), 462
add_coupling_term() (tenpy.models.tf_ising.TFIChain method), 434
add_coupling_term() (tenpy.models.xxz_chain.XXZChain2 method), 448
add_coupling_term() (tenpy.networks.terms.CouplingTerms method), 590
add_coupling_term() (tenpy.networks.terms.MultiCouplingTerms method), 598
add_exponentially_decaying_coupling() (tenpy.models.fermions_spinless.FermionChain method), 478
add_exponentially_decaying_coupling() (tenpy.models.hubbard.BoseHubbardChain method), 492
add_exponentially_decaying_coupling() (tenpy.models.hubbard.FermiHubbardChain method), 505
add_exponentially_decaying_coupling() (tenpy.models.model.CouplingModel method), 408
add_exponentially_decaying_coupling() (tenpy.models.model.MultiCouplingModel method), 419
add_exponentially_decaying_coupling() (tenpy.models.spins.SpinsChain method), 463
add_exponentially_decaying_coupling() (tenpy.models.tf_ising.TFIChain method), 435
add_exponentially_decaying_coupling() (tenpy.models.xxz_chain.XXZChain2 method), 449
add_leg() (tenpy.linalg.np_conserved.Array method), 228
add_local_term() (tenpy.models.fermions_spinless.FermionChain method), 479
add_local_term() (tenpy.models.hubbard.BoseHubbardChain method), 493
add_local_term() (tenpy.models.hubbard.FermiHubbardChain method), 506
add_local_term() (tenpy.models.model.CouplingModel method), 403
add_local_term() (tenpy.models.model.MultiCouplingModel method), 420
add_local_term() (tenpy.models.spins.SpinsChain method), 463
add_local_term() (tenpy.models.tf_ising.TFIChain method), 436
add_local_term() (tenpy.models.xxz_chain.XXZChain2 method), 450
add_missing_IdL_IdR() (tenpy.networks.mpo.MPOGraph method), 585
add_multi_coupling() (tenpy.models.fermions_spinless.FermionChain method), 479
add_multi_coupling() (tenpy.models.hubbard.BoseHubbardChain method), 493
add_multi_coupling() (tenpy.models.hubbard.FermiHubbardChain method), 506
add_multi_coupling() (tenpy.models.model.CouplingModel method), 406
add_multi_coupling() (tenpy.models.model.MultiCouplingModel method), 421
add_multi_coupling() (tenpy.models.spins.SpinsChain method), 464
add_multi_coupling()
(tenpy.models.tf_ising.TFIChain method), 436
add_multi_coupling()
(tenpy.models.xxz_chain.XXZChain2 method), 450
add_multi_coupling_term()
(tenpy.models.fermions_spinless.FermionChain method), 480
add_multi_coupling_term()
(tenpy.models.hubbard.BoseHubbardChain method), 494
add_multi_coupling_term()
(tenpy.models.hubbard.FermiHubbardChain method), 507
add_multi_coupling_term()
(tenpy.models.model.CouplingModel method), 408
add_multi_coupling_term()
(tenpy.models.model.MultiCouplingModel method), 422
add_multi_coupling_term()
(tenpy.models.spins.SpinChain method), 465
add_multi_coupling_term()
(tenpy.models.tf_ising.TFIChain method), 437
add_multi_coupling_term()
(tenpy.models.xxz_chain.XXZChain2 method), 451
add_multi_coupling_term()
(tenpy.networks.terms.MultiCouplingTerms method), 596
add_onsite_term()
(tenpy.models.fermions_spinless.FermionChain method), 481
add_onsite_term()
(tenpy.models.hubbard.BoseHubbardChain method), 495
add_onsite_term()
(tenpy.models.hubbard.FermiHubbardChain method), 508
add_onsite_term()
(tenpy.models.model.CouplingModel method), 404
add_onsite_term()
(tenpy.models.model.MultiCouplingModel method), 423
add_onsite_term()
(tenpy.models.spins.SpinChain method), 466
add_onsite_term()
(tenpy.models.tf_ising.TFIChain method), 438
add_onsite_term()
(tenpy.models.xxz_chain.XXZChain2 method), 452
add_onsite_term()
(tenpy.networks.terms.OnsiteTerms method), 601
add_op()
(tenpy.networks.site.BosonSite method), 530
add_op()
(tenpy.networks.site.FermionSite method), 535
add_op()
(tenpy.networks.site.GroupedSite method), 540
add_op()
(tenpy.networks.site.Site method), 545
add_op()
(tenpy.networks.site.SpinHalfFermionSite method), 550
add_op()
(tenpy.networks.site.SpinHalfSite method), 554
add_op()
(tenpy.networks.site.SpinSite method), 559
add_string()
(tenpy.networks.mpo.MPOGraph method), 585
add_to_graph()
(tenpy.networks.terms.CouplingTerms method), 591
add_to_graph()
(tenpy.networks.terms.ExponentiallyDecayingTerms method), 594
add_to_graph()
(tenpy.networks.terms.MultiCouplingTerms method), 597
add_to_graph()
(tenpy.networks.terms.OnsiteTerms method), 601
add_to_nn_bond_Arrays()
(tenpy.networks.terms.OnsiteTerms method), 601
add_trivial_leg()
(tenpy.linalg.np_conserved.Array method), 227
add_with_None_0()
(in module tenpy.tools.misc), 632
adjoint()
(tenpy.algorithms.mps_common.EffectiveH method), 161
adjoint()
(tenpy.algorithms.mps_common.OneSiteH method), 164
adjoint()
(tenpy.algorithms.mps_common.TwoSiteH method), 167

Index 705
adjoint() (tenpy.algorithms.purification.PurificationTwoSiteU method), 211
adjoint() (tenpy.linalg.sparse.FlatHermitianOperator method), 281
adjoint() (tenpy.linalg.sparse.FlatLinearOperator method), 289
adjoint() (tenpy.linalg.sparse.NpcLinearOperator method), 292
adjoint() (tenpy.linalg.sparse.NpcLinearOperatorWrapper method), 294
adjoint() (tenpy.linalg.sparse.OrthogonalNpcLinearOperator method), 295
adjoint() (tenpy.linalg.sparse.ShiftNpcLinearOperator method), 296
adjoint() (tenpy.networks.mps.TransferMatrix method), 575
alg_decay() (in module tenpy.tools.fit), 643
alg_decay_fit() (in module tenpy.tools.fit), 644
alg_decay_fit_res() (in module tenpy.tools.fit), 644
alg_decay_fits() (in module tenpy.tools.fit), 644
all_coupling_terms() (tenpy.models.fermions_spinless.FermionChain method), 481
all_coupling_terms() (tenpy.models.hubbard.BoseHubbardChain method), 495
all_coupling_terms() (tenpy.models.hubbard.FermiHubbardChain method), 508
all_coupling_terms() (tenpy.models.model.CouplingModel method), 404
all_coupling_terms() (tenpy.models.model.MultiCouplingModel method), 423
all_coupling_terms() (tenpy.models.spins.SpinChain method), 466
all_coupling_terms() (tenpy.models.tf_ising.TFIChain method), 438
all_onsite_terms() (tenpy.models.fermions_spinless.FermionChain method), 481
all_onsite_terms() (tenpy.models.hubbard.BoseHubbardChain method), 495
all_onsite_terms() (tenpy.models.hubbard.FermiHubbardChain method), 508
all_onsite_terms() (tenpy.models.model.CouplingModel method), 404
all_onsite_terms() (tenpy.models.model.MultiCouplingModel method), 423
all_onsite_terms() (tenpy.models.spins.SpinChain method), 466
all_onsite_terms() (tenpy.models.tf_ising.TFIChain method), 438
all_onsite_terms() (tenpy.models.xxz_chain.XXZChain2 method), 452
alg_decay() (in module tenpy.models.hubbard), 444
alg_decay_fit() (in module tenpy.models.hubbard), 444
alg_decay_fit_res() (in module tenpy.models.hubbard), 444
alg_decay_fits() (in module tenpy.models.hubbard), 444
as_completely_blocked() (tenpy.linalg.np_conserved.Array method), 232
atleast_2d_pad() (in module tenpy.models.hubbard), 633
attr_class (in module tenpy.models.hubbard), 622
ATTR_CLASS (in module tenpy.models.hubbard), 622
ATTR_FORMAT (in module tenpy.models.hubbard), 622
ATTR_LEN (in module tenpy.models.hubbard), 622
ATTR_MODULE (in module tenpy.models.hubbard), 622
ATTR_TYPE (in module tenpy.models.hubbard), 622
Array (class in tenpy.linalg.np_conserved), 221
as_completely_blocked() (tenpy.linalg.np_conserved.Array method), 232
asConfig() (in module tenpy.models.hubbard), 625
astype() (tenpy.linalg.np_conserved.Array method), 233
basis (tenpy.models.lattice.Lattice attribute), 352
bc (tenpy.models.lattice.Lattice attribute), 351
bc (tenpy.networks.mpo.MPOGraph attribute), 583
bc_MPS (tenpy.models.lattice.Lattice attribute), 352
bc_shift (tenpy.models.lattice.Lattice attribute), 352
binary_blockwise() (tenpy.linalg.np_conserved.Array method), 236
block_number (tenpy.linalg.charges.LegCharge attribute), 258
bond_energies() (tenpy.models.fermions_spinless.FermionChain method), 481
bond_energies() (tenpy.models.hubbard.BoseHubbardChain method), 495
bond_energies() (tenpy.models.hubbard.FermiHubbardChain method), 508
bond_energies() (tenpy.models.model.NearestNeighborModel method), 428
bond_energies() (tenpy.models.spins.SpinChain method), 466
bond_energies() (tenpy.models.tf_ising.TFIChain method), 438
bond_energies() (tenpy.models.xxz_chain.XXZChain2 method), 453
BoseHubbardChain (class in tenpy.models.hubbard), 489
BosonSite (class in tenpy.networks.site), 530
boundary_conditions() (tenpy.models.lattice.Chain property), 303
boundary_conditions() (tenpy.models.lattice.Honeycomb property), 312
boundary_conditions() (tenpy.models.lattice.IrregularLattice property), 323
boundary_conditions() (tenpy.models.lattice.Kagome property), 330
boundary_conditions() (tenpy.models.lattice.Ladder property), 340
boundary_conditions() (tenpy.models.lattice.Lattice property), 355
boundary_conditions() (tenpy.models.lattice.SimpleLattice property), 362
boundary_conditions() (tenpy.models.lattice.Square property), 371
boundary_conditions() (tenpy.models.lattice.Triangular property), 381
boundary_conditions() (tenpy.models.lattice.TrivialLattice property), 389
boundary_conditions() (tenpy.models.toric_code.DualSquare property), 519
box() (in module tenpy.linalg.random_matrix), 278
build_full_H_from_bonds() (tenpy.algorithms.exact_diag.ExactDiag method), 217
build_full_H_from_mpo() (tenpy.algorithms.exact_diag.ExactDiag method), 217
build_initial_state() (in module tenpy.networks.mps), 575
build_initial_state() (in module tenpy.tools.misc), 634
build_MPO() (tenpy.networks.mpo.MPOGraph method), 585
calc_H_MPO() (tenpy.models.spins.SpinChain method), 466
calc_H_MPO() (tenpy.models.tf_ising.TFIChain method), 438
calc_H_MPO() (tenpy.models.xxz_chain.XXZChain2 method), 433
calc_H_MPO_from_bond() (tenpy.models.fermions_spinless.FermionChain method), 482
calc_H_MPO_from_bond() (tenpy.models.hubbard.BoseHubbardChain method), 496
calc_H_MPO_from_bond() (tenpy.models.hubbard.FermiHubbardChain method), 509
calc_H_MPO_from_bond() (tenpy.models.model.NearestNeighborModel method), 428
calc_H_Oscsite() (tenpy.models.xxz_chain.XXZChain2 method), 466
calc_H_Oscsite() (tenpy.models.tf_ising.TFIChain method), 439
calc_H_Oscsite() (tenpy.models.xxz_chain.XXZChain2 method), 453
calc_H_Oscsite() (tenpy.models.spins.SpinChain method), 482
calc_H_Oscsite() (tenpy.models.hubbard.BoseHubbardChain method), 496
calc_H_Oscsite() (tenpy.models.hubbard.FermiHubbardChain method), 509
calc_H_Oscsite() (tenpy.models.model.CouplingModel method), 409
calc_H_Oscsite() (tenpy.models.model.MultiCouplingModel method), 423
calc_H_Oscsite() (tenpy.models.spins.SpinChain method), 467
calc_H_Oscsite() (tenpy.models.tf_ising.TFIChain method), 439
calc_H_Oscsite() (tenpy.models.xxz_chain.XXZChain2 method), 453
calc_U() (tenpy.algorithms.purification.PurificationTEBDcombine_Heff() (tenpy.algorithms.mps_common.OneSiteH method), 201
calc_U() (tenpy.algorithms.purification.PurificationTEBDcombine_Heff() (tenpy.algorithms.mps_common.TwoSiteH method), 206
callback() (tenpy.tools.events.Listener property), 630
central_charge_from_s_profile() (in module tenpy.tools.fit), 644
Chain (class in tenpy.models.lattice), 303
change() (tenpy.linalg.charges.ChargeInfo class method), 255
change_charge() (tenpy.linalg.np_conserved.Array combine_theta() (tenpy.algorithms.mps_common.TwoSiteH method), 161
change_charge() (tenpy.linalg.np_conserved.Array combine_theta() (tenpy.algorithms.mps_common.OneSiteH method), 161
change_charge() (tenpy.linalg.np_conserved.Array change_charge() (tenpy.networks.site.BosonSite method), 531
change_charge() (tenpy.networks.site.FermionSite method), 535
change_charge() (tenpy.networks.site.GroupedSite method), 540
change_charge() (tenpy.networks.site.Site method), 545
change_charge() (tenpy.networks.site.SpinHalfFermionSite method), 550
change_charge() (tenpy.networks.site.SpinHalfSite method), 555
charge_sector() (tenpy.algorithms.exact_diag.ExactDiag attribute), 216
charge_sector() (tenpy.linalg.sparse.FlatHermitianOperator property), 281
charge_sector() (tenpy.linalg.sparse.FlatLinearOperator property), 287
charge_sectors() (tenpy.linalg.charges.LegCharge method), 264
charge_sectors() (tenpy.linalg.charges.LegPipe method), 269
ChargeInfo (class in tenpy.linalg.charges), 254
charges (tenpy.linalg.charges.LegCharge attribute),
check_valid() (tenpy.linalg.charges.ChargeInfo method), 256
chi_list() (in module tenpy.algorithms.dmrq), 191
chiinfo (tenpy.algorithms.exact_diag.ExactDiag attribute), 215
chiinfo (tenpy.linalg.charges.LegCharge attribute), 258
chiinfo (tenpy.linalg.np_conserved.Array attribute), 222
chiinfo (tenpy.networks.mpo.MPOGraph attribute), 583
COE() (in module tenpy.linalg.random_matrix), 276
combine (tenpy.algorithms.mps_common.EffectiveH attribute), 161
combine (tenpy.algorithms.mps_common.TwoSiteH attribute), 165
combine (tenpy.algorithms.mps_common.TwoSiteH attribute), 166
combine_Heff() (tenpy.algorithms.mps_common.OneSiteH method), 163
combine_Heff() (tenpy.algorithms.mps_common.TwoSiteH method), 166
combine_legs() (tenpy.linalg.np_conserved.Array method), 230
combine_theta() (tenpy.algorithms.mps_common.EffectiveH method), 161
TeNPy, Release 0.7.2.dev55+68eae2c

coupling_term_handle_JW()
(tenpy.networks.terms.CouplingTerms method), 590
coupling_terms()
(tenpy.networks.terms.CouplingTerms method), 598
coupling_terms()
(tenpy.models.models.CouplingModel attribute), 402
coupling_terms()
(tenpy.networks.terms.CouplingTerms attribute), 589
coupling_terms()
(tenpy.models.models.MultiCouplingTerms attribute), 596
CouplingModel (class in tenpy.models.models), 402
CouplingTerms (class in tenpy.networks.terms), 589
create_group_for_obj()
(tenpy.tools.hdf5.io.Hdf5Saver method), 617
CUE () (in module tenpy.linalg.random_matrix), 276

D
DefaultMixer (tenpy.algorithms.dmrg.EngineCombine attribute), 172
DefaultMixer (tenpy.algorithms.dmrg.EngineFracture attribute), 180
del_LP ()
(tenpy.networks.mps.MPSEnvironment method), 581
del_LP ()
(tenpy.networks.mps.MPSEnvironment method), 571
del_RP ()
(tenpy.networks.mpo.MPOEnvironment method), 581
del_RP ()
(tenpy.networks.mps.MPSEnvironment method), 571
DensityMatrixMixer (class in tenpy.algorithms.dmrg), 168
detect_grid_outer_legcharge() (in module tenpy.linalg.np_conserved), 238
detect_legcharge() (in module tenpy.linalg.np_conserved), 238
detect_qtotal() (in module tenpy.linalg.np_conserved), 239
diag () (in module tenpy.linalg.np_conserved), 239
diag ()
(tenpy.algorithms.dmrg.EngineCombine method), 172
diag ()
(tenpy.algorithms.dmrg.EngineFracture method), 180
dim(tenpy.models.lattice.Chain attribute), 303
dim(tenpy.models.lattice.Honeycomb attribute), 310
dim(tenpy.models.lattice.Kagome attribute), 331
dim(tenpy.models.lattice.Ladder attribute), 340
dim(tenpy.models.lattice.Square attribute), 371
dim(tenpy.models.lattice.Triangular attribute), 381
dim ()
(tenpy.models.lattice.IrregularLattice property), 323
dim ()
(tenpy.models.lattice.Lattice property), 353
dim ()
(tenpy.models.lattice.SimpleLattice property), 363
dim ()
(tenpy.models.lattice.TrivialLattice property), 390
dim ()
(tenpy.models.toric_code.DualSquare property), 590
dim ()
(tenpy.networks.site.BosonSite property), 531
dim ()
(tenpy.networks.site.FermionSite property), 535
dim ()
(tenpy.networks.site.GroupedSite property), 540
dim ()
(tenpy.networks.site.SpinHalfFermionSite property), 551
dim ()
(tenpy.networks.site.SpinHalfSite property), 555
dim ()
(tenpy.networks.site.SpinSite property), 559
disconnect ()
(tenpy.tools.events.EventHandler method), 629
disent_iterations ()
(tenpy.algorithms.purification.PurificationTEBD property), 201
disent_iterations ()
(tenpy.algorithms.purification.PurificationTEBD2 property), 206
disentangle ()
(tenpy.algorithms.purification.PurificationTEBD method), 202
disentangle ()
(tenpy.algorithms.purification.PurificationTEBD2 method), 207
disentangle_global ()
(tenpy.algorithms.purification.PurificationTEBD method), 202
disentangle_global ()
(tenpy.algorithms.purification.PurificationTEBD2 method), 207
disentangle_global() (tenpy.algorithms.purification.PurificationTEBD method), 202
disentangle_global() (tenpy.algorithms.purification.PurificationTEBD2 method), 207
disentangle_global_nsite() (tenpy.algorithms.purification.PurificationTEBD method), 202
disentangle_global_nsite() (tenpy.algorithms.purification.PurificationTEBD2 method), 207
disentangle_n_site() (tenpy.algorithms.purification.PurificationTEBD method), 202
disentangle_n_site() (tenpy.algorithms.purification.PurificationTEBD2 method), 207
dispatch_load (tenpy.tools.hdf5.io.Hdf5Loader attribute), 613
dispatch_save (tenpy.tools.hdf5.io.Hdf5Saver attribute), 616
dot ()
(tenpy.linalg.sparse.FlatHermitianOperator method), 281
dot ()
(tenpy.linalg.sparse.FlatLinearOperator method), 289
drop ()
(tenpy.linalg.charges.ChargeInfo class method), 255
drop_charge() (tenpy.linalg.np_conserved.Array method), 229
dtype (tenpy.algorithms.mps_common.EffectiveH attribute), 161
dtype (tenpy.linalg.np_conserved.Array attribute), 222
dtype (tenpy.linalg.sparse.FlatLinearOperator attribute), 286
dtype (tenpy.linalg.sparse.NpcLinearOperator attribute), 292
dtype (tenpy.networks.mps.MPSEnvironment attribute), 569
DualSquare (class in tenpy.models.toric_code), 519

e (tenpy.algorithms.exact_diag.ExactDiag attribute), 216
EffectiveH (class in tenpy.algorithms.mps_common), 160
EffectiveH (tenpy.algorithms.dmrg.EngineCombine attribute), 172
EffectiveH (tenpy.algorithms.dmrg.EngineFracture attribute), 180
EffectiveH (tenpy.algorithms.purification.PurificationApplyMPO attribute), 198
eig() (in module tenpy.linalg.np_conserved), 240
eigenvectors() (tenpy.linalg.sparse.FlatHermitianOperator method), 284
eigenvectors() (tenpy.linalg.sparse.FlatLinearOperator method), 288
eigenvectors() (tenpy.networks.mps.TransferMatrix method), 575
eigh() (in module tenpy.linalg.np_conserved), 240
eigvals() (in module tenpy.linalg.np_conserved), 241
eigvalsh() (in module tenpy.linalg.np_conserved), 241
emit() (tenpy.tools.events.EventHandler method), 630
emit_until_result() (tenpy.tools.events.EventHandler method), 630
EngineCombine (class in tenpy.algorithms.dmrg), 172
EngineFracture (class in tenpy.algorithms.dmrg), 180
enlarge_mps_unit_cell() (tenpy.models.lattice.IrregularLattice method), 323
enlarge_mps_unit_cell() (tenpy.models.lattice.Kagome method), 331
enlarge_mps_unit_cell() (tenpy.models.lattice.Ladder method), 341
enlarge_mps_unit_cell() (tenpy.models.lattice.Lattice method), 355
enlarge_mps_unit_cell() (tenpy.models.lattice.SimpleLattice method), 363
enlarge_mps_unit_cell() (tenpy.models.lattice.Square method), 372
enlarge_mps_unit_cell() (tenpy.models.lattice.Triangular method), 381
enlarge_mps_unit_cell() (tenpy.models.lattice.TrivialLattice method), 390
enlarge_mps_unit_cell() (tenpy.models.model.CouplingModel method), 410
enlarge_mps_unit_cell() (tenpy.models.model.MPOModel method), 412
enlarge_mps_unit_cell() (tenpy.models.model.MultiCouplingModel method), 425
enlarge_mps_unit_cell() (tenpy.models.model.NearestNeighborModel method), 428
enlarge_mps_unit_cell() (tenpy.models.spins.SpinChain method), 468
enlarge_mps_unit_cell() (tenpy.models.if_ising.TFIChain method), 440
enlarge_mps_unit_cell() (tenpy.models.toric_code.DualSquare method), 521
enlarge_mps_unit_cell() (tenpy.models.xxz_chain.XXZChain2 method), 454
entropy() (in module tenpy.tools.math), 639
entropy_profile_from_CFT() (in module tenpy.tools.fit), 645
environment_sweeps() (tenpy.algorithms.dmrg.EngineCombine method), 173
environment_sweeps()
(tenpy.algorithms.dmrg.EngineFracture method), 181
environment_sweeps()
(tenpy.algorithms.purification.PurificationApplyMPO method), 198
eps (tenpy.algorithms.truncation.TruncationError attribute), 155
EventHandler (class in tenpy.tools.events), 628
ExactDiag (class in tenpy.algorithms.exact_diag), 215
exp_decaying_terms
(tenpy.models.model.CouplingModel attribute), 402
exp_decaying_terms
(tenpy.networks.terms.ExponentiallyDecayingTerms attribute), 593
exp_H() (tenpy.algorithms.exact_diag.ExactDiag method), 217
expectation_value()
(tenpy.networks.mpo.MPOEnvironment method), 581
expectation_value()
(tenpy.networks.mps.MPSEnvironment method), 571
explicit_plushc (tenpy.models.model.CouplingModel attribute), 403
expm() (in module tenpy.linalg.np_conserved), 242
ExponentiallyDecayingTerms (class in tenpy.networks.terms), 593
extend() (tenpy.linalg.charges.LegCharge method), 264
extend() (tenpy.linalg.charges.LegPipe method), 269
extend() (tenpy.linalg.np_conserved.Array method), 228
eye_like() (in module tenpy.linalg.np_conserved), 242
FermiHubbardChain (class in tenpy.models.hubbard), 502
FermionChain (class in tenpy.models.fermions_spinless), 475
FermionSite (class in tenpy.networks.site), 534
filling (tenpy.networks.site.BosonSite attribute), 530
filling (tenpy.networks.site.FermionSite attribute), 535
filling (tenpy.networks.site.SpinHalfFermionSite attribute), 550
find_global() (tenpy.tools.hdf5_io.Hdf5Loader static method), 614
fit_with_sum_of_exp() (in module tenpy.tools.fit), 645
flat_linop (tenpy.networks.mps.TransferMatrix attribute), 574
flat_to_npc() (tenpy.linalg.sparse.FlatHermitianOperator method), 281
flat_to_npc() (tenpy.linalg.sparse.FlatLinearOperator method), 287
flat_to_npc_all_sectors()
(tenpy.linalg.sparse.FlatHermitianOperator method), 282
flat_to_npc_all_sectors()
(tenpy.linalg.sparse.FlatLinearOperator method), 288
flat_to_npc_None_sector()
(tenpy.linalg.sparse.FlatHermitianOperator method), 288
FlatHermitianOperator (class in tenpy.linalg.sparse), 281
FlatLinearOperator (class in tenpy.linalg.sparse), 286
flip_charges_qconj()
(tenpy.linalg.charges.LegCharge method), 261
flip_charges_qconj()
(tenpy.linalg.charges.LegPipe method), 269
form (tenpy.networks.mps.TransferMatrix attribute), 574
format_selection (tenpy.tools.hdf5_io.Hdf5Saver attribute), 616
from_add_charge()
(tenpy.linalg.charges.LegCharge class method), 260
from_add_charge()
(tenpy.linalg.charges.LegPipe class method), 269
from_change_charge()
(tenpy.linalg.charges.LegCharge class method), 260
from_change_charge()
(tenpy.linalg.charges.LegPipe class method), 270
from_drop_charge()
(tenpy.linalg.charges.LegCharge class method), 260
from_drop_charge()
(tenpy.linalg.charges.LegPipe class method), 270
from_func()
(tenpy.linalg.np_conserved.Array class method), 224
from_func_square()
(tenpy.linalg.np_conserved.Array class method), 225
from_guess_with_pipe()
(tenpy.linalg.sparse.FlatHermitianOperator class method), 282
from_guess_with_pipe()
from NpcArray() (tenpy.linalg.sparse.FlatHermitianOperator class method), 282
from NpcArray() (tenpy.linalg.sparse.FlatLinearOperator class method), 287
from qdict() (tenpy.linalg.charges.LegCharge class method), 260
from qdict() (tenpy.linalg.charges.LegPipe class method), 270
from qflat() (tenpy.linalg.charges.LegCharge class method), 259
from qflat() (tenpy.linalg.charges.LegPipe class method), 270
from qind() (tenpy.linalg.charges.LegCharge class method), 260
from qind() (tenpy.linalg.charges.LegPipe class method), 271
from S() (tenpy.algorithms.truncation.TruncationError class method), 155
from_term_list() (tenpy.networks.mpo.MPOGraph class method), 584
from_terms() (tenpy.networks.mpo.MPOGraph class method), 584
from_trivial() (tenpy.linalg.charges.LegCharge class method), 259
from_trivial() (tenpy.linalg.charges.LegPipe class method), 271
full_contraction() (tenpy.networks.mpo.MPOEnvironment method), 581
full_contraction() (tenpy.networks.mps.MPSEnvironment method), 571
full_diag_effH() (in module tenpy.algorithms.dmrg), 191
full_diagonalization() (tenpy.algorithms.exact_diag.ExactDiag method), 217
full_H (tenpy.algorithms.exact_diag.ExactDiag attribute), 216
full_to_mps() (tenpy.algorithms.exact_diag.ExactDiag method), 217
full_version (in module tenpy.version), 657

gauge_hopping() (in module tenpy.models.hofstadter), 514
gauge_total_charge() (tenpy.linalg.np_conserved.Array method), 228
gcd() (in module tenpy.tools.math), 640
gcd_array() (in module tenpy.tools.math), 640
get_attr() (tenpy.tools.hdf5_io.Hdf5Loader static method), 614

gcdd() (in module tenpy.models.lattice), 397
get_leg() (tenpy.linalg.np_conserved.Array method), 226
get_leg_index() (tenpy.linalg.np_conserved.Array method), 226
get_leg_indices() (tenpy.linalg.np_conserved.Array method), 226
get_leg_labels() (tenpy.linalg.np_conserved.Array method), 226
get_level() (in module tenpy.tools.optimization), 654
get_LP() (tenpy.networks.mpo.MPOEnvironment method), 580
get_LP() (tenpy.networks.mps.MPSEnvironment method), 570
get_LP_age() (tenpy.networks.mpo.MPOEnvironment method), 581
get_LP_age() (tenpy.networks.mps.MPSEnvironment method), 570
get_op() (tenpy.networks.site.BosonSite method), 531
get_op() (tenpy.networks.site.FermionSite method), 536
load_general_dict() (tenpy.tools.hdf5_io.Hdf5Loader method), 614
load_global() (tenpy.tools.hdf5_io.Hdf5Loader method), 615
load_hdf5exportable() (tenpy.tools.hdf5_io.Hdf5Loader method), 615
load_ignored() (tenpy.tools.hdf5_io.Hdf5Loader method), 615
load_list() (tenpy.tools.hdf5_io.Hdf5Loader method), 614
load_none() (tenpy.tools.hdf5_io.Hdf5Loader method), 614
load_omp_library() (in module tenpy.tools.process), 649
load_range() (tenpy.tools.hdf5_io.Hdf5Loader method), 614
load_reduce() (tenpy.tools.hdf5_io.Hdf5Loader method), 615
load_set() (tenpy.tools.hdf5_io.Hdf5Loader method), 614
load_simple_dict() (tenpy.tools.hdf5_io.Hdf5Loader method), 614
load_str() (tenpy.tools.hdf5_io.Hdf5Loader method), 614
load_tuple() (tenpy.tools.hdf5_io.Hdf5Loader method), 614
Lp (tenpy.algorithms.tdvp.H0_mixed attribute), 193
Lp (tenpy.algorithms.tdvp.H1_mixed attribute), 194
Lp (tenpy.algorithms.tdvp.H2_mixed attribute), 195
Ls (tenpy.models.lattice.Lattice attribute), 351
Lu (tenpy.models.lattice.Honeycomb attribute), 310
Lu (tenpy.models.lattice.Kagome attribute), 338
Lu (tenpy.models.lattice.Ladder attribute), 340
Lu (tenpy.models.lattice.Lattice attribute), 352
Lu (tenpy.models.lattice.SimpleLattice attribute), 362
make_eff_H() (tenpy.algorithms.dmrg.EngineCombine method), 174
make_eff_H() (tenpy.algorithms.dmrg.EngineFracture method), 182
make_eff_H() (tenpy.algorithms.purification.PurificationApplyMPO method), 198
make_pipe() (tenpy.linalg.np_conserved.Array method), 230
make_valid() (tenpy.linalg.charges.ChargeInfo method), 256
make_W_II() (in module tenpy.networks.mpo), 586
map_incoming_flat() (tenpy.linalg.charges.LegPipe method), 269
matmat() (tenpy.linalg.sparse.FlatHermitianOperator method), 283
matmat() (tenpy.linalg.sparse.FlatLinearOperator method), 290
matvec() (tenpy.algorithms.exact_diag.ExactDiag method), 217
matvec() (tenpy.algorithms.mps_common.EffectiveH method), 161
matvec() (tenpy.algorithms.mps_common.OneSiteH method), 163
matvec() (tenpy.algorithms.mps_common.TwoSiteH method), 166
matvec() (tenpy.algorithms.purification.PurificationTwoSiteU method), 211
matvec() (tenpy.linalg.np_conserved.Array method), 236
max_range (tenpy.networks.mpo.MPOGraph attribute), 583
max_range() (tenpy.networks.terms.CouplingTerms method), 590
max_range() (tenpy.networks.terms.ExponentiallyDecayingTerms method), 594
max_range() (tenpy.networks.terms.MultiCouplingTerms method), 597
max_range() (tenpy.networks.terms.OnsiteTerms method), 601
max_size (tenpy.algorithms.exact_diag.ExactDiag attribute), 216
memo_load (tenpy.tools.hdf5_io.Hdf5Loader attribute), 613
memo_save (tenpy.tools.hdf5_io.Hdf5Saver attribute), 616
memory_usage() (in module tenpy.tools.process), 649
mix_rho_L() (tenpy.algorithms.dmrg.DensityMatrixMixer method), 169
mix_rho_R() (tenpy.algorithms.dmrg.DensityMatrixMixer method), 169
mixed_svd() (tenpy.algorithms.dmrg.EngineCombine method), 221

M

make_eff_H() (tenpy.algorithms.dmrg.EngineCombine method), 174
make_eff_H() (tenpy.algorithms.dmrg.EngineFracture method), 182
make_eff_H() (tenpy.algorithms.purification.PurificationApplyMPO method), 198
make_pipe() (tenpy.linalg.np_conserved.Array method), 230
make_valid() (tenpy.linalg.charges.ChargeInfo method), 256
make_W_II() (in module tenpy.networks.mpo), 586
map_incoming_flat() (tenpy.linalg.charges.LegPipe method), 269
matmat() (tenpy.linalg.sparse.FlatHermitianOperator method), 283
matmat() (tenpy.linalg.sparse.FlatLinearOperator method), 290
matvec() (tenpy.algorithms.exact_diag.ExactDiag method), 217
matvec() (tenpy.algorithms.mps_common.EffectiveH method), 161
matvec() (tenpy.algorithms.mps_common.OneSiteH method), 163
matvec() (tenpy.algorithms.mps_common.TwoSiteH method), 166
matvec() (tenpy.algorithms.purification.PurificationTwoSiteU method), 211
matvec() (tenpy.linalg.np_conserved.Array method), 236
max_range (tenpy.networks.mpo.MPOGraph attribute), 583
max_range() (tenpy.networks.terms.CouplingTerms method), 590
max_range() (tenpy.networks.terms.ExponentiallyDecayingTerms method), 594
max_range() (tenpy.networks.terms.MultiCouplingTerms method), 597
max_range() (tenpy.networks.terms.OnsiteTerms method), 601
max_size (tenpy.algorithms.exact_diag.ExactDiag attribute), 216
memo_load (tenpy.tools.hdf5_io.Hdf5Loader attribute), 613
memo_save (tenpy.tools.hdf5_io.Hdf5Saver attribute), 616
memory_usage() (in module tenpy.tools.process), 649
mix_rho_L() (tenpy.algorithms.dmrg.DensityMatrixMixer method), 169
mix_rho_R() (tenpy.algorithms.dmrg.DensityMatrixMixer method), 169
mixed_svd() (tenpy.algorithms.dmrg.EngineCombine method), 221
mixed_svd() (tenpy.algorithms.dmrg.EngineFracture method), 174
mixer_activate() (tenpy.algorithms.dmrg.EngineCombine method), 174
mixer_activate() (tenpy.algorithms.dmrg.EngineFracture method), 182
mixer_cleanup() (tenpy.algorithms.dmrg.EngineCombine method), 175
mixer_cleanup() (tenpy.algorithms.dmrg.EngineFracture method), 182
mkl_get_nthreads() (in module tenpy.tools.process), 649
mkl_set_nthreads() (in module tenpy.tools.process), 650
mod() (tenpy.linalg.charges.ChargeInfo property), 256
Model (class in tenpy.models.model), 414
model (tenpy.algorithms.exact_diag.ExactDiag attribute), 215
module
tenpy, 152
tenpy.algorithms, 153
tenpy.algorithms.dmrg, 191
tenpy.algorithms.exact_diag, 218
tenpy.algorithms.mpo_evolution, 212
tenpy.algorithms.mps_common, 166
tenpy.algorithms.network_contractor, 214
tenpy.algorithms.purification, 211
tenpy.algorithms.tdvp, 195
tenpy.algorithms.tebd, 158
tenpy.linalg, 218
tenpy.linalg.charges, 273
tenpy.linalg.lanczos, 300
tenpy.linalg.np_conserved, 251
tenpy.linalg.random_matrix, 278
tenpy.linalg.sparse, 297
tenpy.linalg.svd, 275
tenpy.models, 300
tenpy.models.fermions_spinless, 486
tenpy.models.haldane, 516
tenpy.models.hofstadter, 515
tenpy.models.hubbard, 513
tenpy.models.lattice, 400
tenpy.models.model, 429
tenpy.models.spins, 471
tenpy.models.spins_nnn, 472
tenpy.models.tf_ising, 443
tenpy.models.toric_code, 527
tenpy.models.xzz_chain, 457
tenpy.networks, 527
tenpy.networks.mpo, 587
tenpy.networks.mps, 576
tenpy.networks.purification_mps, 607
tenpy.networks.site, 566
tenpy.networks.terms, 606
tenpy.tools, 609
tenpy.tools.events, 631
tenpy.tools.fit, 647
tenpy.tools.hdf5_io, 621
tenpy.tools.math, 643
tenpy.tools.misc, 639
tenpy.tools.optimization, 656
tenpy.tools.params, 627
tenpy.tools.process, 650
tenpy.tools.string, 648
tenpy.version, 657
move_right (tenpy.algorithms.mps_common.EffectiveH attribute), 161
MPOEnvironment (class in tenpy.networks.mpo), 579
MPOGraph (class in tenpy.networks.mpo), 583
MPOModel (class in tenpy.models.model), 412
mps2lat_idx() (tenpy.models.lattice.Chain method), 304
mps2lat_idx() (tenpy.models.lattice.Honeycomb method), 314
mps2lat_idx() (tenpy.models.lattice.IrregularLattice method), 324
mps2lat_idx() (tenpy.models.lattice.Kagome method), 332
mps2lat_idx() (tenpy.models.lattice.Ladder method), 342
mps2lat_idx() (tenpy.models.lattice.Lattice method), 355
mps2lat_idx() (tenpy.models.lattice.SimpleLattice method), 364
mps2lat_idx() (tenpy.models.lattice.Square method), 373
mps2lat_idx() (tenpy.models.lattice.Triangular method), 382
mps2lat_idx() (tenpy.models.lattice.TrivialLattice method), 390
mps2lat_idx() (tenpy.models.toric_code.DualSquare method), 522
mps2lat_values() (tenpy.models.lattice.Chain method), 305
mps2lat_values() (tenpy.models.lattice.Honeycomb method), 314
mps2lat_values() (tenpy.models.lattice.IrregularLattice method), 324
mps2lat_values() (tenpy.models.lattice.Kagome method), 332
mps2lat_values() (tenpy.models.lattice.Ladder method), 342
mps2lat_values() (tenpy.models.lattice.Lattice method), 356
mps2lat_values() (tenpy.models.lattice.SimpleLattice method), 390
mps2lat_values() (tenpy.models.toric_code.DualSquare method), 522
mps2lat_values() (tenpy.models.toric_code.DualSquare method), 522
Index 719
mps2lat_values() (tenpy.models.lattice.Square method), 373
mps2lat_values() (tenpy.models.lattice.Triangular method), 382
mps2lat_values() (tenpy.models.lattice.TrivialLattice method), 390
mps2lat_values() (tenpy.models.toric_code.DualSquare method), 522
mps2lat_values_masked() (tenpy.models.lattice.Chain method), 305
mps2lat_values_masked() (tenpy.models.lattice.Honeycomb method), 315
mps2lat_values_masked() (tenpy.models.lattice.IrregularLattice method), 325
mps2lat_values_masked() (tenpy.models.lattice.Kagome method), 333
mps2lat_values_masked() (tenpy.models.lattice.Ladder method), 343
mps2lat_values_masked() (tenpy.models.lattice.Lattice method), 357
mps2lat_values_masked() (tenpy.models.lattice.SimpleLattice method), 364
mps2lat_values_masked() (tenpy.models.lattice.Square method), 373
mps2lat_values_masked() (tenpy.models.lattice.Triangular method), 382
mps2lat_values_masked() (tenpy.models.lattice.TrivialLattice method), 391
mps2lat_values_masked() (tenpy.models.toric_code.DualSquare method), 523
mps_idx_fix_u() (tenpy.models.lattice.Chain method), 305
mps_idx_fix_u() (tenpy.models.lattice.Honeycomb method), 315
mps_idx_fix_u() (tenpy.models.lattice.IrregularLattice method), 325
mps_idx_fix_u() (tenpy.models.lattice.Kagome method), 333
mps_idx_fix_u() (tenpy.models.lattice.Ladder method), 343
mps_idx_fix_u() (tenpy.models.lattice.Lattice method), 356
mps_idx_fix_u() (tenpy.models.lattice.SimpleLattice method), 365
mps_idx_fix_u() (tenpy.models.lattice.Square method), 374
mps_idx_fix_u() (tenpy.models.lattice.Triangular method), 383
mps_idx_fix_u() (tenpy.models.lattice.TrivialLattice method), 392
mps_idx_fix_u() (tenpy.models.toric_code.DualSquare method), 523
mps_sites() (tenpy.models.lattice.Chain method), 306
mps_sites() (tenpy.models.lattice.Honeycomb method), 316
mps_sites() (tenpy.models.lattice.IrregularLattice method), 325
mps_sites() (tenpy.models.lattice.Kagome method), 334
mps_sites() (tenpy.models.lattice.Ladder method), 344
mps_sites() (tenpy.models.lattice.Lattice method), 355
mps_sites() (tenpy.models.lattice.SimpleLattice method), 365
mps_sites() (tenpy.models.lattice.Square method), 374
mps_sites() (tenpy.models.lattice.Triangular method), 383
mps_sites() (tenpy.models.lattice.TrivialLattice method), 392
mps_sites() (tenpy.models.toric_code.DualSquare method), 523
method), 524

mps_to_full() (tenpy.algorithms.exact_diag.ExactDiag method), 217

MPSEnvironment (class in tenpy.networks.mps), 568

multi_coupling_shape() (tenpy.models.lattice.Chain method), 306

multi_coupling_shape() (tenpy.models.lattice.Honeycomb method), 316

multi_coupling_shape() (tenpy.models.lattice.IrregularLattice method), 325

multi_coupling_shape() (tenpy.models.lattice.Kagome method), 334

multi_coupling_shape() (tenpy.models.lattice.Ladder method), 344

multi_coupling_shape() (tenpy.models.lattice.Lattice method), 359

multi_coupling_shape() (tenpy.models.lattice.SimpleLattice method), 365

multi_coupling_shape() (tenpy.models.lattice.Square method), 374

multi_coupling_shape() (tenpy.models.lattice.Triangular method), 383

multi_coupling_shape() (tenpy.models.lattice.TrivialLattice method), 392

multi_coupling_shape() (tenpy.models.toric_code.DualSquare method), 524

multi_coupling_term_handle_JW() (tenpy.networks.terms.MultiCouplingTerms method), 597

multi_sites_combine_charges() (in module tenpy.networks.site), 562

MultiCouplingModel (class in tenpy.models.model), 417

MultiCouplingTerms (class in tenpy.networks.terms), 596

multiply_op_names() (tenpy.networks.site.BosonSite method), 551

multiply_op_names() (tenpy.networks.site.FermionSite method), 555

multiply_op_names() (tenpy.networks.site.SpinHalfFermionSite method), 560

multiply_op_names() (tenpy.networks.site.SpinSite method), 560

multiply_operators() (tenpy.networks.site.BosonSite method), 532

multiply_operators() (tenpy.networks.site.FermionSite method), 536

multiply_operators() (tenpy.networks.site.GroupedSite method), 541

multiply_operators() (tenpy.networks.site.Site method), 547

multiply_operators() (tenpy.networks.site.SpinHalfFermionSite method), 551

multiply_operators() (tenpy.networks.site.SpinHalfSite method), 556

multiply_operators() (tenpy.networks.site.SpinSite method), 560

N

N (tenpy.algorithms.mps_common.EffectiveH attribute), 161

N_cells (tenpy.models.lattice.Lattice attribute), 351

n_optimize() (tenpy.algorithms.dmrg.EngineCombine property), 175

n_optimize() (tenpy.algorithms.dmrg.EngineFracture property), 183

n_optimize() (tenpy.algorithms.purification.PurificationApplyMPO property), 198

N_rings (tenpy.models.lattice.Lattice attribute), 351

N_sites (tenpy.models.lattice.Lattice attribute), 351

n_sites (tenpy.networks.site.GroupedSite attribute), 539

N_sites_per_ring (tenpy.models.lattice.Lattice attribute), 351

name (tenpy.tools.hdf5_io.Hdf5Ignored attribute), 612

names (tenpy.linalg.charges.ChargeInfo attribute), 254

ncon() (in module tenpy.algorithms.network_contractor), 213

ndim() (tenpy.linalg.np_conserved.Array property), 226

NearestNeighborModel (class in tenpy.models.model), 427

need_JW_string (tenpy.networks.site.Site attribute), 544

nlegs (tenpy.linalg.charges.LegPipe attribute), 266

norm() (in module tenpy.linalg.np_conserved), 245
norm() ([tenpy.linalg.np_conserved.Array method], 235)
npc_matvec ([tenpy.linalg.sparse.FlatLinearOperator attribute], 286)
npc_to_flat() ([tenpy.linalg.sparse.FlatLinearOperator method], 283)
npc_to_flat() ([tenpy.linalg.sparse.FlatHermitianOperator method], 288)
npc_to_flat_all_sectors() ([tenpy.linalg.sparse.FlatHermitianOperator method], 283)
npc_to_flat_all_sectors() ([tenpy.linalg.sparse.FlatLinearOperator method], 288)
NpcLinearOperator ([class in tenpy.linalg.sparse], 292)
NpcLinearOperatorWrapper ([class in tenpy.linalg.sparse], 293)
number_nearest_neighbors() ([tenpy.models.lattice.Chain method], 306)
number_nearest_neighbors() ([tenpy.models.lattice.Honeycomb method], 316)
number_nearest_neighbors() ([tenpy.models.lattice.IrregularLattice method], 326)
number_nearest_neighbors() ([tenpy.models.lattice.Kagome method], 334)
number_nearest_neighbors() ([tenpy.models.lattice.Ladder method], 344)
number_nearest_neighbors() ([tenpy.models.lattice.SimpleLattice method], 365)
number_nearest_neighbors() ([tenpy.models.lattice.Square method], 374)
number_nearest_neighbors() ([tenpy.models.lattice.Triangular method], 383)
number_nearest_neighbors() ([tenpy.models.lattice.TrivialLattice method], 393)
number_nearest_neighbors() ([tenpy.models.toric_code.DualSquare method], 524)
O_close_1() ([in module tenpy.linalg.random_matrix], 277)
omp_get_nthreads() ([in module tenpy.tools.process], 650)
omp_set_nthreads() ([in module tenpy.tools.process], 650)
one() ([in module tenpy.linalg.np_conserved], 246)
OneSiteH ([class in tenpy.algorithms.mps_common], 162)
onsite_ops() ([tenpy.networks.site.BosonSite property], 532)
onsite_ops() ([tenpy.networks.site.FermionSite property], 536)
onsite_ops() ([tenpy.networks.site.GroupedSite property], 541)
onsite_ops() ([tenpy.networks.site.Site property], 545)
onsite_ops() ([tenpy.networks.site.SpinHalfFermionSite property], 552)
onsite_ops() ([tenpy.networks.site.SpinHalfSite property], 556)
onsite_ops() ([tenpy.networks.site.SpinSite property], 560)
onsite_terms ([tenpy.models.model.CouplingModel attribute], 402)
onsite_terms ([tenpy.networks.terms.OnsiteTerms attribute], 601)
OnsiteTerms ([class in tenpy.networks.terms], 600)
op_needs_JW() ([tenpy.networks.site.BosonSite method], 532)
op_needs_JW() ([tenpy.networks.site.FermionSite method], 536)
op_needs_JW() ([tenpy.networks.site.GroupedSite method], 541)
plot_basis() (tenpy.models.lattice.SimpleLattice method), 367
plot_basis() (tenpy.models.lattice.Square method), 376
plot_basis() (tenpy.models.lattice.Triangular method), 385
plot_basis() (tenpy.models.lattice.TrivialLattice method), 393
plot_basis() (tenpy.models.model_code.DualSquare method), 524
plot_bc_identified() (tenpy.models.lattice.Chain method), 306
plot_bc_identified() (tenpy.models.lattice.Honeycomb method), 316
plot_bc_identified() (tenpy.models.lattice.IrregularLattice method), 326
plot_bc_identified() (tenpy.models.lattice.Kagome method), 336
plot_bc_identified() (tenpy.models.lattice.Ladder method), 346
plot_bc_identified() (tenpy.models.lattice.Lattice method), 359
plot_bc_identified() (tenpy.models.lattice.SimpleLattice method), 367
plot_bc_identified() (tenpy.models.lattice.Square method), 376
plot_bc_identified() (tenpy.models.lattice.Triangular method), 385
plot_bc_identified() (tenpy.models.lattice.TrivialLattice method), 395
plot_bc_identified() (tenpy.models.model_code.DualSquare method), 524
plot_coupling() (tenpy.models.lattice.Chain method), 307
plot_coupling() (tenpy.models.lattice.Honeycomb method), 317
plot_coupling() (tenpy.models.lattice.IrregularLattice method), 326
plot_coupling() (tenpy.models.lattice.Kagome method), 337
plot_coupling() (tenpy.models.lattice.Ladder method), 347
plot_coupling() (tenpy.models.lattice.Lattice method), 359
plot_coupling() (tenpy.models.lattice.SimpleLattice method), 367
plot_coupling() (tenpy.models.lattice.Square method), 376
plot_coupling() (tenpy.models.lattice.Triangular method), 385
plot_coupling() (tenpy.models.lattice.TrivialLattice method), 395
plot_coupling() (tenpy.models.model_code.DualSquare method), 525
plot_coupling_terms() (tenpy.models.lattice.CouplingTerms method), 385
plot_coupling_terms() (tenpy.models.lattice.MultiCouplingTerms method), 395
plot_order() (tenpy.models.lattice.Chain method), 307
plot_order() (tenpy.models.lattice.Honeycomb method), 317
plot_order() (tenpy.models.lattice.IrregularLattice method), 326
plot_order() (tenpy.models.lattice.Kagome method), 337
plot_order() (tenpy.models.lattice.Ladder method), 347
plot_order() (tenpy.models.lattice.Lattice method), 359
plot_order() (tenpy.models.lattice.SimpleLattice method), 367
plot_order() (tenpy.models.lattice.Square method), 376
plot_order() (tenpy.models.lattice.Triangular method), 385
plot_order() (tenpy.models.lattice.TrivialLattice method), 395
plot_order() (tenpy.models.model_code.DualSquare method), 525
plot_sites() (tenpy.models.lattice.Chain method), 307
plot_sites() (tenpy.models.lattice.Honeycomb method), 317
plot_sites() (tenpy.models.lattice.IrregularLattice method), 326
plot_sites() (tenpy.models.lattice.Kagome method), 337
plot_sites() (tenpy.models.lattice.Ladder method), 347
plot_sites() (tenpy.models.lattice.Lattice method), 359
plot_sites() (tenpy.models.lattice.SimpleLattice method), 367
plot_sites() (tenpy.models.lattice.Square method), 376
plot_sites() (tenpy.models.lattice.Triangular method), 385
plot_sites() (tenpy.models.lattice.TrivialLattice method), 395
plot_sites()  (tenpy.models.toric_code.DualSquare method), 525
plot_stats()  (in module tenpy.linalg.lanczos), 299
plot_sweep_stats()  
(tenpy.algorithms.dmrg.EngineCombine method), 175
plot_sweep_stats()  
(tenpy.algorithms.dmrg.EngineFracture method), 183
plot_update_stats()  
(tenpy.algorithms.dmrg.EngineCombine method), 175
plot_update_stats()  
(tenpy.algorithms.dmrg.EngineFracture method), 183
position()  
(tenpy.models.lattice.Chain method), 307
position()  
(tenpy.models.lattice.Honeycomb method), 317
position()  
(tenpy.models.lattice.IrregularLattice method), 327
position()  
(tenpy.models.lattice.Kagome method), 337
position()  
(tenpy.models.lattice.Ladder method), 347
position()  
(tenpy.models.lattice.Lattice method), 355
position()  
(tenpy.models.lattice.SimpleLattice method), 368
position()  
(tenpy.models.lattice.Triangular method), 377
position()  
(tenpy.models.lattice.TrivialLattice method), 386
position()  
(tenpy.models.toric_code.DualSquare method), 525
possible_couplings()  
(tenpy.models.lattice.Chain method), 307
possible_couplings()  
(tenpy.models.lattice.Honeycomb method), 317
possible_couplings()  
(tenpy.models.lattice.IrregularLattice method), 327
possible_couplings()  
(tenpy.models.lattice.Kagome method), 337
possible_couplings()  
(tenpy.models.lattice.Ladder method), 347
possible_couplings()  
(tenpy.models.lattice.Lattice method), 355
possible_couplings()  
(tenpy.models.lattice.SimpleLattice method), 368
possible_couplings()  
(tenpy.models.lattice.Triangular method), 377
possible_couplings()  
(tenpy.models.toric_code.DualSquare method), 525
possible_couplings()  
(tenpy.models.toric_code.Triangular method), 386
possible_multi_couplings()  
(tenpy.models.lattice.Chain method), 308
possible_multi_couplings()  
(tenpy.models.lattice.Honeycomb method), 318
possible_multi_couplings()  
(tenpy.models.lattice.IrregularLattice method), 327
possible_multi_couplings()  
(tenpy.models.lattice.Kagome method), 338
possible_multi_couplings()  
(tenpy.models.lattice.Ladder method), 348
possible_multi_couplings()  
(tenpy.models.lattice.Lattice method), 359
possible_multi_couplings()  
(tenpy.models.lattice.SimpleLattice method), 368
possible_multi_couplings()  
(tenpy.models.lattice.Triangular method), 377
possible_multi_couplings()  
(tenpy.models.toric_code.DualSquare method), 526
post_update_local()  
(tenpy.algorithms.dmrg.EngineCombine method), 175
post_update_local()  
(tenpy.algorithms.dmrg.EngineFracture method), 183
post_update_local()  
(tenpy.algorithms.purification.PurificationApplyMPO method), 198
prepare_svd()  
(tenpy.algorithms.dmrg.EngineCombine method), 176
prepare_svd()  
(tenpy.algorithms.dmrg.EngineFracture method), 183
prepare_update()  
(tenpy.algorithms.dmrg.EngineCombine method), 176
prepare_update() (tenpy.algorithms.dmrgetm.EngineFracture method), 183
prepare_update() (tenpy.algorithms.purification.PurificationApplyMPO method), 198
priority() (tenpy.tools.events.Listener property), 631
project() (tenpy.linalg.charges.LegCharge method), 263
project() (tenpy.linalg.charges.LegPipe method), 268
PurificationApplyMPO (class in tenpy.algorithms.purification), 198
PurificationTEBD (class in tenpy.algorithms.purification), 200
PurificationTEBD2 (class in tenpy.algorithms.purification), 206
PurificationTwoSiteU (class in tenpy.algorithms.purification), 211
Python Enhancement Proposals
PEP 257, 148
PEP 8, 148

Q
q_map (tenpy.linalg.charges.LegPipe attribute), 267
q_map_slices (tenpy.linalg.charges.LegPipe attribute), 267
qconj (tenpy.linalg.charges.LegCharge attribute), 258
QCUTOFF (in module tenpy.linalg.np_conserved), 251
qnumber() (tenpy.linalg.charges.ChargeInfo property), 256
qr() (in module tenpy.linalg.np_conserved), 247
qr_li() (in module tenpy.tools.math), 641
qtotal (tenpy.linalg.np_conserved.Array attribute), 222
qtotal (tenpy.networks.mps.TransferMatrix attribute), 574
QTYPE (in module tenpy.linalg.charges), 273
QTYPE (in module tenpy.linalg.np_conserved), 251

R
rank (tenpy.linalg.np_conserved.Array attribute), 222
regular_lattice (tenpy.models.lattice.IrregularLattice attribute), 321
released (in module tenpy.version), 657
remove_op() (tenpy.networks.site.BosonSite method), 532
remove_op() (tenpy.networks.site.FermionSite method), 537
remove_op() (tenpy.networks.site.GroupedSite method), 541
remove_op() (tenpy.networks.site.Site method), 546
remove_op() (tenpy.networks.site.SpinHalfFermionSite method), 552
remove_op() (tenpy.networks.site.SpinHalfSite method), 556

726
Square (class in tenpy.models.lattice), 371
squeeze() (tenpy.linalg.np_conserved.Array method), 232
standard_normal_complex() (in module tenpy.linalg.random_matrix), 278
state_index() (tenpy.networks.site.BosonSite method), 533
state_index() (tenpy.networks.site.FermionSite method), 537
state_index() (tenpy.networks.site.GroupedSite method), 542
state_index() (tenpy.networks.site.Site method), 546
state_index() (tenpy.networks.site.SpnhalfFermionSite method), 552
state_index() (tenpy.networks.site.SpnhalfSite method), 557
state_index() (tenpy.networks.site.SpnhalfSite method), 561
state_indices() (tenpy.networks.site.BosonSite method), 533
state_indices() (tenpy.networks.site.FermionSite method), 537
state_indices() (tenpy.networks.site.GroupedSite method), 542
state_indices() (tenpy.networks.site.Site method), 546
state_indices() (tenpy.networks.site.SpnhalfFermionSite method), 552
state_indices() (tenpy.networks.site.SpnhalfSite method), 557
state_indices() (tenpy.networks.site.SpnhalfSite method), 561
state_labels (tenpy.networks.site.Site attribute), 544
states (tenpy.networks.mpo.MPOGraph attribute), 583
stored_blocks() (tenpy.linalg.np_conserved.Array property), 226
strengths (tenpy.networks.terms.TermList attribute), 603
subqshape (tenpy.linalg.charges.LegPipe attribute), 267
subshape (tenpy.linalg.charges.LegPipe attribute), 266
subspace_expand() (tenpy.algorithms.dmrg.SingleSiteMixer method), 188
subspace_expand() (tenpy.algorithms.dmrg.TwoSiteMixer method), 190
sum_of_exp() (in module tenpy.tools.fit), 646
SumNpcLinearOperator (class in tenpy.linalg.sparse), 296
suzuki_trotter_decomposition() (tenpy.algorithms.purification.PurificationTEBD static method), 203
suzuki_trotter_decomposition() (tenpy.algorithms.purification.PurificationTEBD2 static method), 208
suzuki_trotter_time_steps() (tenpy.algorithms.purification.PurificationTEBD static method), 203
suzuki_trotter_time_steps() (tenpy.algorithms.purification.PurificationTEBD2 static method), 208
svd() (in module tenpy.linalg.np_conserved), 248
svd() (in module tenpy.linalg.svd_robust), 274
svd_gesvd() (in module tenpy.linalg.svd_robust), 274
svd_theta() (in module tenpy.algorithms.truncation), 156
sweep() (tenpy.algorithms.dmrg.EngineCombine method), 177
sweep() (tenpy.algorithms.dmrg.EngineFracture method), 185
sweep() (tenpy.algorithms.purification.PurificationApplyMPO method), 199
T
T() (tenpy.linalg.sparse.FlatHermitianOperator property), 281
T() (tenpy.linalg.sparse.FlatLinearOperator property), 289
take_slice() (tenpy.linalg.np_conserved.Array method), 227
temporary_level (class in tenpy.tools.optimization), 653
temporary_level (tenpy.tools.optimization.temporary_level attribute), 653
tenpy
  module, 152
tenpy.algorithms
    module, 153
tenpy.algorithms.dmrg
      module, 191
tenpy.algorithms.exact_diag
        module, 218
tenpy.algorithms.mpo_evolution
          module, 212
tenpy.algorithms.mps_common
            module, 166
tenpy.algorithms.network_contractor
              module, 214
tenpy.algorithms.purification
                module, 211
tenpy.algorithms.tdvp
                  module, 195
tenpy.algorithms.tebd
                    module, 158
tenpy.algorithms.truncation
                      module, 157
<table>
<thead>
<tr>
<th>Module Name</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>tenpy.linalg</td>
<td>218</td>
</tr>
<tr>
<td>tenpy.linalg.charges</td>
<td>273</td>
</tr>
<tr>
<td>tenpy.linalg.lanczos</td>
<td>300</td>
</tr>
<tr>
<td>tenpy.linalg.np_conserved</td>
<td>251</td>
</tr>
<tr>
<td>tenpy.linalg.random_matrix</td>
<td>278</td>
</tr>
<tr>
<td>tenpy.linalg.sparse</td>
<td>297</td>
</tr>
<tr>
<td>tenpy.linalg.svd_robust</td>
<td>275</td>
</tr>
<tr>
<td>tenpy.models</td>
<td>300</td>
</tr>
<tr>
<td>tenpy.models.fermions_spinless</td>
<td>486</td>
</tr>
<tr>
<td>tenpy.models.haldane</td>
<td>516</td>
</tr>
<tr>
<td>tenpy.models.hofstadter</td>
<td>515</td>
</tr>
<tr>
<td>tenpy.models.hubbard</td>
<td>513</td>
</tr>
<tr>
<td>tenpy.models.lattice</td>
<td>400</td>
</tr>
<tr>
<td>tenpy.models.model</td>
<td>429</td>
</tr>
<tr>
<td>tenpy.models.spins</td>
<td>471</td>
</tr>
<tr>
<td>tenpy.models.spins_nnn</td>
<td>472</td>
</tr>
<tr>
<td>tenpy.models.tf_ising</td>
<td>443</td>
</tr>
<tr>
<td>tenpy.models.toric_code</td>
<td>527</td>
</tr>
<tr>
<td>tenpy.models.xxz_chain</td>
<td>457</td>
</tr>
<tr>
<td>tenpy.networks</td>
<td>527</td>
</tr>
<tr>
<td>tenpy.networks.mpo</td>
<td>587</td>
</tr>
<tr>
<td>tenpy.networks.mps</td>
<td>576</td>
</tr>
<tr>
<td>tenpy.networks.purification_mps</td>
<td>607</td>
</tr>
<tr>
<td>tenpy.networks.site</td>
<td>566</td>
</tr>
<tr>
<td>tenpy.networks.terms</td>
<td>606</td>
</tr>
<tr>
<td>tenpy.tools</td>
<td>609</td>
</tr>
<tr>
<td>tenpy.tools.events</td>
<td>631</td>
</tr>
<tr>
<td>tenpy.tools.fit</td>
<td>647</td>
</tr>
<tr>
<td>tenpy.tools.hdf5_io</td>
<td>621</td>
</tr>
<tr>
<td>tenpy.tools.math</td>
<td>643</td>
</tr>
<tr>
<td>tenpy.tools.misc</td>
<td>639</td>
</tr>
<tr>
<td>tenpy.tools.optimization</td>
<td>656</td>
</tr>
<tr>
<td>tenpy.tools.params</td>
<td>627</td>
</tr>
<tr>
<td>tenpy.tools.process</td>
<td>650</td>
</tr>
<tr>
<td>tenpy.tools.string</td>
<td>648</td>
</tr>
<tr>
<td>tenpy.version</td>
<td>657</td>
</tr>
<tr>
<td>tensordot()</td>
<td>249</td>
</tr>
<tr>
<td>TermList</td>
<td>603</td>
</tr>
<tr>
<td>terms</td>
<td>603</td>
</tr>
<tr>
<td>test_contractible()</td>
<td>261</td>
</tr>
<tr>
<td>test_contractible()</td>
<td>272</td>
</tr>
<tr>
<td>test_equal()</td>
<td>262</td>
</tr>
<tr>
<td>test_equal()</td>
<td>272</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>256</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>261</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>268</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>222</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>486</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>500</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>513</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>308</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>318</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>328</td>
</tr>
<tr>
<td>test_sanity()</td>
<td>338</td>
</tr>
</tbody>
</table>
transpose() (tenpy.linalg.np_conserved.Array method), 234
transpose() (tenpy.linalg.sparse.FlatHermitianOperator method), 284
transpose() (tenpy.linalg.sparse.FlatLinearOperator method), 291
transpose_list_list() (in module tenpy.tools.misc), 638
Triangular (class in tenpy.models.lattice), 380
trivial_like_NNModel() (tenpy.models.fermions_spinless.FermionChain method), 486
trivial_like_NNModel() (tenpy.models.hubbard.BoseHubbardChain method), 500
trivial_like_NNModel() (tenpy.models.hubbard.FermiHubbardChain method), 513
trivial_like_NNModel() (tenpy.models.model.NearestNeighborModel method), 428
trivial_like_NNModel() (tenpy.models.spins.SpinChain method), 471
trivial_like_NNModel() (tenpy.models.tf_ising.TFIChain method), 443
trivial_like_NNModel() (tenpy.models.xxz_chain.XXZChain2 method), 457
TrivialLattice (class in tenpy.models.lattice), 389
trunc_err_bonds() (tenpy.algorithms.purification.PurificationTEBD property), 203
trunc_err_bonds() (tenpy.algorithms.purification.PurificationTEBD2 property), 208
TruncationError (class in tenpy.algorithms.truncation), 154
TwoSiteH (class in tenpy.algorithms.mps_common), 165
TwoSiteMixer (class in tenpy.algorithms.dmrg), 189
TYPES_FOR_HDF5_DATASETS (in module tenpy.tools.hdf5_io), 623

U
U_close_1() (in module tenpy.linalg.random_matrix), 278
unary_blockwise() (tenpy.linalg.np_conserved.Array method), 235
unit_cell (tenpy.models.lattice.Lattice attribute), 351
unit_cell_positions (tenpy.models.lattice.Lattice attribute), 352
unused_parameters() (in module tenpy.tools.params), 626
unwrapped() (tenpy.linalg.sparse.NpcLinearOperatorWrapper method), 293
unwrapped() (tenpy.linalg.sparse.OrthogonalNpcLinearOperator method), 295
unwrapped() (tenpy.linalg.sparse.ShiftNpcLinearOperator method), 296
unwrapped() (tenpy.linalg.sparse.SumNpcLinearOperator method), 297
update() (tenpy.algorithms.purification.PurificationTEBD method), 204
update() (tenpy.algorithms.purification.PurificationTEBD2 method), 206
update_amplitude() (tenpy.algorithms.dmrg.DensityMatrixMixer method), 170
update_amplitude() (tenpy.algorithms.dmrg.SingleSiteMixer method), 188
update_amplitude() (tenpy.algorithms.dmrg.TwoSiteMixer method), 190
update_bond() (tenpy.algorithms.purification.PurificationTEBD method), 201
update_bond() (tenpy.algorithms.purification.PurificationTEBD2 method), 208
update_bond_imag() (tenpy.algorithms.purification.PurificationTEBD method), 201
update_bond_imag() (tenpy.algorithms.purification.PurificationTEBD2 method), 209
update_imag() (tenpy.algorithms.purification.PurificationTEBD method), 204
update_imag() (tenpy.algorithms.purification.PurificationTEBD2 method), 209
update_local() (tenpy.algorithms.dmrg.EngineCombine method), 178
update_local() (tenpy.algorithms.dmrg.EngineFracture method), 186
update_local() (tenpy.algorithms.purification.PurificationApplyMPO method), 198
update_LP() (tenpy.algorithms.dmrg.EngineCombine method), 178
update_LP() (tenpy.algorithms.dmrg.EngineFracture method), 185
update_RP() (tenpy.algorithms.dmrg.EngineCombine method), 178
update_RP() (tenpy.algorithms.dmrg.EngineFracture method), 186
update_step() (tenpy.algorithms.purification.PurificationTEBD method), 205

Index
method), 204
update_step() (tenpy.algorithms.purification.PurificationTEBD2
method), 206
use_cython() (in module tenpy.tools.optimization),
655
used_disentangler
  (tenpy.algorithms.purification.PurificationTEBD
attribute), 201
V
  V (tenpy.algorithms.exact_diag.ExactDiag attribute), 216
valid_hdf5_path_component() (in module
tenpy.tools.hdf5_io), 621
valid_opname() (tenpy.networks.site.BosonSite
method), 533
valid_opname() (tenpy.networks.site.FermionSite
method), 537
valid_opname() (tenpy.networks.site.GroupedSite
method), 542
valid_opname() (tenpy.networks.site.Site method),
546
valid_opname() (tenpy.networks.site.SpinHalfFermionSite
method), 553
valid_opname() (tenpy.networks.site.SpinHalfSite
method), 557
valid_opname() (tenpy.networks.site.SpinSite
method), 561
vec_label (tenpy.linalg.sparse.FlatLinearOperator
attribute), 286
version (in module tenpy.version), 657
version_summary (in module tenpy.version), 657
vert_join() (in module tenpy.tools.string), 647
W
  W (tenpy.algorithms.tdvp.H1_mixed attribute), 194
W0 (tenpy.algorithms.tdvp.H2_mixed attribute), 195
W1 (tenpy.algorithms.tdvp.H2_mixed attribute), 195
X
  XXZChain2 (class in tenpy.models.xxz_chain), 446
Z
  zero_if_close() (in module tenpy.tools.misc), 638
zeros() (in module tenpy.linalg.np_conserved), 250
zeros_like() (tenpy.linalg.np_conserved.Array
method), 225

Index 733