TeNPy

Release 0.6.0

TeNPy Developers

May 16, 2020

USER GUIDE

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?

Follow the instructions in the file `doc/INSTALL.rst`, online at https://tenpy.readthedocs.io/en/latest/INSTALL.html. 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 formated 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 intective 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`.

CHAPTER

THREE

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 annoucements, for example when we release a new version.

CHAPTER

FOUR

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

FIVE

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.):

```
@Article{tenpy,
    title={{Efficient numerical simulations with Tensor Networks: Tensor Network ␣
↪Python (TeNPy)}},
    author={Johannes Hauschild and Frank Pollmann},
    journal={SciPost Phys. Lect. Notes},
    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}},
}
```

CHAPTER

SIX

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).

CHAPTER

SEVEN

LICENSE

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

There are several ways to install TeNPy.

A very comfortable way is to simply use [pip] with:

```
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 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 speficy 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 master branch, you can use:

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

This should already have the lastest features described in /changelog/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
```

7.1.2 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`), and to start over with downloading and installing the newest version.

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` 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
```

7.1.3 Installation from source

Minimal Requirements

This code works with a minimal requirement of pure Python>=3.5 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 offical repository is at 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 `~/.bashrc`.

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

```
>>> import tenpy
/home/username/TeNPy/tenpy/tools/optimization.py:276: UserWarning: Couldn't load␣
↪compiled cython code. Code will run a bit slower.
  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_conseved`, 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 one `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 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:

```
>>> 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`*.

7.1.4 Extra requirements

We have some extra requirements that you don't need to install to use TeNPy, but that you might find usefull 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 successfull 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*.

7.1.5 Checking the installation

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

```
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.

7.1.6 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
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.
```

7.1.7 License

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

```
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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 /changelog/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 developed (closed source) TeNPy version.

7.2.1 [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 differnt order, and in that case raise a warning that we will transpose in the future.
- Made `tenpy.linalg.np_conserved.Array.get_block()` public (previously `tenpy.linalg.np_conserved.Array._get_block`).
- `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_sweeps* 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 possiple 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.dmrg.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_sweeps.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_sweeps.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()`.

7.2.2 [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.

7.2.3 [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, site1, label0, label1` of the __init__ can be replaced with `[site0, site1], [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_hubbbard_chain.BoseHubbardModel` (and `tenpy.models.bose_hubbbard_chain.BoseHubbardChain`) did not correspond to $U/2N(N-1)$ 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_bond into H_MPO and vice versa.
- `tenpy.algorithms.tebd.RandomUnitaryEvolution` for random unitary circuits
- Allow documentation links to github issues, arXiv, papers by doi and the forum with e.g. `:issue:`5`, :arxiv:`1805.00055`, :doi:`10.21468/SciPostPhysLectNotes.5`, :forum:`3``
- *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_conserved* 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)|psi0>`
- Warning for poorly conditioned Lanczos; to overcome this enable the new parameter *reortho*.
- Simplified call strucutre 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`.

7.2.4 [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.

7.2.5 [0.2.0] - 2017-02-24

- Compatible with python2 and python3 (using the 2to3 tool).
- Development version.
- Includes TEBD and DMRG.

7.2.6 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 allmost 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 consitent 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 puplic 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.
- withing 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

  Files outside of the library (and in *tests/*, *examples/*) should use absolute imports, e.g. `import tenpy.algorithms.tebd`
- renamed *tenpy/mps/* to *tenpy/networks*, since it containes various tensor networks.
- added `Site` describing the local physical sites by providing the physical LegCharge and onsite operators.

np_conserved

- pure python, no need to compile!
- in module `tenpy.linalg` instead of `algorithms/linalg`.
- moved functionality for charges to `charges`
- Introduced the classes `ChargeInfo` (basically the old `q_number`, and `mod_q`) and `LegCharge` (the old `qind, qconj`).

- 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
- more functions, e.g. `grid_outer()`

TEBD

- 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 orthoganalized 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 this 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`.

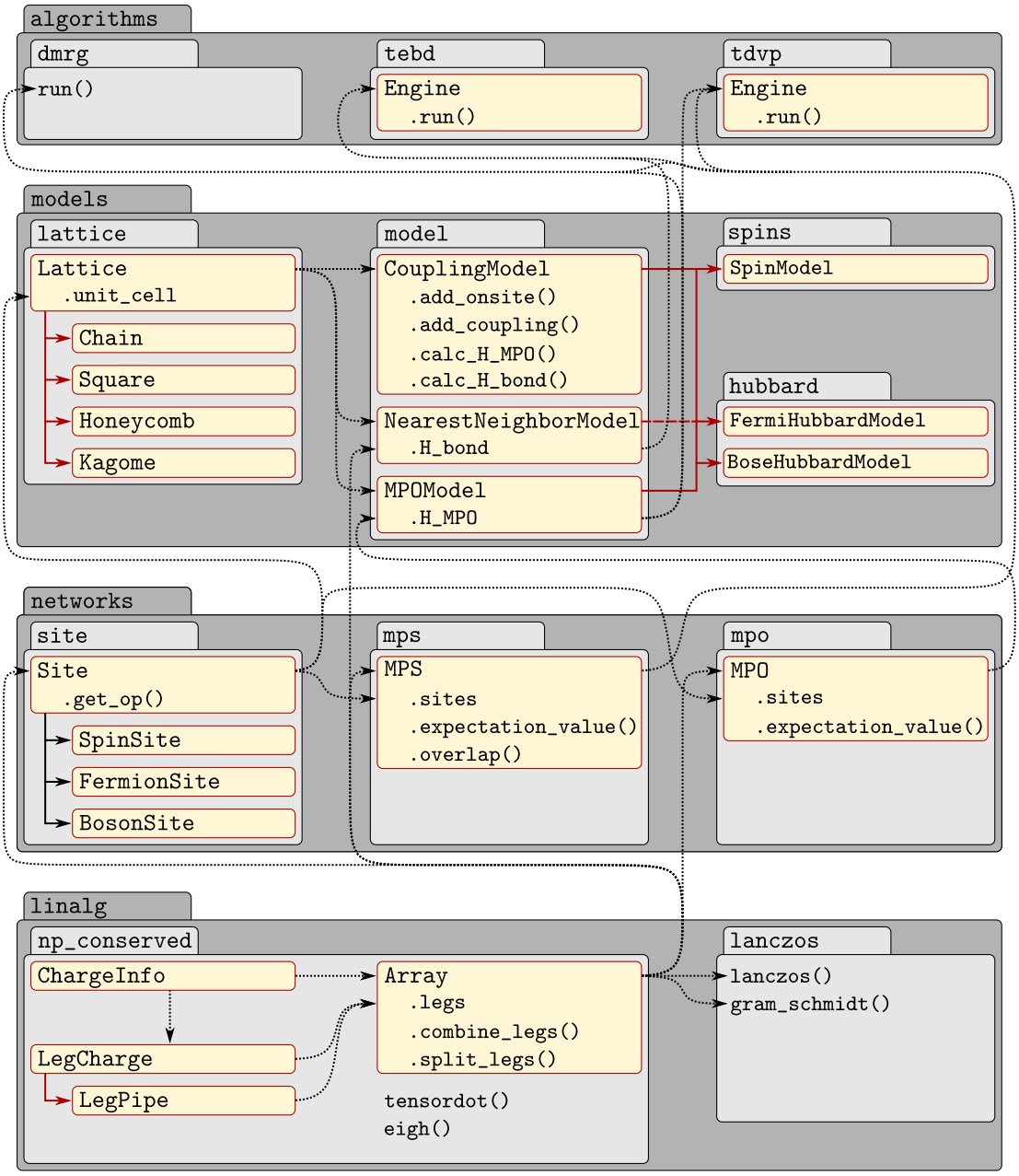
tests Contains files with test routines, to be used with *pytest*. If you are set up correctly and have *pytest* installed, you can run the test suite with `pytest` from within the `tests/` folder.

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 in the `linalg` module, which provides basic features of linear algebra. In particular, the `np_conserved` submodule implements an `Array` class which is used to represent the tensors. The basic interface of `np_conserved` is very similar to that of the NumPy and SciPy libraries. However, the `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.

```
"""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 indiviual 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 `ChargeInfo` class. An `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 `LegCharge` instance for each leg, which contains the *charges* and sign *qconj* for each leg. We can combine multiple legs into a single larger `LegPipe`, which is derived from the `LegCharge` and stores all the information necessary to later split the pipe.

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

```
"""Explicit definition of charges and spin-1/2 operators."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3

import tenpy.linalg.np_conserved as npc

# 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])
# 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,...), `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.

```
"""Initialization of sites, MPS and MPO."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3

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␣
↪* Sz],
          [None, None, None, None, Id]]
W_first = [W_bulk[0]]  # first row
W_last = [[row[-1]] for row in W_bulk]  # last column
Ws = [W_first] + [W_bulk] * (N - 2) + [W_last]
H = MPO.from_grids([spin] * N, Ws, bc='finite', IdL=0, IdR=-1)
print("<psi|H|psi> =", H.expectation_value(psi))
# <psi|H|psi> = -1.25
```

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.

```
"""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_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.

```
"""Initialization of the Heisenberg model on a kagome lattice."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3

from tenpy.models.spins import SpinModel

model_params = {
    "S": 0.5,  # Spin 1/2
    "lattice": "Kagome",
```

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```
    "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.

```
"""Call of (finite) DMRG."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3

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.

```
"""Call of infinite DMRG."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3

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

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
```

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```
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.

```
"""Call of (infinite) TEBD."""
# Copyright 2019-2020 TeNPy Developers, GNU GPLv3

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 Toy Codes

The following "toy codes" are included in the TeNPy repository in the folder `toycodes/`, we include them here in the documentation for reference. They are meant to give you a flavor of the different algorithms, while keeping the codes as readable and simple as possible. The only requirements to run them are Python 3, Numpy, and Scipy. Simply go to the folder where you downloaded them, and execute them with python.

Toycode `a_mps.py`

```
"""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.
```

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```
    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)
        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_theta1(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_theta1(i), self.Bs[j], [2, 0])  # vL i [vR],␣
↪[vL] j vR

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

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```
        return [self.Bs[i].shape[2] for i in range(self.nbonds)]

    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_theta1(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], [1, 2]])
            # i j [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 = []
        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*
        T = np.transpose(T, [0, 2, 1, 3])  # vL vL* vR vR*
        for i in range(1, self.L):
            B = self.Bs[i]
            T = np.tensordot(T, B, axes=[2, 0])  # vL vL* [vR] vR*, [vL] i vR
            T = np.tensordot(T, np.conj(B), axes=[[2, 3], [0, 1]])
            # vL vL* [vR*] [i] vR, [vL*] [i*] vR*
        T = np.reshape(T, (chi**2, chi**2))
        # Obtain the 2nd largest eigenvalue
        eta = arp.eigs(T, k=2, which='LM', return_eigenvectors=False, ncv=20)
        return -self.L / np.log(np.min(np.abs(eta)))
```

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```
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::
          vL --(theta)-- vR     =>    vL --(A)--diag(S)--(B)-- vR
                |   |                       |              |
                i   j                       i              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
    -------
    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
```

Toycode `b_model.py`

```
"""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 :
        Local operators, namely the Pauli matrices and identity.
    H_bonds : list of np.Array[ndim=4]
        The Hamiltonian written in terms of local 2-site operators, ``H = sum_i H_
↪bonds[i]``.
        Each ``H_bonds[i]`` has (physical) legs (i out, (i+1) out, i in, (i+1) in),
        in short ``i j i* j*``.
    H_mpo : lit of np.Array[ndim=4]
        The Hamiltonian written as an MPO.
        Each ``H_mpo[i]`` has legs (virutal left, virtual right, physical out,␣
↪physical in),
        in short ``wL wR i i*``.
    """
    def __init__(self, L, J, g, bc='finite'):
        assert bc in ['finite', 'infinite']
        self.L, self.d, self.bc = L, 2, bc
        self.J, self.g = J, g
        self.sigmax = np.array([[0., 1.], [1., 0.]])
        self.sigmay = np.array([[0., -1j], [1j, 0.]])
        self.sigmaz = np.array([[1., 0.], [0., -1.]])
        self.id = np.eye(2)
        self.init_H_bonds()
        self.init_H_mpo()

    def init_H_bonds(self):
        """Initialize `H_bonds` hamiltonian.
```

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```
        Called by __init__().
        """
        sx, sz, id = self.sigmax, self.sigmaz, self.id
        d = self.d
        nbonds = self.L - 1 if self.bc == 'finite' else self.L
        H_list = []
        for i in range(nbonds):
            gL = gR = 0.5 * self.g
            if self.bc == 'finite':
                if i == 0:
                    gL = self.g
                if i + 1 == self.L - 1:
                    gR = self.g
            H_bond = -self.J * np.kron(sx, sx) - gL * np.kron(sz, id) - gR * np.
↪kron(id, sz)
            # H_bond has legs ``i, j, i*, j*``
            H_list.append(np.reshape(H_bond, [d, d, d, d]))
        self.H_bonds = H_list

    # (note: not required for TEBD)
    def init_H_mpo(self):
        """Initialize `H_mpo` Hamiltonian.

        Called by __init__().
        """
        w_list = []
        for i in range(self.L):
            w = np.zeros((3, 3, self.d, self.d), dtype=np.float)
            w[0, 0] = w[2, 2] = self.id
            w[0, 1] = self.sigmax
            w[0, 2] = -self.g * self.sigmaz
            w[1, 2] = -self.J * self.sigmax
            w_list.append(w)
        self.H_mpo = w_list
```

Toycode `c_tebd.py`

```
"""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*H_bonds[i])``.

    Each local operator has legs (i out, (i+1) out, i in, (i+1) in), in short ``i j␣
↪i* j*``.
    Note that no imaginary 'i' is included, thus real `dt` means 'imaginary time'␣
↪evolution!
    """
    d = H_bonds[0].shape[0]
    U_bonds = []
```

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```
    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` time 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]))  # i j [i*] [j*], vL␣
↪[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 = np.tensordot(np.diag(psi.Ss[i]**(-1)), Ai, axes=[1, 0])  # vL [vL*], [vL] i␣
↪vC
    psi.Bs[i] = np.tensordot(Gi, np.diag(Sj), axes=[2, 0])  # vL i [vC], [vC] vC
    psi.Ss[j] = Sj  # vC
    psi.Bs[j] = Bj  # vC j vR


def example_TEBD_gs_tf_ising_finite(L, g):
    print("finite TEBD, imaginary time evolution, 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)
    for dt in [0.1, 0.01, 0.001, 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, 1., g)
```

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```
        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={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)
    for dt in [0.1, 0.01, 0.001, 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(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_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',
```

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```
                interpolation='nearest',
                extent=(0, L - 1., -0.5 * dt, (Nsteps + 0.5) * dt))
    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)


if __name__ == "__main__":
    example_TEBD_gs_tf_ising_finite(L=10, g=1.)
    print("-" * 100)
    example_TEBD_gs_tf_ising_infinite(g=1.5)
    print("-" * 100)
    example_TEBD_tf_ising_lightcone(L=20, g=1.5, tmax=3., dt=0.01)
```

Toycode `d_dmrg.py`

```
"""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 `SimpleDMRGEnginge.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  # vL wL* vL*
        self.RP = RP  # vR* wR* vR
        self.W1 = W1  # wL wC i i*
        self.W2 = W2  # wC wR j j*
        chi1, chi2 = LP.shape[0], RP.shape[2]
        d1, d2 = W1.shape[2], W2.shape[2]
        self.theta_shape = (chi1, d1, d2, chi2)  # vL i j vR
        self.shape = (chi1 * d1 * d2 * chi2, chi1 * d1 * d2 * chi2)
        self.dtype = W1.dtype

    def _matvec(self, theta):
        """Calculate |theta'> = H_eff |theta>.
```

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```
        This function is used by :func:scipy.sparse.linalg.eigen.arpack.eigsh` to␣
↪diagonalize
        the effective Hamiltonian with a Lanczos method, withouth generating the full␣
↪matrix."""
        x = np.reshape(theta, self.theta_shape)  # vL i j vR
        x = np.tensordot(self.LP, x, axes=(2, 0))  # vL wL* [vL*], [vL] i j vR
        x = np.tensordot(x, self.W1, axes=([1, 2], [0, 3]))  # vL [wL*] [i] j vR,␣
↪[wL] wC i [i*]
        x = np.tensordot(x, self.W2, axes=([3, 1], [0, 3]))  # vL [j] vR [wC] i, [wC]␣
↪wR j [j*]
        x = np.tensordot(x, self.RP, axes=([1, 3], [0, 1]))  # vL [vR] i [wR] j,␣
↪[vR*] [wR*] vR
        x = np.reshape(x, self.shape[0])
        return x


class SimpleDMRGEngine:
    """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``
    """
    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
```

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```
        # 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 = np.reshape(v[:, 0], Heff.theta_shape)
        # split and truncate
        Ai, Sj, Bj = split_truncate_theta(theta, self.chi_max, self.eps)
        # put back into MPS
        Gi = np.tensordot(np.diag(self.psi.Ss[i]**(-1)), Ai, axes=[1, 0])  # vL [vL*],
↪ [vL] i vC
        self.psi.Bs[i] = np.tensordot(Gi, np.diag(Sj), axes=[2, 0])  # vL i [vC],␣
↪[vC*] vC
        self.psi.Ss[j] = Sj  # vC
        self.psi.Bs[j] = Bj  # vC j vR
        self.update_LP(i)
        self.update_RP(j)

    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*] wR* vR
        RP = np.tensordot(RP, W, axes=[[1, 2], [3, 1]])  # vL [i] [wR*] vR, wL [wR] i␣
↪[i*]
        RP = np.tensordot(RP, Bc, axes=[[1, 3], [2, 1]])  # vL [vR] wL [i], vL* [i*]␣
↪[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] i␣
↪vR
        A = np.tensordot(G, np.diag(self.psi.Ss[j]**-1), axes=[2, 0])  # vL i [vR],␣
↪[vR*] vR
        Ac = A.conj()  # vL* i* vR*
        W = self.H_mpo[i]  # wL wR i i*
```

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```
        LP = np.tensordot(LP, A, axes=[2, 0])  # vL wL* [vL*], [vL] i vR
        LP = np.tensordot(W, LP, axes=[[0, 3], [1, 2]])  # [wL] wR i [i*], vL [wL*]␣
↪[i] vR
        LP = np.tensordot(Ac, LP, axes=[[0, 1], [2, 1]])  # [vL*] [i*] vR*, wR [i]␣
↪[vL] vR
        self.LPs[j] = LP  # vR* wR vR (== vL wL* vL* on site i+1)


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))
        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
```

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```
if __name__ == "__main__":
    example_DMRG_tf_ising_finite(L=10, g=1.)
    print("-" * 100)
    example_DMRG_tf_ising_infinite(g=1.5)
```

Toycode `tfi_exact.py`

```
"""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` <~ 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):
```

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```
        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
```

7.3.3 Example codes

The following "examples" are included in the TeNPy repository in the folder `examples/`, we include them here in the documentation for reference. Theses examples are meant to give an idea how to use the library and demonstrate parts of the interface. It might be helpful to compare some of them (e.g., *c_tebd.py* and *d_dmrg.py*) to the *Toy Codes*. To run these examples, you have to have TeNPy installed, see *Installation instructions*. You do not need to save the examples inside the tenpy folder/repository, but you can execute them from anywhere (if TeNPy is installed correctly).

Example code `a_np_conserved.py`

```
"""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
```

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```
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-
```

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```
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")

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

envL = npc.zeros([W.get_leg('wL').conj(), Bs[0].get_leg('vL').conj(), Bs[0].get_leg(
↪'vL')],
                 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')],
                 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*'])
```

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```
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 originial 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")
```

Example code `b_mps.py`

```
"""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`,
```

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```
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

# 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[:1, :]
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)
```

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```
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*')], 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 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 originial labels ['p0', 'p1', 'p0*', 'p1*'] of `H2` in `exp_H2`)

# alternative way: use :func:`~tenpy.linalg.np_conserved.expm`
exp_H2_alternative = npc.expm(-1.j * dt * H2).split_legs()
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],␣
↪qconj=[+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")
```

Example code `c_tebd.py`

```
"""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


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
    # alternative: directly measure E2 = np.sum(psi.expectation_value(M.H_bond[1:]))
    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
```

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```
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,
            'svd_min': 1.e-10
        },
        'verbose': verbose,
    }
    eng = tebd.Engine(psi, M, tebd_params)
    eng.run_GS()  # the main work...
    E = np.sum(M.bond_energies(psi))  # M.bond_energies() works only a for␣
↪NearestNeighborModel
    # 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))
    return E, psi, M


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,
```

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```
        '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
    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
```

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```
    # 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
        },
        'verbose': verbose,
    }
    eng = tebd.Engine(psi, M_nn, tebd_params)  # use M_nn and grouped psi
    eng.run_GS()  # the main work...

    # expectation values:
    E = np.sum(M_nn.bond_energies(psi))  # bond_energies() works only a for␣
↪NearestNeighborModel
    print("E = {E:.13f}".format(E=E))
    print("final bond dimensions: ", psi.chi)
    # we can split the sites of the state again for an easier evaluation of␣
↪expectation values
    psi.group_split()
    mag_x = 2. * np.sum(psi.expectation_value("Sx"))  # factor of 2 for Sx vs Sigmax
    mag_z = 2. * np.sum(psi.expectation_value("Sz"))
    print("magnetization in X = {mag_x:.5f}".format(mag_x=mag_x))
    print("magnetization in Z = {mag_z:.5f}".format(mag_z=mag_z))
    return E, psi, M


if __name__ == "__main__":
    example_TEBD_gs_tf_ising_finite(L=10, g=1.)
    print("-" * 100)
    example_TEBD_gs_tf_ising_infinite(g=1.5)
    print("-" * 100)
    example_TEBD_tf_ising_lightcone(L=20, g=1.5, tmax=3., dt=0.01)
    print("-" * 100)
    example_TEBD_gs_tf_ising_next_nearest_neighbor(L=10, g=1.0, Jp=0.1)
```

Example code `d_dmrg.py`

```
"""Example illustrating the use of DMRG in tenpy.

The example functions in this class do the same as the ones in `toycodes/d_dmrg.py`,
but make use of the classes defined in tenpy.

.. todo ::
Docstrings?
"""
```

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```
# 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.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)
    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␣
↪to work.
        'max_E_err': 1.e-10,
        'trunc_params': {
```

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```
            '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
```

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```
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␣
↪to work.
        'trunc_params': {
            'chi_max': 30,
            'svd_min': 1.e-10
        },
        '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,
        },
```

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```
        '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)
    example_DMRG_heisenberg_xxz_infinite(Jz=1.5)
```

Example code `e_tdvp.py`

```
"""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 can
not 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
```

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```
    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()
```

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```
if __name__ == "__main__":
    run_out_of_equilibrium()
```

Example code `tfi_exact.py`

```
"""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` <~ 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)
```

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```
    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
```

Example code `z_exact_diag.py`

```
"""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 dmrg


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␣
↪sector!
    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()
    # ED.build_full_H_from_bonds()  # 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")
```

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```
    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)
    ov2 = psi_ED_mps.overlap(psi_DMRG)
    print("<psi_ED_mps|psi_DMRG> =", ov2)
    assert (abs(abs(ov2) - 1.) < 1.e-13)
    assert (abs(ov - ov2) < 1.e-13)
    # -> advantage: expectation_value etc. of MPS are available!
    print("<Sz> =", psi_ED_mps.expectation_value('Sz'))


if __name__ == "__main__":
    example_exact_diagonalization(10, 1.)
```

Advanced examples

The following "advanced examples" are included in the TeNPy repository in the folder `examples/advanced`, we include them here in the documentation for reference. Theses "advanced examples" go beyond the basic usage of the algorithm, but can give you an idea for certain tasks. It's a somewhat random collection, feel free to suggest further examples.

Advanced example `xxz_corr_length.py`

```
"""Calculate the correleation legnth of the transferse field Ising model for various␣
↪h_z.

This example uses DMRG to find the ground state of the transverse field Ising model␣
↪when tuning
through the phase transition by changing the field `hz`. It uses
:meth:`~tenpy.networks.mps.MPS.correlation_length` to extract the correlation length␣
↪of the ground
state, and plots it vs. hz in the end.
"""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

import numpy as np

from tenpy.models.spins import SpinChain
from tenpy.networks.mps import MPS, TransferMatrix
from tenpy.algorithms import dmrg
import matplotlib.pyplot as plt


def run(Jzs):
    L = 2
    model_params = dict(L=L, Jx=1., Jy=1., Jz=Jzs[0], bc_MPS='infinite', conserve='Sz
↪', verbose=0)
```

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```
    chi = 300
    dmrg_params = {
        'trunc_params': {
            'chi_max': chi,
            'svd_min': 1.e-10,
            'trunc_cut': None
        },
        'update_env': 20,
        'start_env': 20,
        'max_E_err': 0.0001,
        'max_S_err': 0.0001,
        'verbose': 1,
        'mixer': False
    }

    M = SpinChain(model_params)
    psi = MPS.from_product_state(M.lat.mps_sites(), (["up", "down"] * L)[:L], M.lat.
↪bc_MPS)

    engine = dmrg.TwoSiteDMRGEngine(psi, M, dmrg_params)
    np.set_printoptions(linewidth=120)
    corr_length = []
    for Jz in Jzs:
        print("-" * 80)
        print("Jz =", Jz)
        print("-" * 80)
        model_params['Jz'] = Jz
        M = SpinChain(model_params)
        engine.init_env(model=M)  # (re)initialize DMRG environment with new model
        # this uses the result from the previous DMRG as first initial guess
        engine.run()
        # psi is modified by engine.run() and now represents the ground state for the␣
↪current `Jz`.
        corr_length.append(psi.correlation_length(tol_ev0=1.e-3))
        print("corr. length", corr_length[-1])
        print("<Sz>", psi.expectation_value('Sz'))
        dmrg_params['start_env'] = 0  # (some of) the parameters are read out again
    corr_length = np.array(corr_length)
    results = {
        'model_params': model_params,
        'dmrg_params': dmrg_params,
        'Jzs': Jzs,
        'corr_length': corr_length,
        'eval_transfermatrix': np.exp(-1. / corr_length)
    }
    return results


def plot(results, filename):
    corr_length = results['corr_length']
    Jzs = results['Jzs']
    plt.plot(Jzs, np.exp(-1. / corr_length))
    plt.xlabel(r'$J_z/J_x$')
    plt.ylabel(r'$t = \exp(-\frac{1}{\xi})$')
    plt.savefig(filename)
    print("saved to " + filename)
```

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```
if __name__ == "__main__":
    filename = 'xxz_corrlength.pkl'
    import pickle
    import os.path
    if not os.path.exists(filename):
        results = run(list(np.arange(4.0, 1.5, -0.25)) + list(np.arange(1.5, 0.8, -0.
↪05)))
        with open(filename, 'wb') as f:
            pickle.dump(results, f)
    else:
        print("just load the data")
        with open(filename, 'rb') as f:
            results = pickle.load(f)
    plot(results, filename[:-4] + '.pdf')
```

Advanced example `central_charge_ising.py`

```
"""Example to extract the central charge from the entranglement scaling.

This example code evaluate the central charge of the transverse field Ising model␣
↪using IDMRG.
The expected value for the central charge c = 1/2. The code always recycle the␣
↪environment from
the previous simulation, which can be seen at the "age".
"""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

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


def example_DMRG_tf_ising_infinite_S_xi_scaling(g):
    model_params = dict(L=2, J=1., g=g, bc_MPS='infinite', conserve='best', verbose=0)
    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 = {
        'start_env': 10,
        'mixer': False,
        #  'mixer_params': {'amplitude': 1.e-3, 'decay': 5., 'disable_after': 50},
        'trunc_params': {
            'chi_max': 5,
            'svd_min': 1.e-10
        },
        'max_E_err': 1.e-9,
        'max_S_err': 1.e-6,
        'update_env': 0,
        'verbose': 0
    }
```

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```
    chi_list = np.arange(7, 31, 2)
    s_list = []
    xi_list = []
    eng = dmrg.TwoSiteDMRGEngine(psi, M, dmrg_params)

    for chi in chi_list:

        t0 = time.time()
        eng.reset_stats(
        )  # necessary if you for example have a fixed numer of sweeps, if you don't␣
↪set this you option your simulation stops after initial number of sweeps!
        eng.trunc_params['chi_max'] = chi
        ##   DMRG Calculation    ##
        print("Start IDMRG CALCULATION")
        eng.run()
        eng.engine_params['mixer'] = None
        psi.canonical_form()

        ##   Calculating bond entropy and correlation length  ##
        s_list.append(np.mean(psi.entanglement_entropy()))
        xi_list.append(psi.correlation_length())

        print(chi,
              time.time() - t0,
              np.mean(psi.expectation_value(M.H_bond)),
              s_list[-1],
              xi_list[-1],
              flush=True)
        tenpy.tools.optimization.optimize(3)  # quite some speedup for small chi

        print("SETTING NEW BOND DIMENSION")

    return s_list, xi_list


def fit_plot_central_charge(s_list, xi_list, filename):
    """Plot routine in order to determine the cental charge."""
    import matplotlib.pyplot as plt
    from scipy.optimize import curve_fit

    def fitFunc(Xi, c, a):
        return (c / 6) * np.log(Xi) + a

    Xi = np.array(xi_list)
    S = np.array(s_list)
    LXi = np.log(Xi)  # Logarithm of the correlation length xi

    fitParams, fitCovariances = curve_fit(fitFunc, Xi, S)

    # Plot fitting parameter and covariances
    print('c =', fitParams[0], 'a =', fitParams[1])
    print('Covariance Matrix', fitCovariances)

    # plot the data as blue circles
    plt.errorbar(LXi,
                 S,
```

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```
                 fmt='o',
                 c='blue',
                 ms=5.5,
                 markerfacecolor='white',
                 markeredgecolor='blue',
                 markeredgewidth=1.4)
    # plot the fitted line
    plt.plot(LXi,
             fitFunc(Xi, fitParams[0], fitParams[1]),
             linewidth=1.5,
             c='black',
             label='fit c={c:.2f}'.format(c=fitParams[0]))

    plt.xlabel(r'$\log{\,}\xi_{\chi}$', fontsize=16)
    plt.ylabel(r'$S$', fontsize=16)
    plt.legend(loc='lower right', borderaxespad=0., fancybox=True, shadow=True,␣
↪fontsize=16)
    plt.savefig(filename)


if __name__ == "__main__":
    s_list, xi_list = example_DMRG_tf_ising_infinite_S_xi_scaling(g=1)
    fit_plot_central_charge(s_list, xi_list, "central_charge_ising.pdf")
```

Advanced example `mpo_exponential_decay.py`

```
"""Demonstration of the mpo.MPO.from_grids method.

We construct a MPO model for a spin 1/2 Heisenberg chain with an infinite number of
2-sites interactions, with strength that decays exponentially with the distance␣
↪between the sites.

Because of the infinite number of couplings it is not possible to construct the MPO␣
↪from a
coupling model. However the tensors that form the MPO have a surprisingly simple
form (see the grid below).

We run the iDMRG algorithm to find the ground state and energy density of the
system in the thermodynamic limit.
"""
# Copyright 2018-2020 TeNPy Developers, GNU GPLv3

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

from tenpy.networks.mpo import MPO
from tenpy.networks.mps import MPS
from tenpy.networks.site import SpinHalfSite
from tenpy.models.model import MPOModel
from tenpy.models.lattice import Chain
from tenpy.algorithms import dmrg
from tenpy.tools.params import asConfig
```

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```
class ExponentiallyDecayingHeisenberg(MPOModel):
    r"""Spin-1/2 Heisenberg Chain with exponentially decaying interactions.

    The Hamiltonian reads:

    .. math ::

        H = \sum_i \sum_{j>i} \exp(-\frac{|j-i-1|}{\mathtt{xi}}) (
                  \mathtt{Jxx}/2 (S^{+}_i S^{-}_j + S^{-}_i S^{+}_j)
              + \mathtt{Jz} S^z_i S^z_j                          ) \\
            - \sum_i \mathtt{hz} S^z_i

    All parameters are collected in a single dictionary `model_params`.

    Parameters
    ----------
    L : int
        Length of the chain.
    Jxx, Jz, hz, xi: float
        Coupling parameters as defined for the Hamiltonian above.
    bc_MPS : {'finite' | 'infinte'}
        MPS boundary conditions.
    conserve : 'Sz' | 'parity' | None
        What should be conserved. See :class:`~tenpy.networks.Site.SpinHalfSite`.
    """
    def __init__(self, model_params):
        # model parameters
        model_params = asConfig(model_params, "ExponentiallyDecayingHeisenberg")
        L = model_params.get('L', 2)
        xi = model_params.get('xi', 0.5)
        Jxx = model_params.get('Jxx', 1.)
        Jz = model_params.get('Jz', 1.5)
        hz = model_params.get('hz', 0.)
        conserve = model_params.get('conserve', 'Sz')
        if xi == 0.:
            g = 0.
        elif xi == np.inf:
            g = 1.
        else:
            g = np.exp(-1 / (xi))

        # Define the sites and the lattice, which in this case is a simple uniform␣
↪chain
        # of spin 1/2 sites
        site = SpinHalfSite(conserve=conserve)
        lat = Chain(L, site, bc_MPS='infinite', bc='periodic')

        # The operators that appear in the Hamiltonian. Standard spin operators are
        # already defined for the spin 1/2 site, but it is also possible to add new
        # operators using the add_op method
        Sz, Sp, Sm, Id = site.Sz, site.Sp, site.Sm, site.Id

        # yapf:disable
        # The grid (list of lists) that defines the MPO. It is possible to define the
        # operators in the grid in the following ways:
        # 1) NPC arrays, defined above:
        grid = [[Id,    Sp,    Sm,    Sz,    -hz*Sz    ],
```

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```
                [None, g*Id, None, None, 0.5*Jxx*Sm],
                [None, None, g*Id, None, 0.5*Jxx*Sp],
                [None, None, None, g*Id, Jz*Sz     ],
                [None, None, None, None, Id        ]]
        # 2) In the form [("OpName", strength)], where "OpName" is the name of the
        # operator (e.g. "Sm" for Sm) and "strength" is a number that multiplies it.
        grid = [[[("Id", 1)], [("Sp",1)], [("Sm",1)], [("Sz",1)], [("Sz", -hz)]    ],
                [None       , [("Id",g)], None      , None      , [("Sm", 0.5*Jxx)]],
                [None       , None      , [("Id",g)], None      , [("Sp", 0.5*Jxx)]],
                [None       , None      , None      , [("Id",g)], [("Sz",Jz)]      ],
                [None       , None      , None      , None      , [("Id",1)]       ]]
        # 3) It is also possible to write a single "OpName", equivalent to
        # [("OpName", 1)].
        grid = [["Id"       , "Sp"      , "Sm"      , "Sz"      , [("Sz", -hz)]    ],
                [None       , [("Id",g)], None      , None      , [("Sm", 0.5*Jxx)]],
                [None       , None      , [("Id",g)], None      , [("Sp", 0.5*Jxx)]],
                [None       , None      , None      , [("Id",g)], [("Sz",Jz)]      ],
                [None       , None      , None      , None      , "Id"             ]]
        # yapf:enable
        grids = [grid] * L

        # Generate the MPO from the grid. Note that it is not necessary to specify
        # the physical legs and their charges, since the from_grids method can extract
        # this information from the position of the operators inside the grid.
        H = MPO.from_grids(lat.mps_sites(), grids, bc='infinite', IdL=0, IdR=-1)
        MPOModel.__init__(self, lat, H)


def example_run_dmrg():
    """Use iDMRG to extract information about the ground state of the system."""
    model_params = dict(L=2, Jxx=1, Jz=1.5, xi=0.8, verbose=1)
    model = ExponentiallyDecayingHeisenberg(model_params)
    psi = MPS.from_product_state(model.lat.mps_sites(), ["up", "down"], bc='infinite')
    dmrg_params = {
        'mixer': True,
        'chi_list': {
            0: 100
        },
        'trunc_params': {
            'svd_min': 1.e-10
        },
        'verbose': 1
    }
    results = dmrg.run(psi, model, dmrg_params)
    print("Energy per site: ", results['E'])
    print("<Sz>: ", psi.expectation_value('Sz'))


if __name__ == "__main__":
    example_run_dmrg()
```

7.3.4 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). Ref. [Singh2009] explains why it works form a mathematical point of view, [Singh2010] has the focus on a $U(1)$ symmetry and might be easier to read.

Notations

Lets 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:

$$T_{a_0,a_1,...a_{rank-1}} \quad \text{with} \quad a_i \in \{0, ..., n_i - 1\}$$

Each **leg** a_i corresponds the a vector space of dimension *n_i*.

An **index** of a leg is a particular value $a_i \in \{0, ..., n_i - 1\}$.

The **rank** is the number of legs, the **shape** is $(n_0, ..., n_{rank-1})$.

We restrict ourselfes 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 refered 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 $c_i \to c_i e^{i\phi}$. 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 $S^z = \sum_i S_i^z$ as the conserved quantity, with values $S_i^z = \pm\frac{1}{2}$. Obviously, if S^z is conserved, then so is $2S^z$, so you can use the charges $q_i = 2S_i^z \in \{-1, +1\}$ for the *down* and *up* states, respectively. Alternatively, you can also use a shift and define $q_i = S_i^z + \frac{1}{2} \in \{0, 1\}$.

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 considereing 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:

```
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], ..., [3]` for the indices `0, 1, 2, 3,..., 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:

```
slices = [0, 1, 3, 7, 9]
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:

```
{(-2,): slice(0, 1),
 (-1,): slice(1, 3),
 (0,) : slice(3, 7),
 (3,) : 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:

```
slices = [0, 1, 3, 5, 7, 9]
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 diveds 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:

charges	bunched	sorted	blocked
`[[-2], [-1], [0], [1], [3]]`	`True`	`True`	`True`
`[[-2], [-1], [0], [0], [3]]`	`False`	`True`	`False`
`[[-2], [0], [-1], [1], [3]]`	`True`	`False`	`True`
`[[-2], [0], [-1], [0], [3]]`	`True`	`False`	`False`

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, ...]` of the tensor is defined as:

```
qtotal[ia, ib, ic, ...] = a.to_qflat()[ia] * a.qconj + b.to_qflat()[ib] * b.qconj + c.
↪to_qflat()[ic] * c.qconj + ...  modulo qmod
```

The rule which entries of the a `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, ...` of a *Array* can only be non-zero, if `qtotal[ia, ib, ic, ...]` 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, ...` for which the above defined `qtotal[ia, ib, ic, ...]` 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 straigth-forward 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 whats 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  modulo qmod
B.qtotal == B.legs[0].to_qflat()[ib] * B.legs[0].qconj + B.legs[1].to_qflat()[ic] * B.
↪legs[1].qconj  modulo 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  modulo 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:

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, *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 acchive).

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:

```
|
|    x->-  | A |  ->-y->-  | B |  ->-z
|          -----            -----
|            ^                ^
|            |p               |p
```

The two legs `p` are the physical legs and share the same charge, as they both describe the same local Hilbert space. For better distincition, 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:

```
chinfo = npc.ChargeInfo([1], ['2*Sz'])
p  = 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 acchieved 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:

```
A[up, :, :]   = [[1/2.**0.5, 0]]      B[up, :, :]   = [[0], [-1]]
A[down, :, :] = [[0, 1/2.**0.5]]      B[down, :, :] = [[1], [0]]
```

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:

```
A.qtotal = 0 = p.to_qflat()[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)
```

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.from_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:

```
B.qtotal = 0 = p.to_qflat()[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)
```

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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 fullfilled! This is an implication of the fact that the singlet has a well defined value for $S_a^z + S_b^z$. For other states without fixed magnetization (e.g., $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$) 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*).

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 exisiting 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 permution 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:

```
legs[0].slices = np.array([0, 1, 4, ...])
legs[0].charges = np.array([[-2], [1], ...])
```

Each row of *charges* gives the charges for a *charge block* of the leg, with the actual indices of the total tensor determined by the *slices*. The *qindex* simply enumerates the charge blocks of a lex. Picking a qindex (and thus a *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 *rank* qindices, we put a corresponding entry in `_qdata`, which is a 2D array of shape `(#stored_blocks, rank)`. Each row corresponds to a non-zero subblock, and there are rank columns giving the corresponding qindex for each leg.

Example: for a rank 3 tensor we might have:

```
T._data = [t1, t2, t3, t4, ...]
T._qdata = np.array([[3, 2, 1],
                     [1, 1, 1],
                     [4, 2, 2],
                     [2, 1, 2],
                     ...       ])
```

The third subblock has an ndarray `t3`, and qindices `[4 2 2]` for the three legs.

- To find the position of `t3` in the actual tensor you can use `get_slice()`:

  ```
  T.legs[0].get_slice(4), T.legs[1].get_slice(2), T.legs[2].get_slice(2)
  ```

  The function `leg.get_charges(qi)` simply returns `slice(leg.slices[qi], leg.slices[qi+1])`

- To find the charges of t3, we an use `get_charge()`:

  ```
  T.legs[0].get_charge(2), T.legs[1].get_charge(2), T.legs[2].get_charge(2)
  ```

  The function `leg.get_charge(qi)` simply returns `leg.charges[qi]*leg.qconj`.

Note: Outside of *np_conserved*, you should use the API to access the entries. If you really need to iterate over all blocks of an Array `T`, try `for (block, blockslices, charges, qindices) in T: 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 `isort_qdata()`, the `_qdata` example above goes to

```
_qdata = np.array([[1, 1, 1],
                   [3, 2, 1],
                   [2, 1, 2],
                   [4, 2, 2],
                   ...       ])
```

Note that *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 gaurantee. If an algorithm modifies `_qdata`, it **must** set `_qdata_sorted = False` (unless it gaurantees it is still sorted). The routine `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 *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 arrarys (described here). Unlike numpy arrays, our Array class does not broadcast existing index arrays – this would be terribly slow. Also, *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[i0, i1, ...]`. If all indices `i0, i1, ...` are integers, the single corresponding entry (of type *dtype*) is returned.

However, the individual 'indices' `i0` 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 *take_slice()*.
- a `slice(None)` or `:`: keep the complete axis
- an `Ellipsis` or `...`: shorthand for `slice(None)` for missing axes to fix the len
- an 1D bool *ndarray* `mask`: apply a mask to that axis, see *iproject()*.
- a `slice(start, stop, step)` or `start:stop:step`: keep only the indices specified by the slice. This is also implemented with *iproject*.
- an 1D int *ndarray* `mask`: keep only the indices specified by the array. This is also implemented with *iproject*.

For slices and 1D arrays, additional permuations may be perfomed with the help of *permute()*.

If the number of indices is less than *rank*, the remaining axes remain free, so for a rank 4 Array `A`, `A[i0, i1] == A[i0, i1, ...] == A[i0, i1, :, :]`.

Note that indexing always **copies** the data – even if *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 `a0` and `a1` the following holds

```
A[a0, a1].to_ndarray() == A.to_ndarray()[np.ix_(a0, a1)] != A.to_ndarray()[a0, a1]
```

For a combination of slices and arrays, things get more complicated with numpys advanced indexing. In that case, a simple `np.ix_(...)` 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 perfom a SVD, a tensor needs to be viewed as a matrix. For a flat array, this can be done with `np.reshape`, e.g., if `A` has shape `(10, 3, 7)` then `B = np.reshape(A, (30, 7))` will result in a (view of the) array with one less dimension, but a "larger" first leg. By default (`order='C'`), this results in

```
B[i*3 + j , k] == A[i, j, k] for i in range(10) for j in range(3) for k in range(7)
```

While for a np.array, also a reshaping `(10, 3, 7) -> (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

```
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 = {label: leg_position, ...}`. Not all legs need a label.
- To set the labels, call

  ```
  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 sourrounded 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 contians 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.)

```
"""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.
"""
```

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```
# 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
#         |
#         ^
#         |
```

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```
#         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")

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

envL = npc.zeros([W.get_leg('wL').conj(), Bs[0].get_leg('vL').conj(), Bs[0].get_leg(
↪'vL')],
                 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')],
                 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
```

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```
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 originial 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")
```

7.3.5 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) strucuture: above, we spoke of a 1D "chain".
- The boundary conditions: do we have open or periodic boundary conditions? The "chain" suggests open boundaries, 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. Each algorithm requires the model and Hamiltonian to be specified in a particular form. We have one class for each such required form. For example `dmrg` requires an `MPOModel`, which contains the Hamiltonian written as an `MPO`. On the other hand, if we want to evolve a state with `tebd` we need a `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.

Implmenting you own model ultimatley means to get an instance of `MPOModel` or `NearestNeighborModel`. The predefined classes in the other modules under `models` are subclasses of at least one of those, you will see examples later down below.

The Hilbert space

The **local Hilbert** space is represented by a `Site` (read its doc-string!). In particular, the *Site* contains the local `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 `tenpy.networks.site`, but if necessary you can easily extend them by adding further local operators or completely write your own subclasses of `Site`.

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

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

An example where `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 *np_conserved* yet, but want to get started with models right away, you can set `conserve=None` in the existing sites or use `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 *Charge conservation with np_conserved*.

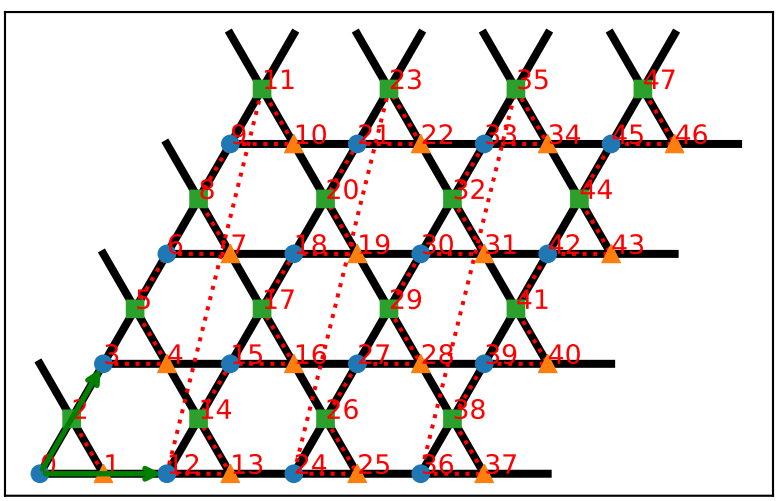
The geometry : lattices

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. (More details on that can be found in the doc-string of `Lattice`, read it!)

Visualization of the lattice can help a lot to understand which sites are connected by what couplings. The methods `plot_...` of the `Lattice` can do a good job for a quick illustration. We include a small image in the documation of each of the lattices. For example, the following small script can generate the image of the Kagome lattice shown below:

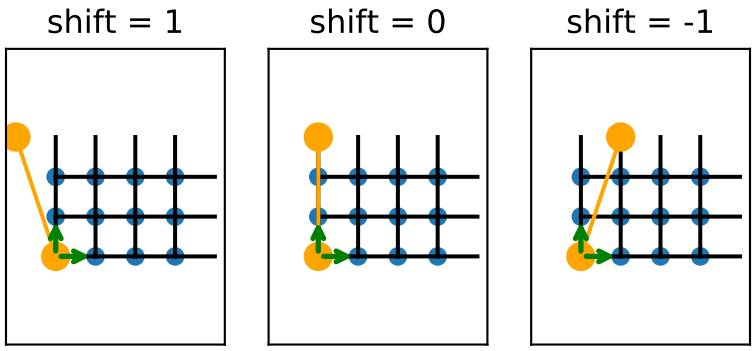
```
import matplotlib.pyplot as plt
from tenpy.models.lattice import Kagome

ax = plt.gca()
lat = Kagome(4, 4, None, bc='periodic')
lat.plot_coupling(ax, lat.nearest_neighbors, linewidth=3.)
lat.plot_order(ax=ax, linestyle=':')
lat.plot_sites()
lat.plot_basis(ax, color='g', linewidth=2.)
ax.set_aspect('equal')
ax.get_xaxis().set_visible(False)
ax.get_yaxis().set_visible(False)
plt.show()
```



The lattice contains also the **boundary conditions** *bc* in each direction. It can be one of the usual `'open'` or `'periodic'` in each direcetion. Instead of just saying "periodic", you can also specify a *shift* (except in the first direction). This is easiest to understand at its standard usecase: DMRG on a infinite cylinder. Going around the

cylinder, you have a degree of freedom which sites to connect. The orange markers in the following figures illustrates sites identified for a Square lattice with `bc=['periodic', shift]` (see `plot_bc_shift()`):



Note that the "cylinder" axis (and direction for k_x) is perpendicular to the orange line connecting these sites. The line where the cylinder is "cut open" therefore winds around the the cylinder for a non-zero *shift* (or more complicated lattices without perpendicular basis).

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 in by the lattice, as it defines an **order** (*order*) of the sites. The methods *mps2lat_idx()* and *lat2mps_idx()* map indices of the MPS to and from indices of the lattice. If you obtained and array with expectation values for a given MPS, you can use *mps2lat_values()* to map it to lattice indices, thereby reverting the ordering.

Performing this mapping of the Hamiltonain from a 2D lattice to a 1D chain by hand can be a tideous process. Therefore, we have automated this mapping in TeNPy as explained in the next section. (Nevertheless it's a good exercise you should do at least once in your life to understand how it works!)

Note: 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 strate 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.

Implementing you own model

When you want to simulate a model not provided in *models*, you need to implement your own model class, lets call it `MyNewModel`. The idea is that you define a new subclass of one or multiple of the model base classes. For example, when you plan to do DMRG, you have to provide an MPO in a `MPOModel`, so your model class should look like this:

```
class MyNewModel(MPOModel):
    """General strucutre for a model suitable for DMRG.

    Here is a good place to document the represented Hamiltonian and parameters.

    In the models of TeNPy, we usually take a single dictionary `model_params`
    containing all parameters, and read values out with ``model_params.get(key,␣
↪default)``.
    The model needs to provide default values if the parameters was not specified.
    """
```

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```
    def __init__(self, model_params):
        # some code here to read out model parameters and generate H_MPO
        lattice = somehow_generate_lattice(model_params)
        H_MPO = somehow_generate_MPO(lattice, model_params)
        # initialize MPOModel
        MPOModel.__init__(self, lattice, H_MPO)
```

TEBD requires another representation of H in terms of bond terms *H_bond* given to a `NearestNeighborModel`, so in this case it would look so like this instead:

```
class MyNewModel2(NearestNeighborModel):
    """General strucutre for a model suitable for TEBD."""
    def __init__(self, model_params):
        # some code here to read out model parameters and generate H_bond
        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`. Moreover, it's quite annoying 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 *CouplingModel*!

The easy way to new models: the (Multi)CouplingModel

The *`CouplingModel`* provides a general, quite abstract way to specify a Hamiltonian of two-site 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 forumla $H = \sum_i A_i B_{i+dx} + ...$ with onsite operators A, B,... into a model class.

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

```
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:

```
self.add_onsite(-np.asarray(h), 0, 'Sz')
for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
    self.add_coupling(0.5*J, u1, 'Sp', u2, 'Sm', dx, plus_hc=True)
    self.add_coupling(    J, u1, 'Sz', u2, 'Sz', dx)
```

Note: The method *add_coupling()* adds the coupling only in one direction, i.e. not switching *i* and *j* in a $\sum_{\langle i,j \rangle}$. 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 $J/2(S_i^+ S_j^- + h.c.)$ 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 multipliy 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_MPO()* to initialze 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*.

The *CouplingModel* works for Hamiltonians which are a sum of terms involving at most two sites. The generalization *MultiCouplingModel* can be used for Hamlitonians with coupling terms acting on more than 2 sites at once. Follow the exact same steps in the initialization, and just use the *add_multi_coupling()* instead or in addition to the *add_coupling()*. 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 outline above. The *XXZChain2* implements the very same model, but based on the `CouplingMPOModel` explained in the next section.

```
"""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 Config
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:
```

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```
    .. 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' | 'infinte'}
            MPS boundary conditions. Coupling boundary conditions are chosen␣
↪appropriately.

    """
    def __init__(self, model_params):
        # 0) read out/set default parameters
        if not isinstance(model_params, Config):
            model_params = Config(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'
```

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```
        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.setdefault('lattice', "Chain")
        if not isinstance(model_params, Config):
            model_params = Config(model_params, "XXZChain2")
        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 easy easy 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 the class is like this:

```
class CouplingMPOModel(CouplingModel,MPOModel):
    def __init__(self, model_param):
        # ... follow 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):
        sites = self.init_sites(self, model_param) # for steps 1-3
        # initialize an arbitrary pre-defined lattice
        # using model_params['lattice']

    def init_terms(self, model_param):
        # does nothing.
        # You should overwrite this
```

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 a e.g. 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 Neigbors 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
```

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```
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 ::
        H = - \sum_{\langle i,j\rangle, i < j} \mathtt{J} \sigma^x_i \sigma^x_{j}
            - \sum_{i} \mathtt{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'
            What should be conserved. See :class:`~tenpy.networks.Site.SpinHalfSite`.
        J, g : float | array
            Coupling as defined for the Hamiltonian above.

    """
    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']:
```

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```
            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.
    """
    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:

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

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:

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

```
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:

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

Some final remarks

- 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`.

7.3.6 Fermions and the Jordan-Wigner transformation

The Jordan-Wigner tranformation 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 $\sigma_j^{x,y,z}$ and $\sigma_j^{\pm} = (\sigma_j^x \pm \mathrm{i}\sigma_j^y)/2$ on each site, we can map

$$\begin{aligned} n_j &\leftrightarrow (\sigma_j^z + 1)/2 \\ c_j &\leftrightarrow (-1)^{\sum_{l<j} n_l} \sigma_j^- \\ c_j^\dagger &\leftrightarrow (-1)^{\sum_{l<j} n_l} \sigma_j^+ \end{aligned}$$

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 `l <= j`! Thus, clearly the operators `C` and `Cd` 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 $JW := (-1)^{n_l}$ acting all sites `l < 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 `l < j` *and* the local operator `C` (or `Cd`, respectively) on site `j`.

On the sites itself, the onsite operators `C` and `Cd` 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 entry in the list acting on site *i*, the relations are thus:

```
["JW", ..., "JW", "C",  "Id", ..., "Id"]   # for the annihilation operator
["JW", ..., "JW", "Cd", "Id", ..., "Id"]   # for the creation operator
```

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:

```
["JW", ..., "JW", "Cd",  "Id", ..., "Id"] * ["JW", ..., "JW", "C", "Id", ..., "Id"]
== ["JW JW", ..., "JW JW", "Cd C",  "Id Id", ..., "Id Id"]      # by definition of␣
↪the tensorproduct
== ["Id",    ..., "Id",    "N",     "Id",    ..., "Id"]         # by definition of␣
↪the local operators
# ("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.)
```

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`, $c_i^\dagger c_j \leftrightarrow \sigma_i^+ (-1)^{\sum_{i<=l<j} n_l} \sigma_j^-$. More explicitly, for `j = i+2` we get:

```
["JW", ..., "JW", "Cd", "Id", "Id", "Id", ..., "Id"] * ["JW", ..., "JW", "JW", "JW",
↪"C", "Id", ..., "Id"]
== ["JW JW", ..., "JW JW", "Cd JW",  "Id JW", "Id C", ..., "Id"]
== ["Id",    ..., "Id",    "Cd JW",  "JW",    "C",    ..., "Id"]
```

In other words, the Jordan-Wigner string appears only in the range `i <= 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`.)

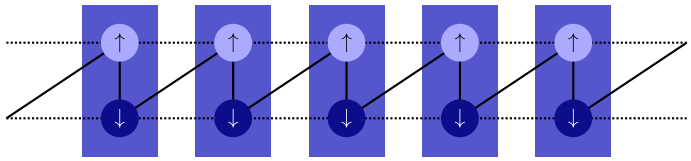
This is also the case for `j < i`, say `j = i-2`: $c_i^\dagger c_j \leftrightarrow (-1)^{\sum_{j<=l<i} n_l} \sigma_i^+ \sigma_j^-$. As shown in the following, the `JW` again appears on the left site, but this time acting *after* `C`:

```
["JW", ..., "JW", "JW", "JW", "Cd", "Id", ..., "Id"] * ["JW", ..., "JW", "C", "Id",
↪"Id", "Id", ..., "Id"]
== ["JW JW", ..., "JW JW", "JW C",  "JW", "Cd Id", ..., "Id"]
== ["Id",    ..., "Id",    "JW C",  "JW", "Cd",    ..., "Id"]
```

Higher dimensions

For an MPO or MPS, you always have to define an ordering of all your sites. This ordering effectifely maps the higher-dimensional lattice to a 1D chain, usually at the expence of long-range hopping/interactions. With this mapping, the Jordan-Wigner transformation generalizes to higher dimensions in a straight-forward 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 `SpinHalfFermionSite` which is composed of two `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 $(-1)^{n_l}$ 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 `FermionSite`):

$$
\begin{aligned}
n_{\uparrow,j} &\leftrightarrow (\sigma^z_{\uparrow,j} + 1)/2 \\
n_{\downarrow,j} &\leftrightarrow (\sigma^z_{\downarrow,j} + 1)/2 \\
c_{\uparrow,j} &\leftrightarrow (-1)^{\sum_{l<j} n_{\uparrow,l} + n_{\downarrow,l}} \sigma^-_{\uparrow,j} \\
c^\dagger_{\uparrow,j} &\leftrightarrow (-1)^{\sum_{l<j} n_{\uparrow,l} + n_{\downarrow,l}} \sigma^+_{\uparrow,j} \\
c_{\downarrow,j} &\leftrightarrow (-1)^{\sum_{l<j} n_{\uparrow,l} + n_{\downarrow,l}} (-1)^{n_{\uparrow,j}} \sigma^-_{\downarrow,j} \\
c^\dagger_{\downarrow,j} &\leftrightarrow (-1)^{\sum_{l<j} n_{\uparrow,l} + n_{\downarrow,l}} (-1)^{n_{\uparrow,j}} \sigma^+_{\downarrow,j}
\end{aligned}
$$

In each of the above mappings the operators on the right hand sides commute; we can rewrite $(-1)^{\sum_{l<j} n_{\uparrow,l} + n_{\downarrow,l}} = \prod_{l<j} (-1)^{n_{\uparrow,l}} (-1)^{n_{\downarrow,l}}$, 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 $\sigma^-_{\uparrow,j}$, `Cdu` is $\sigma^+_{\uparrow,j}$, `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 asymetry 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 $c_{\downarrow,j}, c^\dagger_{\downarrow,j}, c_{\downarrow,j}, c^\dagger_{\downarrow,j}$ 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 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", "Cdd",  "Id", ..., "Id"]   # for the creation operator spin-down
```

As you can see, the asymmetry regaring the spins in the definition of the local onsite operators `"Cu", "Cd", "Cdu", "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 $(-1)^{n_{\uparrow,2}}$ 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 operators. 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 $c_i^\dagger c_j$ 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. $c_i^\dagger c_j^\dagger c_k c_l$ 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 $j < m < k$.

Note: 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 correspondlingly set `op_string='JW', str_on_first=True`, if necessary. For *add_multi_coupling*, you cann'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 $\sum_i (c_i^\dagger c_{i+1} + h.c.) = \sum_i (c_i^\dagger c_{i+1} + c_i^\dagger c_{i-1})$ in a 1D chain of *FermionSite* with *add_coupling()*. The recoomended way is just:

```
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:

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

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

```
for (dx, dy) in [(1, 0), (0, 1)]:
    add_coupling(strength, 0, 'Cdu', 0, 'Cu', (dx, dy), plus_hc=True)  # spin up
    add_coupling(strength, 0, 'Cdd', 0, 'Cd', (dx, dy), plus_hc=True)  # spin down

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

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

7.3.7 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:

```
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):

```
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:

```
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(data, 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")
```

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:

0. 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).
1. 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.
2. Allow to save (nested) python lists, tuples and dictionaries with values (and keys) which can be saved.
3. 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.
4. 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`.
5. 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.
7. Loading a dataset should be (fairly) secure and not execute arbitrary python code (even if the dataset was manipulated), as it is the case for pickle.

   Disclaimer: I'm not an security expert, so I can't guarantee that... Also, loading a HDF5 file can import other python modules, so importing a manipulated file is not secure if you downloaded a malicious python file as well.

The full format specification is given by the 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

7.4 Literature

This is a (by far non-exhaustive) list of some references for the various ideas behind the code. They can be cited from the python doc-strings using the format `[Author####]_`. Within each category, we sort the references by year and author.

7.4.1 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. [TeNPyDoc] is where the location is hosted online. [TeNPyForum] is the place where you can ask questions and look for help, when you are stuck with implementing something.

7.4.2 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]. [Hubig2019] 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 [Verstraete2009], [Eisert2013] and [Orus2014]. [Stoudenmire2011] reviews the use of DMRG for 2D systems. [Cirac2009] discusses the different groups of tensor network states.

7.4.3 Algorithm developments

[White1992] is the invention of DMRG, which started everything. [Vidal2004] introduced TEBD. [White2005] and [Hubig2015] solved problems for single-site DMRG. [McCulloch2008] was a huge step forward to solve convergence problems for infinite DMRG. [Singh2009], [Singh2010] explain how to incorporate Symmetries. [Haegeman2011] introduced TDVP, again explained more accessible in [Haegeman2016]. [Karrasch2013] gives some tricks to do finite-temperature simulations (DMRG), which is a bit extended in [Hauschild2018]. [Vidal2007] introduced MERA.

7.4.4 Related theory

The following are referenced from somewhere in the algorithms.

7.4.5 Software-related

The following are not physics-related, but are good to know if you want to work with TeNPy (or more generally Python).

7.5 Contributing

There are lots of things where you can help, even if you don't wont 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. 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]. If you want to become a member of the developer team, just ask ;-)

Thank You!

7.5.1 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 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 master 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 abouth 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
:class:`~tenpy.linalg.np_conserved.Array`, :meth:`~tenpy.linalg.np_conserved.
↪Array.to_ndarray`,
: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` and :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`.


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`.
"""
```

- Use relative imports within TeNPy. Example:

```
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 /changelog/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.

7.5.2 Bulding 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, install the extra requirements, i.e., Sphinx, with:

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

Note: Plotting the inheritance graphs also requires Graphviz. If you have *conda*, installing it requires just `conda install graphviz`.

Afterwards, simply go to the folder `doc/` and run the following command:

```
make html
```

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 webbroser 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 modules. The *conf.py* adjusts the python path to include the *tenpy* from root directory of the repository.

7.5.3 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: Write UserGuide!!!

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/algorithms/dmrg.py:do
of tenpy.algorithms.dmrg, line 30.)

Todo: Rebuild TDVP engine as subclasses of sweep Do testing

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/algorithms/mps_sweep
of tenpy.algorithms.mps_sweeps, line 18.)

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 corresponding npc function first.

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/algorithms/network_co
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/v0.6.0/tenpy/algorithms/tdvp.py:doc
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/v0.6.0/tenpy/algorithms/tdvp.py:doc
of tenpy.algorithms.tdvp, line 16.)

Todo: add further terms (e.g. c^dagger c^dagger + h.c.) to the Hamiltonian.

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/fermions_spinl
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 Jx, Jy.

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/hofstadter.py:d
of tenpy.models.hofstadter, line 3.)

Todo: make sure this function is used for expectation values…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/lattice.py:docs
of tenpy.models.lattice.Honeycomb.mps2lat_values, line 53.)

Todo:

- this doesn't fully work yet…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/lattice.py:docs
of tenpy.models.lattice.IrregularLattice, line 3.)

Todo: make sure this function is used for expectation values…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/lattice.py:docs
of tenpy.models.lattice.IrregularLattice.mps2lat_values, line 53.)

Todo: make sure this function is used for expectation values…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/lattice.py:docs
of tenpy.models.lattice.Kagome.mps2lat_values, line 53.)

Todo: make sure this function is used for expectation values…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/lattice.py:docs
of tenpy.models.lattice.Ladder.mps2lat_values, line 53.)

Todo: make sure this function is used for expectation values…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/lattice.py:docs
of tenpy.models.lattice.Lattice.mps2lat_values, line 53.)

Todo: make sure this function is used for expectation values…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/lattice.py:docs
of tenpy.models.lattice.TrivialLattice.mps2lat_values, line 53.)

Todo: implement MPO for time evolution…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/model.py:docs
of tenpy.models.model.MPOModel, line 7.)

Todo: make sure this function is used for expectation values…

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/models/toric_code.py:
of tenpy.models.toric_code.DualSquare.mps2lat_values, line 53.)

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/v0.6.0/tenpy/networks/mpo.py:docs
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/v0.6.0/tenpy/networks/mpo.py:docs
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/v0.6.0/tenpy/networks/mps.py:docs
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 Barthel (2016), arXiv:1607.01696 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/v0.6.0/tenpy/networks/purification_
of tenpy.networks.purification_mps, line 104.)

Todo: Check if Jordan-Wigner strings for 4x4 operators are correct.

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/tenpy/checkouts/v0.6.0/tenpy/networks/site.py:docst
of tenpy.networks.site.SpinHalfFermionSite, line 61.)

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/v0.6.0/tenpy/tools/hdf5_io.py:docst
of tenpy.tools.hdf5_io, line 60.)

7.6 Tenpy main module

- full name: tenpy
- parent module: *tenpy*
- type: module

Submodules

algorithms	A collection of algorithms such as TEBD and DMRG.
linalg	Linear-algebra tools for tensor networks.
models	Definition of the various models.
networks	Definitions of tensor networks like MPS and MPO.
tools	A collection of tools: mostly short yet quite useful functions.
version	Access to version of this library.

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.

`tenpy.__version__ = '0.6.0'`
hard-coded version string

`tenpy.__full_version__ = '0.6.0'`
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

algorithms	A collection of algorithms such as TEBD and DMRG.
linalg	Linear-algebra tools for tensor networks.
models	Definition of the various models.
networks	Definitions of tensor networks like MPS and MPO.
tools	A collection of tools: mostly short yet quite useful functions.
version	Access to version of this library.

7.7 algorithms

- full name: tenpy.algorithms
- parent module: *tenpy*
- type: module

Module description

A collection of algorithms such as TEBD and DMRG.

Submodules

truncation	Truncation of Schmidt values.
dmrg	Density Matrix Renormalization Group (DMRG).
mps_sweeps	'Sweep' algorithm and effective Hamiltonians.
tebd	Time evolving block decimation (TEBD).
tdvp	Time Dependant Variational Principle (TDVP) with MPS (finite version only).
purification_tebd	Time evolving block decimation (TEBD) for MPS of purification.
network_contractor	Network Contractor.
exact_diag	Full diagonalization (ED) of the Hamiltonian.

7.7.1 truncation

- full name: tenpy.algorithms.truncation
- parent module: *tenpy.algorithms*
- type: module

Classes

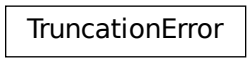
TruncationError

TruncationError([eps, ov])	Class representing a truncation error.

TruncationError

- full name: tenpy.algorithms.truncation.TruncationError
- parent module: *tenpy.algorithms.truncation*
- type: class

Inheritance Diagram



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_norm(norm_new[, norm_old])	Construct TruncationError from norm after and before the truncation.

Class Attributes and Properties

TruncationError.ov_err	Error `1.-ov` of the overlap with the correct state.

class tenpy.algorithms.truncation.**TruncationError**(*eps=0.0*, *ov=1.0*)

Bases: `object`

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 **ov** (*eps,*) – See below.

eps

The total sum of all discared 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 $|\langle\psi_{trunc}|\psi_{correct}\rangle|^2$ (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

Examples

```
>>> TE = TruncationError()
>>> TE += tebd.time_evolution(...)  # add `eps`, multiply `ov`
```

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, $\sqrt{\sum_{akept}\lambda_a^2}$ (before renormalization).
- **norm_old** (*float*) – Norm of all Schmidt values before truncation, $\sqrt{\sum_a \lambda_a^2}$.

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, $\sqrt{\sum_a \lambda_a^2}$. Default (None) is 1.

property ov_err
Error 1.-ov of the overlap with the correct state.

Functions

svd_theta(theta, trunc_par[, qtotal_LR, ...])	Performs SVD of a matrix *theta* (= the wavefunction) and truncates it.
truncate(S, options)	Given a Schmidt spectrum *S*, determine which values to keep.

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 re-

sult 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 singluar values of the array. If no *cutoff* is given, it has lenght `min(M, N)`. Normalized to `np.linalg.norm(S)==1`.
- **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 `truncate()` picks exactly those from a given Schmidt spectrum λ_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 χ_c of the initially χ Schmidt values.

Then we decompose the untruncated state as $|\psi\rangle = \sqrt{1-\epsilon}|\psi_{tr}\rangle + \sqrt{\epsilon}|\psi_{tr}^{\perp}\rangle$ 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), $|\psi_{tr}^{\perp}\rangle = \frac{1}{\sqrt{\epsilon}} \sum_{a>=\chi_c} \lambda_a |L_a\rangle|R_a\rangle$ is the discarded part (orthogonal to the kept part) and the *truncation error of a single truncation* is defined as $\epsilon = 1 - |\langle\psi|\psi_{tr}\rangle|^2 = \sum_{a>=\chi_c} \lambda_a^2$.

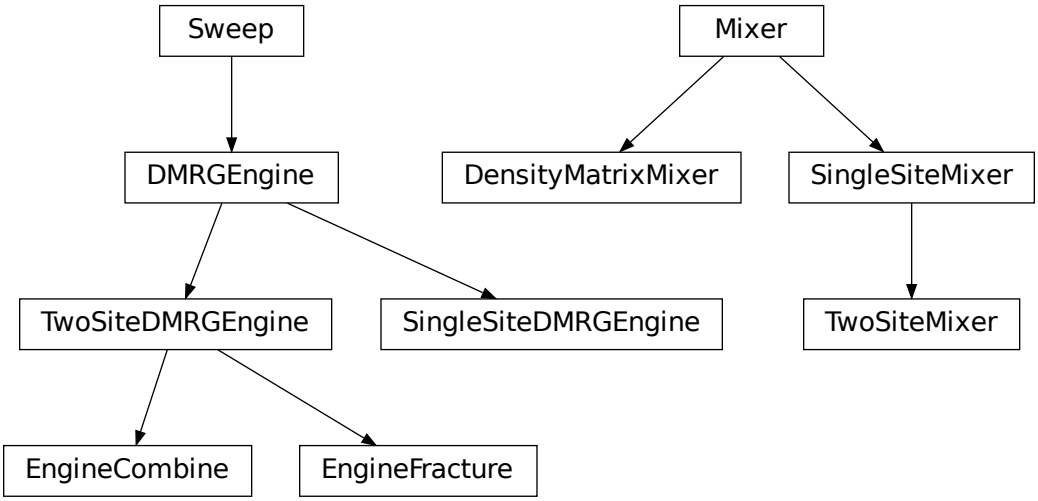
> **Warning:** For imaginary time evolution (e.g. with TEBD), you try to project out the ground state. Then, looking at the truncation error defined in this module does *not* give you any information how good the found state coincides with the actual ground state! (Instead, the returned truncation error 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.

7.7.2 dmrg

- full name: tenpy.algorithms.dmrg
- parent module: *tenpy.algorithms*
- type: module

Classes

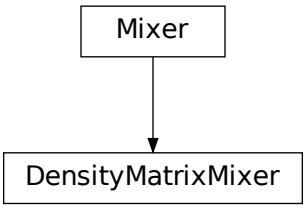


DMRGEngine(psi, model, options)	DMRG base class.'Engine' for the DMRG algorithm.
DensityMatrixMixer(options)	Mixer based on density matrices.
EngineCombine(psi, model, DMRG_params)	Engine which combines legs into pipes as far as possible.
EngineFracture(psi, model, DMRG_params)	Engine which keeps the legs separate.
Mixer(options)	Base class of a general Mixer.
SingleSiteDMRGEngine(psi, model, options)	'Engine' for the single-site DMRG algorithm.
SingleSiteMixer(options)	Mixer for single-site DMRG.
TwoSiteDMRGEngine(psi, model, options)	'Engine' for the two-site DMRG algorithm.
TwoSiteMixer(options)	Mixer for two-site DMRG.

DensityMatrixMixer

- full name: tenpy.algorithms.dmrg.DensityMatrixMixer
- parent module: *tenpy.algorithms.dmrg*
- type: class

Inheritance Diagram



Methods

`DensityMatrixMixer.__init__`(options)	Initialize self.
DensityMatrixMixer.get_xL(wL_leg, Id_L, Id_R)	Generate the coupling of the MPO legs for the reduced density matrix.
DensityMatrixMixer.get_xR(wR_leg, Id_L, Id_R)	Generate the coupling of the MPO legs for the reduced density matrix.
DensityMatrixMixer.mix_rho_L(engine, theta, ...)	Calculated mixed reduced density matrix for left site.
DensityMatrixMixer.mix_rho_R(engine, theta, ...)	Calculated mixed reduced density matrix for left site.
DensityMatrixMixer.perturb_svd(engine, ...)	Mix extra terms to theta and perform an SVD.
DensityMatrixMixer.update_amplitude(sweeps)	Update the amplitude, possibly disable the mixer.

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 singluar 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---.            .---theta-------.
|    |   |   |   |            |   |   |       |
|            |   |           LP---H0--H1--.   |
|    |   |   |   |            |   |   |   |   |
|    .---theta*--.                    |   xR  |
|                             |   |   |   |   |
|                            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---.            .------theta---.
|    |   |   |   |            |      |   |   |
```

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```
|     |    |                     |    .--H0--H1--RP
|     |    |    |    |           |    |  |    |    |
|     .---theta*--.               |  wL  |
|                                 |    |  |    |    |
|                                 |    .--H0*-H1*-RP*
|                                 |       |    |    |
|                                 .------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_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.

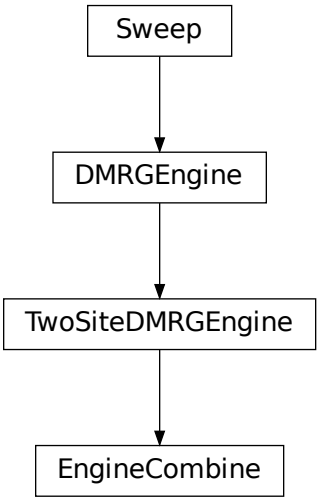
Returns **mixer** – Returns *self* if we should continue mixing, or `None`, if the mixer should be disabled.

Return type `Mixer` | None

EngineCombine

- full name: tenpy.algorithms.dmrg.EngineCombine
- parent module: *tenpy.algorithms.dmrg*
- type: class

Inheritance Diagram



Methods

`EngineCombine.__init__`(psi, model, DMRG_params)	Initialize self.
EngineCombine.diag(theta_guess)	Diagonalize the effective Hamiltonian represented by self.
EngineCombine.environment_sweeps(N_sweeps)	Perform *N_sweeps* sweeps without optimization to update the environment.
EngineCombine.get_sweep_schedule()	Define the schedule of the sweep.
EngineCombine.init_env([model])	(Re-)initialize the environment.

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Table 10 – continued from previous page

EngineCombine.make_eff_H()	Create new instance of *self.EffectiveH* at *self.i0* and set it to *self.eff_H*.
EngineCombine.mixed_svd(theta)	Get (truncated) *B* from the new theta (as returned by diag).
EngineCombine.mixer_activate()	Set *self.mixer* to the class specified by *options['mixer']*.
EngineCombine.mixer_cleanup()	Cleanup the effects of a mixer.
EngineCombine.plot_sweep_stats([axes, ...])	Plot `sweep_stats` to display the convergence with the sweeps.
EngineCombine.plot_update_stats(axes[, ...])	Plot `update_stats` to display the convergence during the sweeps.
EngineCombine.post_update_local(update_data)	Perform post-update actions.
EngineCombine.prepare_svd(theta)	Transform theta into matrix for svd.
EngineCombine.prepare_update()	Prepare *self* to represent the effective Hamiltonian on sites `(i0, i0+1)`.
EngineCombine.reset_stats()	Reset the statistics, useful if you want to start a new sweep run.
EngineCombine.run()	Run the DMRG simulation to find the ground state.
EngineCombine.set_B(U, S, VH)	Update the MPS with the `U, S, VH` returned by *self.mixed_svd*.
EngineCombine.sweep([optimize, meas_E_trunc])	One 'sweep' of a sweeper algorithm.
EngineCombine.update_LP(U)	Update left part of the environment.
EngineCombine.update_RP(VH)	Update right part of the environment.
EngineCombine.update_local(theta[, ...])	Perform bond-update on the sites `(i0, i0+1)`.

Class Attributes and Properties

EngineCombine.DMRG_params
EngineCombine.engine_params

class tenpy.algorithms.dmrg.**EngineCombine**(*psi*, *model*, *DMRG_params*)

Bases: tenpy.algorithms.dmrg.TwoSiteDMRGEngine

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, $O(2d^3\chi^3 D)$.

Deprecated since version 0.5.0: Directly use the `TwoSiteDMRGEngine` with the DMRG parameter `combine=True`.

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 folloing 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.`**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 `Sweep.`**init_env_data**: **dict**
Dictionary as returned by `self.env.get_initialization_data()` from `get_initialization_data()`.

option `Sweep.`**orthogonal_to**: **list of** ***MPSEnvironment***
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 hte 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 singluar 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 originial form, this function simply performs one sweep with disabled mixer.

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()`
- **yaxis** (*xaxis,*) – 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-axisof 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*, *meas_E_trunc=False*)
Perform post-update actions.

Compute truncation energy, remove *LP*/*RP* that are no longer needed and collect statistics.

Parameters

- **update_data** (*dict*) – Data computed during the local update, as described in the following list.
- **meas_E_trunc** (*bool, optional*) – Wheter to measure the energy after truncation.

prepare_svd(*theta*)
Transform theta into matrix for svd.

prepare_update()

Prepare *self* to represent the effective Hamiltonian on sites `(i0, i0+1)`.

Returns **theta** – Current best guess for the ground state, which is to be optimized. Labels `'vL', 'p0', 'vR', 'p1'`.

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 simluation, i.e. just a reference to `psi`.

Options

option DMRGEngine.**diag_method: str**

Method to be used for diagonalzation, 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 optimizaiton 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

- **VH** (*`U,`*) – 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(*optimize=True*, *meas_E_trunc=False*)
One 'sweep' of a sweeper algorithm.

Iteratate 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

- **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*, *meas_E_trunc=False*)

Perform bond-update on the sites `(i0, i0+1)`.

Parameters

- **theta** (*Array*) – Initial guess for the ground state of the effective Hamiltonian.
- **optimize** (*bool*) – Wheter we actually optimize to find the ground state of the effective Hamiltonian. (If False, just update the environments).
- **meas_E_trunc** (*bool*) – Wheter to measure the energy after truncation.

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()*.

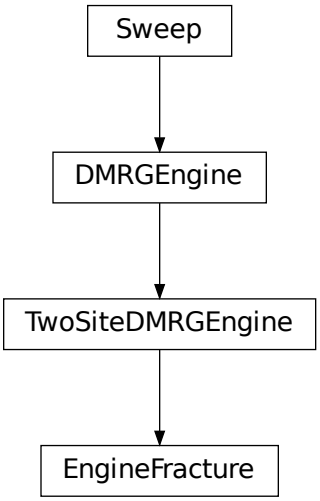
ov_change: float Change in the wave function `1. - abs(<theta_guess|theta>)` induced by *diag()*, *not* including the truncation!

Return type dict

EngineFracture

- full name: tenpy.algorithms.dmrg.EngineFracture
- parent module: *tenpy.algorithms.dmrg*
- type: class

Inheritance Diagram



Methods

`EngineFracture.__init__`(psi, model, DMRG_params)	Initialize self.
`EngineFracture.diag`(theta_guess)	Diagonalize the effective Hamiltonian represented by self.
`EngineFracture.environment_sweeps`(N_sweeps)	Perform *N_sweeps* sweeps without optimization to update the environment.
`EngineFracture.get_sweep_schedule`()	Define the schedule of the sweep.
`EngineFracture.init_env`([model])	(Re-)initialize the environment.
`EngineFracture.make_eff_H`()	Create new instance of *self.EffectiveH* at *self.i0* and set it to *self.eff_H*.
`EngineFracture.mixed_svd`(theta)	Get (truncated) *B* from the new theta (as returned by diag).
`EngineFracture.mixer_activate`()	Set *self.mixer* to the class specified by *options['mixer']*.
`EngineFracture.mixer_cleanup`()	Cleanup the effects of a mixer.
`EngineFracture.plot_sweep_stats`([axes, ...])	Plot `sweep_stats` to display the convergence with the sweeps.
`EngineFracture.plot_update_stats`(axes[, ...])	Plot `update_stats` to display the convergence during the sweeps.
`EngineFracture.post_update_local`(update_data)	Perform post-update actions.
`EngineFracture.prepare_svd`(theta)	Transform theta into matrix for svd.
`EngineFracture.prepare_update`()	Prepare *self* to represent the effective Hamiltonian on sites `(i0, i0+1)`.

continues on next page

Table 12 – continued from previous page

EngineFracture.reset_stats()	Reset the statistics, useful if you want to start a new sweep run.
EngineFracture.run()	Run the DMRG simulation to find the ground state.
EngineFracture.set_B(U, S, VH)	Update the MPS with the `U, S, VH` returned by *self.mixed_svd*.
EngineFracture.sweep([optimize, meas_E_trunc])	One 'sweep' of a sweeper algorithm.
EngineFracture.update_LP(U)	Update left part of the environment.
EngineFracture.update_RP(VH)	Update right part of the environment.
EngineFracture.update_local(theta[, ...])	Perform bond-update on the sites `(i0, i0+1)`.

Class Attributes and Properties

`EngineFracture.DMRG_params`
`EngineFracture.engine_params`

class `tenpy.algorithms.dmrg.`**`EngineFracture`**(*psi*, *model*, *DMRG_params*)

Bases: `tenpy.algorithms.dmrg.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 $O(2\chi^3 d^2 W + 2\chi^2 d^3 W^2)$.

Deprecated since version 0.5.0: Directly use the `TwoSiteDMRGEngine` with the DMRG parameter `combine=False`.

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 folloing 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.`**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 `Sweep.`**init_env_data: dict**

Dictionary as returned by `self.env.get_initialization_data()` from `get_initialization_data()`.

option `Sweep.`**orthogonal_to: list of** ***MPSEnvironment***

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 hte 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 singluar 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 originial form, this function simply performs one sweep with disabled mixer.

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()`
- **yaxis** (*xaxis,*) – 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-axisof 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*, *meas_E_trunc=False*)

Perform post-update actions.

Compute truncation energy, remove *LP*/*RP* that are no longer needed and collect statistics.

Parameters

- **update_data** (*dict*) – Data computed during the local update, as described in the following list.
- **meas_E_trunc** (*bool, optional*) – Wheter to measure the energy after truncation.

prepare_svd(*theta*)

Transform theta into matrix for svd.

prepare_update()

Prepare *self* to represent the effective Hamiltonian on sites `(i0, i0+1)`.

Returns **theta** – Current best guess for the ground state, which is to be optimized. Labels `'vL', 'p0', 'vR', 'p1'`.

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 simluation, i.e. just a reference to `psi`.

Options

option `DMRGEngine.`**`diag_method: str`**
Method to be used for diagonalzation, 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 optimizaiton 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

- **VH** (*U,*) – 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(*optimize=True*, *meas_E_trunc=False*)
One 'sweep' of a sweeper algorithm.

Iteratate 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

- **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*, *meas_E_trunc=False*)
Perform bond-update on the sites `(i0, i0+1)`.

Parameters

- **theta** (*Array*) – Initial guess for the ground state of the effective Hamiltonian.

- **optimize** (*bool*) – Wheter we actually optimize to find the ground state of the effective Hamiltonian. (If False, just update the environments).
- **meas_E_trunc** (*bool*) – Wheter to measure the energy after truncation.

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()`.

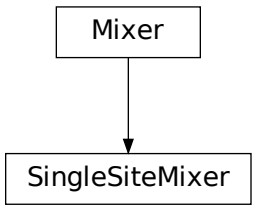
ov_change: float Change in the wave function `1. - abs(<theta_guess|theta>)` induced by `diag()`, *not* including the truncation!

Return type dict

SingleSiteMixer

- full name: tenpy.algorithms.dmrg.SingleSiteMixer
- parent module: `tenpy.algorithms.dmrg`
- type: class

Inheritance Diagram



Methods

`SingleSiteMixer.__init__`(options)	Initialize self.
`SingleSiteMixer.perturb_svd`(engine, theta, ...)	Mix extra terms to theta and perform an SVD.
`SingleSiteMixer.subspace_expand`(engine, ...)	Expand the MPS subspace, to allow the bond dimension to increase.
`SingleSiteMixer.update_amplitude`(sweeps)	Update the amplitude, possibly disable the mixer.

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.

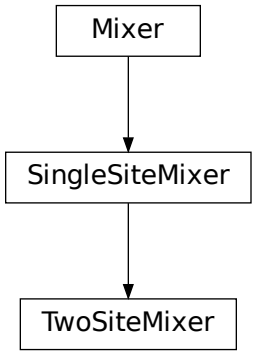
Returns **mixer** – Returns *self* if we should continue mixing, or `None`, if the mixer should be disabled.

Return type `Mixer` | None

TwoSiteMixer

- full name: tenpy.algorithms.dmrg.TwoSiteMixer
- parent module: *tenpy.algorithms.dmrg*
- type: class

Inheritance Diagram



Methods

`TwoSiteMixer.__init__`(options)	Initialize self.
`TwoSiteMixer.perturb_svd`(engine, theta, i0, ...)	Mix extra terms to theta and perform an SVD.
`TwoSiteMixer.subspace_expand`(engine, theta, ...)	Expand the MPS subspace, to allow the bond dimension to increase.
`TwoSiteMixer.update_amplitude`(sweeps)	Update the amplitude, possibly disable the mixer.

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'`.
- **S** (1D ndarray | 2D *`Array`*) – Without mixer just the singluar values of the array; with mixer it might be a general matrix; see comment above.
- **VH** (*`Array`*) – Right-canonical part of *theta*. Labels `'vL', '(vR.p1)'`.
- **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

Functions

chi_list(chi_max[, dchi, nsweeps])	Compute a 'ramping-up' chi_list.
full_diag_effH(effH, theta_guess[, keep_sector])	Perform an exact diagonalization of *effH*.
run(psi, model, options)	Run the DMRG algorithm to find the ground state of the given model.

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 preffered in the end is not obvious a priori and might depend on the used model. Just try both of them.

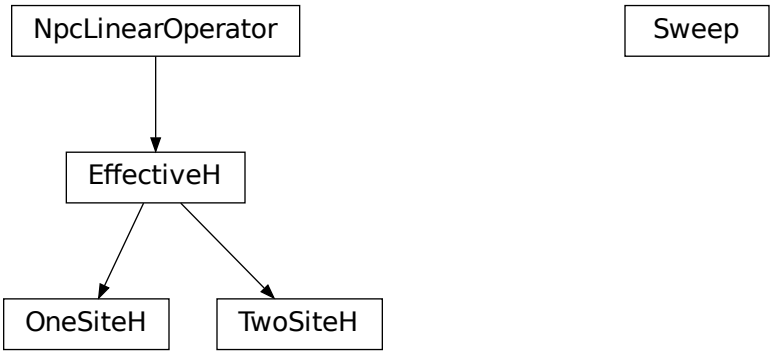
A `Mixer` should be used initially to avoid that the algorithm gets stuck in local energy minima, and then slowly turned off in the end. For `SingleSiteDMRGEngine`, using a mixer is crucial, as the one-site algorithm cannot increase the MPS bond dimension by itself.

Todo: Write UserGuide!!!

7.7.3 mps_sweeps

- full name: tenpy.algorithms.mps_sweeps
- parent module: *tenpy.algorithms*
- type: module

Classes

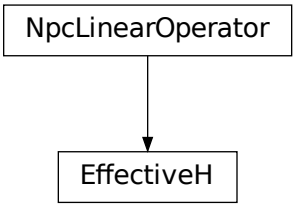


EffectiveH(env, i0[, combine, move_right])	Prototype class for local effective Hamiltonians used in sweep algorithms.
OneSiteH(env, i0[, combine, move_right])	Class defining the one-site effective Hamiltonian for Lanczos.
Sweep(psi, model, options)	Prototype class for a 'sweeping' algorithm.
TwoSiteH(env, i0[, combine, move_right])	Class defining the two-site effective Hamiltonian for Lanczos.

EffectiveH

- full name: tenpy.algorithms.mps_sweeps.EffectiveH
- parent module: *tenpy.algorithms.mps_sweeps*
- type: class

Inheritance Diagram



Methods

`EffectiveH.__init__`(env, i0[, combine, ...])	Initialize self.
`EffectiveH.adjoint`()	Return the hermitian conjugate of *self*
`EffectiveH.combine_theta`(theta)	Combine the legs of *theta*, such that it fits to how we combined the legs of *self*.
`EffectiveH.matvec`(vec)	Calculate the action of the operator on a vector *vec*.
`EffectiveH.to_matrix`()	Contract *self* to a matrix.

Class Attributes and Properties

`EffectiveH.acts_on`
`EffectiveH.length`

class `tenpy.algorithms.mps_sweeps.`**`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 `H0` and `H1` are MPO tensors.

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, 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`x`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 uncombined 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.

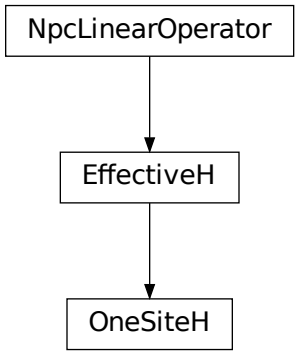
Returns **matrix** – Contraction of the represented operator.

Return type *Array*

OneSiteH

- full name: tenpy.algorithms.mps_sweeps.OneSiteH
- parent module: *tenpy.algorithms.mps_sweeps*
- type: class

Inheritance Diagram



Methods

`OneSiteH.__init__`(env, i0[, combine, move_right])	Initialize self.
`OneSiteH.adjoint`()	Return the hermitian conjugate of *self*.
`OneSiteH.combine_Heff`()	Combine LP and RP with W to form LHeff and RHeff, depending on the direction.
`OneSiteH.combine_theta`(theta)	Combine the legs of *theta*, such that it fits to how we combined the legs of *self*.
`OneSiteH.matvec`(theta)	Apply the effective Hamiltonian to *theta*.
`OneSiteH.to_matrix`()	Contract *self* to a matrix.

Class Attributes and Properties

`OneSiteH.acts_on`
`OneSiteH.length`

class `tenpy.algorithms.mps_sweeps.`**`OneSiteH`**(*env*, *i0*, *combine=False*, *move_right=True*)

Bases: *`tenpy.algorithms.mps_sweeps.EffectiveH`*

Class defining the one-site effective Hamiltonian for Lanczos.

The effective one-site Hamiltonian looks like this:

```
|         .---    ---.
|         |     |     |
|        LP----W0----RP
|         |     |     |
|         .---    ---.
```

If *combine* is True, we define either *LHeff* as contraction of *LP* with *W* (in the case *move_right* is True) or *RHeff*

as contraction of *RP* and *W*.

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, $O(2d^3\chi^3 D)$. Is originally from the wo-site method; unclear if it works well for 1 site.
- **move_right** (*bool*) – Whether the 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

LHeff, RHeff

Only set if `combine`, and only one of them depending on `move_right`. If *move_right* was True, *LHeff* is set with labels `'(vR*.p0)', 'wR', '(vR.p0*)'` for bra, MPO, ket; otherwise *RHeff* 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 LHeff and RHeff, depending on the direction.

In a move to the right, we need LHeff. In a move to the left, we need RHeff. 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*

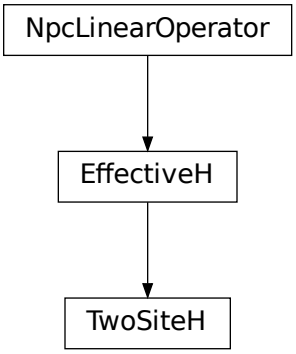
to_matrix()
Contract *self* to a matrix.

adjoint()
Return the hermitian conjugate of *self*.

TwoSiteH

- full name: tenpy.algorithms.mps_sweeps.TwoSiteH
- parent module: *tenpy.algorithms.mps_sweeps*
- type: class

Inheritance Diagram



Methods

TwoSiteH.__init__(env, i0[, combine, move_right])	Initialize self.
TwoSiteH.adjoint()	Return the hermitian conjugate of *self*.
TwoSiteH.combine_Heff()	Combine LP and RP with W to form LHeff and RHeff.
TwoSiteH.combine_theta(theta)	Combine the legs of *theta*, such that it fits to how we combined the legs of *self*.
TwoSiteH.matvec(theta)	Apply the effective Hamiltonian to *theta*.
TwoSiteH.to_matrix()	Contract *self* to a matrix.

Class Attributes and Properties

`TwoSiteH.acts_on`
`TwoSiteH.length`

class tenpy.algorithms.mps_sweeps.**TwoSiteH**(*env*, *i0*, *combine=False*, *move_right=True*)

Bases: `tenpy.algorithms.mps_sweeps.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 *LHeff* and *RHeff*, 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

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, $O(2d^3\chi^3D)$.

Type bool

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

LHeff

Left part of the effective Hamiltonian. Labels `'(vR*.p0)', 'wR', '(vR.p0*)'` for bra, MPO, ket.

Type `Array`

RHeff

Right part of the effective Hamiltonian. Labels `'(p1*.vL)', 'wL', '(p1.vL*)'` for ket, MPO, bra.

Type `Array`

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.

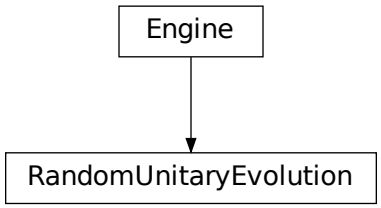
The `Sweep` class attempts to generalize as many aspects of 'sweeping' algorithms as possible. *EffectiveH* and its subclasses implement the effective Hamiltonians mentioned above. Currently, effective Hamiltonians for 1-site and 2-site optimization are implemented.

Todo: Rebuild TDVP engine as subclasses of sweep Do testing

7.7.4 tebd

- full name: tenpy.algorithms.tebd
- parent module: `tenpy.algorithms`
- type: module

Classes



`Engine`(psi, model, options)	Time Evolving Block Decimation (TEBD) algorithm.
`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 evoltion of an MPS. It works only for nearest-neighbor hamiltonians (in tenpy given by a `NearestNeighborModel`), which can be written as $H = H^{even} + H^{odd}$, such that H^{even} contains the the terms on even bonds (and similar H^{odd} the terms on odd bonds). In the simplest case, we apply first $U = \exp(-i * dt * H^{even})$, then $U = \exp(-i * dt * H^{odd})$ 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 *Ui*, 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.

7.7.5 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

H1_mixed

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.

Parameters

- **Lp** (*tenpy.linalg.np_conserved.Array*) – left part of the environment
- **Rp** (*tenpy.linalg.np_conserved.Array*) – right part of the environment
- **M** (*tenpy.linalg.np_conserved.Array*) – MPO which is applied to the 'p' leg of theta

Lp

left part of the environment

Type *tenpy.linalg.np_conserved.Array*

Rp

right part of the environment

Type *tenpy.linalg.np_conserved.Array*

W

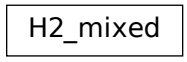
MPO which is applied to the 'p0' leg of theta

Type *tenpy.linalg.np_conserved.Array*

H2_mixed

- full name: tenpy.algorithms.tdvp.H2_mixed
- parent module: *tenpy.algorithms.tdvp*
- type: class

Inheritance Diagram



Methods

`H2_mixed.__init__`(Lp, Rp, W0, W1)	Initialize self.
`H2_mixed.matvec`(theta)	

class `tenpy.algorithms.tdvp.`**`H2_mixed`**(*Lp*, *Rp*, *W0*, *W1*)

Bases: `object`

Class defining the two sites 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
- **W** (*tenpy.linalg.np_conserved.Array*) – MPO which is applied to the 'p0' leg of theta

Lp

left part of the environment

Type *tenpy.linalg.np_conserved.Array*

Rp

right part of the environment

Type *tenpy.linalg.np_conserved.Array*

W0

MPO which is applied to the 'p0' leg of theta

Type *tenpy.linalg.np_conserved.Array*

W1

MPO which is applied to the 'p1' leg of theta

Type *tenpy.linalg.np_conserved.Array*

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 manyfold 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.

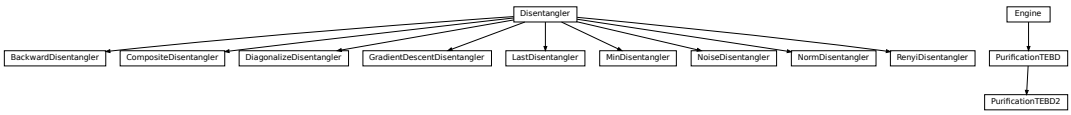
Todo: This is still a beta version, use with care. The interface might still change.

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.

7.7.6 purification_tebd

- full name: tenpy.algorithms.purification_tebd
- parent module: `tenpy.algorithms`
- type: module

Classes

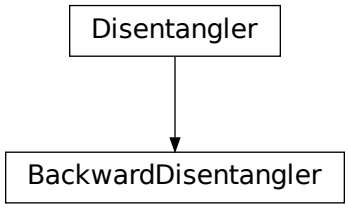


`BackwardDisentangler`(parent)	Disentangle with backward time evolution.
`CompositeDisentangler`(disentanglers)	Concatenate multiple disentanglers.
`DiagonalizeDisentangler`(parent)	Disentangle by diagonalizing the two-site density matrix in the auxiliar space.
`Disentangler`(parent)	Prototype for a disentangler.
`GradientDescentDisentangler`(parent)	Gradient-descent optimization, similar to `RenyiDisentangler`.
`LastDisentangler`(parent)	Use the last total 'U' used in `disentangle()` for the same _update_index as guess.
`MinDisentangler`(disentanglers, parent)	Chose the disentangler giving the smallest entropy.
`NoiseDisentangler`(parent)	Apply a little bit of random noise.
`NormDisentangler`(parent)	Find optimal U for which the truncation of Ultheta> has maximal overlap with Ultheta>.
`PurificationTEBD`(psi, model, options)	Time evolving block decimation (TEBD) for purification MPS.
`PurificationTEBD2`(psi, model, options)	Similar as PurificationTEBD, but perform sweeps instead of brickwall.
`RenyiDisentangler`(parent)	Iterative find U which minimized the second Renyi entropy.

BackwardDisentangler

- full name: tenpy.algorithms.purification_tebd.BackwardDisentangler
- parent module: `tenpy.algorithms.purification_tebd`
- type: class

Inheritance Diagram



Methods

`BackwardDisentangler.__init__`(parent)	Initialize self.

class `tenpy.algorithms.purification_tebd.`**`BackwardDisentangler`**(*parent*)

Bases: *`tenpy.algorithms.purification_tebd.Disentangler`*

Disentangle with backward time evolution.

See [Karrasch2013] for details; only useful during real-time evolution.

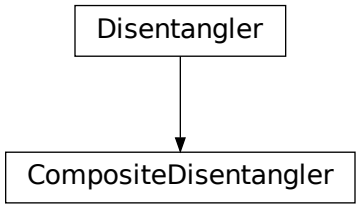
For the infinite temperature state, `theta = delta_{p0, q0}*delta_{p1, q1}`. Thus, an application of *U_bond* to `p0, p1` can be reverted completely by applying `U_bond^{dagger}` to `q0, q1`, resulting in the same state. This works also for finite temperatures, since *exp(-beta H)* and *exp(-i H t)* commute. Once we apply an operator to measure correlation function, the disentangling breaks down, yet for a local operator only in it's light-cone.

Arguments and return values are the same as for *`Disentangler`*.

CompositeDisentangler

- full name: tenpy.algorithms.purification_tebd.CompositeDisentangler
- parent module: *`tenpy.algorithms.purification_tebd`*
- type: class

Inheritance Diagram



Methods

`CompositeDisentangler.__init__`(disentanglers)	Initialize self.

class `tenpy.algorithms.purification_tebd.`**`CompositeDisentangler`**(*disentanglers*)

Bases: *`tenpy.algorithms.purification_tebd.Disentangler`*

Concatenate multiple disentanglers.

Applies multiple disentanglers, one after another (in iteration order).

Parameters **`disentanglers`** (list of *`Disentangler`*) – The disentanglers to be used.

`disentanglers`

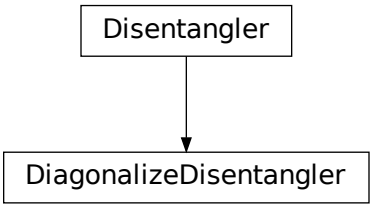
The disentanglers to be used.

Type list of *`Disentangler`*

DiagonalizeDisentangler

- full name: tenpy.algorithms.purification_tebd.DiagonalizeDisentangler
- parent module: *`tenpy.algorithms.purification_tebd`*
- type: class

Inheritance Diagram



Methods

`DiagonalizeDisentangler.__init__`(parent)	Initialize self.

class `tenpy.algorithms.purification_tebd.`**`DiagonalizeDisentangler`**(*parent*)

Bases: *`tenpy.algorithms.purification_tebd.Disentangler`*

Disentangle by diagonalizing the two-site density matrix in the auxiliar space.

See arXiv:1704.01974. Problem: Sorting by eigenvalues breaks the charge conservation! Instead we just sort within the charge blocks. For non-trivial charges, this might increase the entropy!

Arguments and return values are the same as for *`Disentangler`*.

Disentangler

- full name: tenpy.algorithms.purification_tebd.Disentangler
- parent module: *`tenpy.algorithms.purification_tebd`*
- type: class

Inheritance Diagram

Methods

`Disentangler.__init__`(parent)	Initialize self.

class `tenpy.algorithms.purification_tebd.`**`Disentangler`**(*parent*)

Bases: `object`

Prototype for a disentangler. Trivial, does nothing.

In 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 physical expectation values.

Note: We have to apply the *same* unitary to the 'bra' and 'ket' used for expectation values / correlation functions!

However, the unitary can strongly influence the entanglement structure of $|\psi >$. Therefore, the `PurificationTEBD` includes a hook in `PurificationTEBD.update_bond()` (and similar methods) to find and apply a disentangling unitary to the auxiliar indices of a two-site wave function by calling (`__call__` method) a *Disentangler*.

This class is a 'trivial' disentangler which does *nothing* to the two-site wave function; derived classes use different strategies to find various disentanglers.

Parameters **`parent`** (`Engine`) – The parent class calling the disentangler.

`parent`

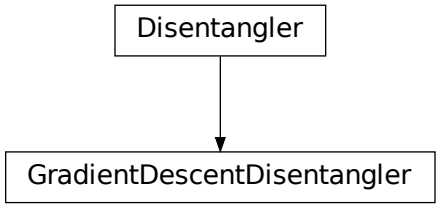
The parent class calling the disentangler.

Type `Engine`

GradientDescentDisentangler

- full name: tenpy.algorithms.purification_tebd.GradientDescentDisentangler
- parent module: `tenpy.algorithms.purification_tebd`
- type: class

Inheritance Diagram



Methods

`GradientDescentDisentangler.__init__`(parent)	Initialize self.
`GradientDescentDisentangler.iter`(theta)	Given *theta*, find a unitary U towards minimizing the n-th Renyi entropy.

class `tenpy.algorithms.purification_tebd.`**`GradientDescentDisentangler`**(*parent*)

Bases: `tenpy.algorithms.purification_tebd.Disentangler`

Gradient-descent optimization, similar to `RenyiDisentangler`.

Reads of the following *TEBD_params*:

key	type	description
disent_eps	float	Break, if the change in the Renyi entropy `S(n=2)` per iteration is smaller than this value.
disent_max_iter	float	Maximum number of iterations to perform.
disent_n	float	Renyi index of the entropy to be used. `n=1` for von-Neumann entropy.

Arguments and return values are the same as for `Disentangler`.

iter(*theta*)

Given *theta*, find a unitary U towards minimizing the n-th Renyi entropy.

This function calulates the gradiant $dS = \partial S(Utheta, n)/\partial U$. and then `U(t) = exp(-t*dS)`, where we choose the t from stepsizes which minimizes the entropy of `U(t) theta`.

When `R[i]` is the derivative $\partial S(Y, n)\partial Y_i$ of the (n-th Renyi) entropy, `dS` is given by:

```
|      .----X--R--Z----.
|      |    |     |    |
|      |    q0    q1   |
|      |               |
|      |    q0*   q1*  |
|      |    |     |    |
|      .----X*-Y--Z*---.
```

Parameters **theta** (`Array`) – Two-site wave function to be disentangled

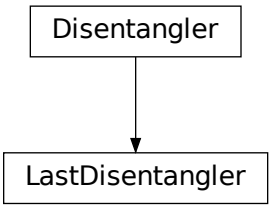
Returns

- **S** (*float*) – n-th Renyi entopy of new_theta
- **theta** (`Array`) – The *disentangled* wave function `new_U theta`.
- **new_U** (`Array`) – Unitary with legs `'q0', 'q1', 'q0*', 'q1*'`, which was used to disentangle *theta*.

LastDisentangler

- full name: tenpy.algorithms.purification_tebd.LastDisentangler
- parent module: *tenpy.algorithms.purification_tebd*
- type: class

Inheritance Diagram



Methods

`LastDisentangler.__init__`(parent)	Initialize self.

class tenpy.algorithms.purification_tebd.**LastDisentangler**(*parent*)

Bases: *tenpy.algorithms.purification_tebd.Disentangler*

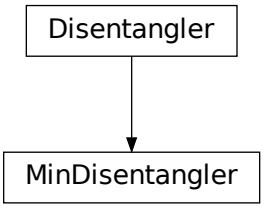
Use the last total 'U' used in `disentangle()` for the same _update_index as guess.

Useful as a starting point in a *CompositeDisentangler* to reduce the number of iterations for a following disentangler.

MinDisentangler

- full name: tenpy.algorithms.purification_tebd.MinDisentangler
- parent module: *tenpy.algorithms.purification_tebd*
- type: class

Inheritance Diagram



Methods

`MinDisentangler.__init__`(disentanglers, parent)	Initialize self.

class `tenpy.algorithms.purification_tebd.`**`MinDisentangler`**(*disentanglers*, *parent*)

Bases: *`tenpy.algorithms.purification_tebd.Disentangler`*

Chose the disentangler giving the smallest entropy.

Apply each of the disentanglers to the given *theta*, use the result with smallest entropy. Reads the TEBD_param `'disent_min_n'` which selects the *`entropy()`* to be used for comparison.

Parameters

- **`disentanglers`** (list of *`Disentangler`*) – The disentanglers to be used.
- **`parent`** (`Engine`) – The parent class calling the disentangler.

`n`

Selects the entropy to be used for comparison.

Type float

`disentanglers`

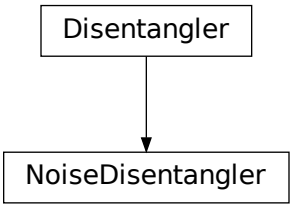
The disentanglers to be used.

Type list of *`Disentangler`*

NoiseDisentangler

- full name: tenpy.algorithms.purification_tebd.NoiseDisentangler
- parent module: *`tenpy.algorithms.purification_tebd`*
- type: class

Inheritance Diagram



Methods

`NoiseDisentangler.__init__`(parent)	Initialize self.

class `tenpy.algorithms.purification_tebd.`**`NoiseDisentangler`**(*parent*)

Bases: *`tenpy.algorithms.purification_tebd.Disentangler`*

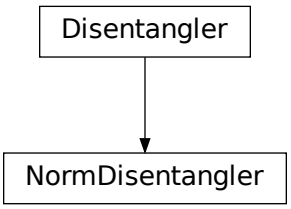
Apply a little bit of random noise. Useful as pre-step to *`RenyiDisentangler`*.

Arguments and return values are the same as for *`Disentangler`*.

NormDisentangler

- full name: tenpy.algorithms.purification_tebd.NormDisentangler
- parent module: *`tenpy.algorithms.purification_tebd`*
- type: class

Inheritance Diagram



Methods

`NormDisentangler.__init__`(parent)	Initialize self.
`NormDisentangler.iter`(theta, U, trunc_params)	Given *theta* and *U*, find *U2* maximizing `<theta|U2 truncate(U |theta>)`.

class `tenpy.algorithms.purification_tebd.`**`NormDisentangler`**(*parent*)

Bases: *`tenpy.algorithms.purification_tebd.Disentangler`*

Find optimal *U* for which the truncation of U|theta> has maximal overlap with U|theta>.

Reads of the following *options* as break criteria for the iteration:

key	type	description
disent_eps	float	Break, if the change in the Renyi entropy `S(n=2)` per iteration is smaller than this value.
disent_max_iter	float	Maximum number of iterations to perform.
disent_trunc_par	dict	Truncation parameters; defaults to *trunc_params*.
disent_norm	iter-chi-able	To find the optimal U it can help to increase *chi_max* of *disent_trunc_par* slowly, the default is `range(1, disent_trunc_par['chi_max']+1)`. However, that's **very** slow for large *chi_max*, so we allow to change it. (In fact, it makes the disentangler *scale* worse than the rest of TEBD.)

Arguments and return values are the same as for `disentangle()`.

iter(*theta*, *U*, *trunc_params*)

Given *theta* and *U*, find *U2* maximizing `<theta|U2 truncate(U |theta>)`.

Finds unitary *U2* which maximizes Tr(U

Parameters

- **theta** (*`Array`*) – Two-site wave function to be disentangled.
- **U** (*`Array`*) – The previous guess for *U*; with legs `'q0', 'q1', 'q0*', 'q1*'`.
- **trunc_params** (*`dict`*) – The truncation parameters (similar as *self.trunc_params*) used to truncate *U|theta>*.

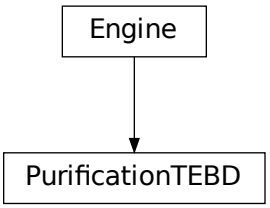
Returns

- **trunc_err** (*TruncationError*) – Norm error discarded during the truncation of `U|theta>`.
- **new_U** (*`Array`*) – Unitary with legs `'q0', 'q1', 'q0*', 'q1*'`. Chosen such that `new_U|theta>` has maximal overlap with the truncated `U|theta>`.

PurificationTEBD

- full name: tenpy.algorithms.purification_tebd.PurificationTEBD
- parent module: *tenpy.algorithms.purification_tebd*
- type: class

Inheritance Diagram



Methods

`PurificationTEBD.__init__`(psi, model, options)	Initialize self.
PurificationTEBD.calc_U(order, delta_t[, ...])	see `calc_U()`
PurificationTEBD.disentangle(theta)	Disentangle *theta* before splitting with svd.
PurificationTEBD.disentangle_global([pair])	Try global disentangling by determining the maximally entangled pairs of sites.
PurificationTEBD.disentangle_global_nsite([n])	Perform a sweep through the system and disentangle with `disentangle_n_site()`.
PurificationTEBD.disentangle_n_site(i, n, theta)	Generalization of `disentangle()` to *n* sites.
PurificationTEBD.run()	(Real-)time evolution with TEBD (time evolving block decimation).
PurificationTEBD.run_GS()	TEBD algorithm in imaginary time to find the ground state.
PurificationTEBD.run_imaginary(beta)	Run imaginary time evolution to cool down to the given *beta*.
PurificationTEBD.suzuki_trotter_decomposition(...)	Returns list of necessary steps for the suzuki trotter decomposition.
PurificationTEBD.suzuki_trotter_time_steps(order)	Return time steps of U for the Suzuki Trotter decomposition of desired order.
PurificationTEBD.update(N_steps)	Evolve by `N_steps * U_param['dt']`.
PurificationTEBD.update_bond(i, U_bond)	Updates the B matrices on a given bond.
PurificationTEBD.update_bond_imag(i, U_bond)	Update a bond with a (possibly non-unitary) *U_bond*.

continues on next page

Table 39 – continued from previous page

PurificationTEBD.update_imag(N_steps)	Perform an update suitable for imaginary time evolution.
PurificationTEBD.update_step(U_idx_dt, odd)	Updates either even *or* odd bonds in unit cell.

Class Attributes and Properties

PurificationTEBD.TEBD_params	
PurificationTEBD.disent_iterations	For each bond the total number of iterations performed in any *Disentangler*.
PurificationTEBD.trunc_err_bonds	truncation error introduced on each non-trivial bond.

class tenpy.algorithms.purification_tebd.**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 *run()* and *run_GS()* for more details.

used_disentangler

The disentangler to be used on the auxiliar indices. Chosen by *get_disentangler()*, called with the TEBD parameter 'disentangle'. Defaults to the trivial disentangler for options['disentangle']=None.

Type *Disentangler*

_disent_iterations

Number of iterations performed on all bonds, including trivial bonds; lenght *L*.

Type 1D ndarray

_guess_U_disent

Same index strucuture as *self._U*: for each two-site U of the physical time evolution the disentangler from the last application. Initialized to identities.

Type list of list of npc.Array

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.

property disent_iterations

For each bond the total number of iterations performed in any *Disentangler*.

calc_U(*order*, *delta_t*, *type_evo='real'*, *E_offset=None*)
see `calc_U()`

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:

```
|            |              |
|     ... - B1  -  s  -  B2 - ...
|            |              |
|            |--------------|
|            |      U       |
|            |--------------|
|            |              |
```

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*

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.

Caclulate 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^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) --> |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 $\exp(tH) \approx prod_{(j,k)\in ST} \exp(d[j]tH[k]) + O(t^{order+1})$.

Parameters **order** (*int*) – The desired order of the Suzuki-Trotter decomposition.

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_steps t H[k]) + O(N_steps t^{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 H_{even/odd} delta_t * 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 -
|       |    |    |    |    |    |    |
|       |    |----|    |----|    |----|
```

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```
|        |     |  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

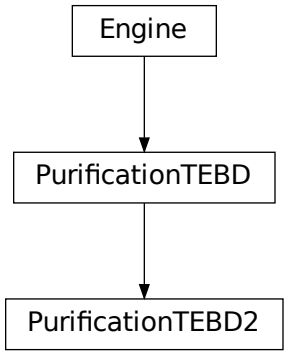
Returns **trunc_err** – The error of the represented state which is introduced due to the truncation during this sequence of update steps.

Return type *TruncationError*

PurificationTEBD2

- full name: tenpy.algorithms.purification_tebd.PurificationTEBD2
- parent module: *tenpy.algorithms.purification_tebd*
- type: class

Inheritance Diagram



Methods

PurificationTEBD2.__init__(psi, model, options)	Initialize self.
PurificationTEBD2.calc_U(order, delta_t[, ...])	see calc_U()
PurificationTEBD2.disentangle(theta)	Disentangle *theta* before splitting with svd.
PurificationTEBD2.disentangle_global([pair])	Try global disentangling by determining the maximally entangled pairs of sites.
PurificationTEBD2.disentangle_global_nsite([n])	Perform a sweep through the system and disentangle with disentangle_n_site().
PurificationTEBD2.disentangle_n_site(i, n, theta)	Generalization of disentangle() to *n* sites.
PurificationTEBD2.run()	(Real-)time evolution with TEBD (time evolving block decimation).
PurificationTEBD2.run_GS()	TEBD algorithm in imaginary time to find the ground state.
PurificationTEBD2.run_imaginary(beta)	Run imaginary time evolution to cool down to the given *beta*.
PurificationTEBD2.suzuki_trotter_decomposition(...)	Returns list of necessary steps for the suzuki trotter decomposition.
PurificationTEBD2.suzuki_trotter_time_steps(order)	Return time steps of U for the Suzuki Trotter decomposition of desired order.
PurificationTEBD2.update(N_steps)	Evolve by N_steps * U_param['dt'].
PurificationTEBD2.update_bond(i, U_bond)	Updates the B matrices on a given bond.
PurificationTEBD2.update_bond_imag(i, U_bond)	Update a bond with a (possibly non-unitary) *U_bond*.
PurificationTEBD2.update_imag(N_steps)	Perform an update suitable for imaginary time evolution.
PurificationTEBD2.update_step(U_idx_dt, odd)	Updates bonds in unit cell.

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.

class tenpy.algorithms.purification_tebd.**PurificationTEBD2**(*psi*, *model*, *options*)

Bases: tenpy.algorithms.purification_tebd.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.

Caclulate 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^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) --> |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

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** (*int*) – The desired order of the Suzuki-Trotter decomposition.

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_steps t H[k]) + O(N_steps t^{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 H_{even/odd} delta_t * 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:

```
|            |              |
|     ... - B1  -  s  -  B2 - ...
|            |              |
|            |-------------|
|            |      U      |
|            |-------------|
|            |              |
```

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.

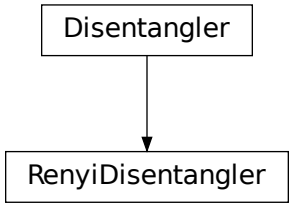
Returns **trunc_err** – The error of the represented state which is introduced due to the truncation during this sequence of update steps.

Return type *TruncationError*

RenyiDisentangler

- full name: tenpy.algorithms.purification_tebd.RenyiDisentangler
- parent module: *tenpy.algorithms.purification_tebd*
- type: class

Inheritance Diagram



Methods

RenyiDisentangler.__init__(parent)	Initialize self.
RenyiDisentangler.iter(theta, U)	Given *theta* and *U*, find another *U* which reduces the 2nd Renyi entropy.

class tenpy.algorithms.purification_tebd.**RenyiDisentangler**(*parent*)

Bases: *tenpy.algorithms.purification_tebd.Disentangler*

Iterative find *U* which minimized the second Renyi entropy.

See [Hauschild2018]

Reads of the following *options* as break criteria for the iteration:

key	type	description
disent_eps	float	Break, if the change in the Renyi entropy `S(n=2)` per iteration is smaller than this value.
disent_max_iter	float	Maximum number of iterations to perform.

Arguments and return values are the same as for `disentangle()`.

iter(*theta*, *U*)

Given *theta* and *U*, find another *U* which reduces the 2nd Renyi entropy.

Temporarily view the different *U* as independt and mimizied one of them - this corresponds to a linearization of the cost function. Defining *Utheta* as the application of *U* to *theata*, and combining the *p* legs of *theta* with `'vL', 'vR'`, this function contracts:

```
|      .----theta----.
|      |    |   |    |
|      |    q0  q1   |
|      |             |
|      |        q1*  |
|      |        |    |
|      |  .-Utheta*-.
|      |  | |
|      |  .-Utheta--.
|      |        |    |
|      |    q0* |    |
|      |    |   |    |
|      .----Utheta*-.
```

The trace yields the second Renyi entropy *S2*. Further, we calculate the unitary *U* with maximum overlap with this network.

Parameters

- **theta** (*Array*) – Two-site wave function to be disentangled.
- **U** (*Array*) – The previous guess for *U*; with legs `'q0', 'q1', 'q0*', 'q1*'`.

Returns

- **S2** (*float*) – Renyi entopy (n=2), $S2 = \frac{1}{1-2} \log tr(\rho_L^2)$ of *U theta*.
- **new_U** (*Array*) – Unitary with legs `'q0', 'q1', 'q0*', 'q1*'`, which should disentangle *theta*.

Functions

get_disentangler(method, parent)	Parse the parameter *method* and construct a *Disentangler* instance.

get_disentangler

- full name: tenpy.algorithms.purification_tebd.get_disentangler
- parent module: *tenpy.algorithms.purification_tebd*
- type: function

`tenpy.algorithms.purification_tebd.`**`get_disentangler`**(*method*, *parent*)

Parse the parameter *method* and construct a *Disentangler* instance.

Parameters

- **method** (str | None) – The method to be used, of the form 'method1-method2-min(method3,method4-method5)'. The usage should be clear from the examples, the precise rule follows: We parse the full *method* string as a *composite*, and define `composite := min_atom ['-' min_atom ...], min_atom := { 'min(' composite [',' composite ...] ')' } | atom`, and `atom := {any key of `disentanglers_atom_parse_dict`}`.
- **parent** (Engine) – The parent class calling the disentangler.

Returns **disentangler** – Disentangler instance, which can be called to disentangle a 2-site *theta* with the specified *method*.

Return type *Disentangler*

Examples

```
>>> get_disentangler(None, p)
Disentangler(p)
>>> get_disentangler('last-renyi', p)
Disentangler([LastDisentangler(p), RenyiDisentangler(p)], p)
>>> get_disentangler('min(None,noise-renyi,min(backwards,last)-graddesc)')
MinDisentangler([Disentangler,
                 CompositeDisentangler([NoiseDisentangler(p),␣
↪RenyiDisentangler(p)], p),
                 CompositeDisentangler([MinDisentangler([BackwardDisentangler(p),
                                                         LastDisentangler(p)]),
                                        GradientDescentDisentangler(p)], p), p)
```

Module description

Time evolving block decimation (TEBD) for MPS of purification.

See introduction in *purification_mps*. Time evolution for finite-temperature ensembles. This can be used to obtain correlation functions in time.

`tenpy.algorithms.purification_tebd.`**`disentanglers_atom_parse_dict = {'None': <class 'tenpy`**

Dictionary to translate the 'disentangle' TEBD parameter into a *Disentangler*.

If you define your own disentanglers, you can dynamically append them to this dictionary. CompositeDisentangler and MinDisentangler separate: they have non-default constructor and special syntax.

7.7.7 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

`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 `l1` of tensor `n1` with leg `l2` of tensor `n2`.
- **`open_legs`** (list of `[n1, l1, l]`) – A list of instructions for "open" (uncontracted) legs. `[n1, l1, l]` implies that leg `l1` of tensor `n1` is not contracted and is labelled `l` 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

`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 corresponding npc function first.

7.7.8 exact_diag

- full name: tenpy.algorithms.exact_diag
- parent module: *tenpy.algorithms*
- type: module

Classes

ExactDiag

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

ExactDiag

Methods

`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.

continues on next page

Table 47 – continued from previous page

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`

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_from** (*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 addional extra work.

7.8 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 conservervation in the context of tensor networks.

Relevant contents of `charges` are imported to `np_conserved`, so you propably won't need to import *charges* directly.

Submodules

`np_conserved`	A module to handle charge conservation in tensor networks.
`charges`	Basic definitions of a charge.
`svd_robust`	(More) robust version of singular value decomposition.
`random_matrix`	Provide some random matrix ensembles for numpy.
`sparse`	Providing support for sparse algorithms (using matrix-vector products only).
`lanczos`	Lanczos algorithm for np_conserved arrays.

7.8.1 np_conserved

- full name: tenpy.linalg.np_conserved
- parent module: `tenpy.linalg`
- type: module

Classes

`Array`(legcharges[, dtype, qtotal, labels])	A multidimensional array (=tensor) for using charge conservation.

Array

- full name: tenpy.linalg.np_conserved.Array
- parent module: *tenpy.linalg.np_conserved*
- type: class

Inheritance Diagram

Methods

`Array.__init__`(legcharges[, dtype, qtotal, ...])	see help(self)
Array.add_charge(add_legs[, chinfo, qtotal])	Add charges.
Array.add_leg(leg, i[, axis, label])	Add a leg to *self*, setting the current array as slice for a given index.
Array.add_trivial_leg([axis, label, qconj])	Add a trivial leg (with just one entry) to *self*.
Array.as_completely_blocked()	Gives a version of self which is completely blocked by charges.
Array.astype(dtype[, copy])	Return copy with new dtype, upcasting all blocks in `_data`.
Array.binary_blockwise(func, other, *args, ...)	Roughly `return func(self, other)`, blockwise.
Array.change_charge(charge, new_qmod[, ...])	Change the *qmod* of one charge in *chinfo*.
Array.combine_legs(combine_legs[, new_axes, ...])	Reshape: combine multiple legs into multiple pipes.
Array.complex_conj()	Return copy which is complex conjugated *without* conjugating the charge data.
Array.conj([complex_conj, inplace])	Conjugate: complex conjugate data, conjugate charge data.
Array.copy([deep])	Return a (deep or shallow) copy of self.
Array.drop_charge([charge, chinfo])	Drop (one of) the charges.
Array.extend(axis, extra)	Increase the dimension of a given axis, filling the values with zeros.
Array.from_func(func, legcharges[, dtype, ...])	Create an Array from a numpy func.
Array.from_func_square(func, leg[, dtype, ...])	Create an Array from a (numpy) function.
Array.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
Array.from_ndarray(data_flat, legcharges[, ...])	convert a flat (numpy) ndarray to an Array.
Array.from_ndarray_trivial(data_flat[, ...])	convert a flat numpy ndarray to an Array with trivial charge conservation.

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`Array.gauge_total_charge`(axis[, newqtotal, ...])	Changes the total charge by adjusting the charge on a certain leg.
`Array.get_block`(qindices[, insert])	Return the ndarray in `_data` representing the block corresponding to *qindices*.
`Array.get_leg`(label)	Return `self.legs[self.get_leg_index(label)]`.
`Array.get_leg_index`(label)	translate a leg-index or leg-label to a leg-index.
`Array.get_leg_indices`(labels)	Translate a list of leg-indices or leg-labels to leg indices.
`Array.get_leg_labels`()	Return list of the leg labels, with *None* for anonymous legs.
`Array.has_label`(label)	Check whether a given label exists.
`Array.iadd_prefactor_other`(prefactor, other)	`self += prefactor * other` for scalar *prefactor* and `Array` *other*.
`Array.ibinary_blockwise`(func, other, *args, ...)	Roughly `self = func(self, other)`, block-wise; in place.
`Array.iconj`([complex_conj])	Wraper around `self.conj()` with `inplace=True`.
`Array.idrop_labels`([old_labels])	Remove leg labels from self; in place.
`Array.iproject`(mask, axes)	Applying masks to one or multiple axes; in place.
`Array.ipurge_zeros`([cutoff, norm_order])	Removes `self._data` blocks with *norm* less than cutoff; in place.
`Array.ireplace_label`(old_label, new_label)	Replace the leg label *old_label* with *new_label*; in place.
`Array.ireplace_labels`(old_labels, new_labels)	Replace leg label `old_labels[i]` with `new_labels[i]`; in place.
`Array.is_completely_blocked`()	Return bool whether all legs are blocked by charge.
`Array.iscale_axis`(s[, axis])	Scale with varying values along an axis; in place.
`Array.iscale_prefactor`(prefactor)	`self *= prefactor` for scalar *prefactor*.
`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*.

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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'>*, *qtotal=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 *LegCharges* 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. >>> b = a.copy(deep=False) # shallow copy >>> b[1, 2] = 4.

Other *inplace* operations might have no effect at all (although we don't guarantee that):

```
>>> 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.

Returns **obj** – Newly generated class instance containing the required data.

Return type cls

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*)

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.

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_kwargs={}*, *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_kwargs)`, otherwise as `func(*func_args, `shape_kw`=shape, **func_kwargs)`. *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_kwargs* 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_kwargs** (*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_kwargs={}*, *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_kwargs* as well.
- **func_args** (*iterable*) – Additional arguments given to *func*.
- **func_kwargs** (*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.

ireplace_label(*old_label*, *new_label*)

Replace the leg label *old_label* with *new_label*; in place.

replace_label(*old_label*, *new_label*)

Return a shallow copy with the leg label *old_label* replaced by *new_label*.

ireplace_labels(*old_labels*, *new_labels*)

Replace leg label `old_labels[i]` with `new_labels[i]`; in place.

replace_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 *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:

```
qtotal = 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 exaclty 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 (*add_legs*, *chinfo=None*, *qtotal=None*)

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 (*charge=None*, *chinfo=None*)

Drop (one of) the charges.

Parameters

- **charge** (*int | str*) – Number or *name* of the charge (within *chinfo*) which is to be dropped. `None` means dropping all charges.
- **chinfo** (`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(*charge*, *new_qmod*, *new_name=''*, *chinfo=None*)

Change the *qmod* of one charge in *chinfo*.

Parameters

- **charge** (*int | str*) – Number or *name* of the charge (within *chinfo*) 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.
- **chinfo** (`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 permuation 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, whith 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

```
>>> oldarray.iset_leg_labels(['a', 'b', 'c', 'd', 'e'])
>>> c1 = oldarray.combine_legs([1, 2], qconj=-1)  # only single output pipe
>>> c1.get_leg_labels()
['a', '(b.c)', 'd', 'e']
```

Indices of *combine_legs* refer to the original array. If transposing is necessary, it is performed automatically:

```
>>> c2 = oldarray.combine_legs([[0, 3], [4, 1]], qconj=[+1, -1]) # two output␣
↪pipes
>>> c2.get_leg_labels()
['(a.d)', 'c', '(e.b)']
>>> c3 = oldarray.combine_legs([['a', 'd'], ['e', 'b']], new_axes=[2, 1],
>>>                            pipes=[c2.legs[0], c2.legs[2]])
>>> c3.get_leg_labels()
['c', '(e.b)', '(a.d)']
```

---

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 splited 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 `np.max(np.abs(block)) > 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 *old_array*, you can combine it and split it again:

```
>>> old_array.iset_leg_labels(['a', 'b', 'c', 'd', 'e'])
>>> comb_array = old_array.combine_legs([[0, 3], [2, 4]] )
>>> comb_array.get_leg_labels()
['(a.d)', 'b', '(c.e)']
>>> split_array = comb_array.split_legs([0, 2])
>>> split_array.get_leg_labels()
['a', 'd', 'b', 'c', 'e']
```

---

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 boolen 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 `res[i, ...] = self[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 `new_self[i1, ..., i_axis, ...] = s[i_axis] * 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 `self = f(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!

Parameters

- **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

```
>>> a.iunaray_blockwise(np.real)  # get real part
>>> a.iunaray_blockwise(np.conj)  # same data as a.iconj(), but doesn't␣
↪charge conjugate.
```

unary_blockwise(*func*, **args*, ***kwargs*)

Roughly `return func(self)`, block-wise. Copies.

Same as *iunary_blockwise()*, but makes a **shallow** copy first.

iconj(*complex_conj=True*)

Wraper around `self.conj()` with `inplace=True`.

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.

complex_conj()

Return copy which is complex conjugated *without* conjugating the charge data.

norm(*ord=None*, *convert_to_float=True*)

Norm of flattened data.

See *norm()* for details.

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

```
>>> a.ibinary_blockwise(np.add, b)  # equivalent to ``a += b``, if ``b`` is␣
↪an `Array`.
>>> a.ibinary_blockwise(np.max, b)  # overwrites ``a`` to ``a = max(a, b)``
```

binary_blockwise(*func*, *other*, **args*, ***kwargs*)

Roughly `return func(self, other)`, block-wise. Copies.

Same as *ibinary_blockwise()*, but makes a **shallow** copy first.

matvec(*other*)

This function is used by the Lanczos algorithm needed for DMRG.

It is supposed to calculate the matrix - vector - product for a rank-2 matrix `self` and a rank-1 vector *other*.

iadd_prefactor_other(*prefactor*, *other*)

`self += prefactor * other` for scalar *prefactor* and *Array* *other*.

Note that we allow the type of *self* to change if necessary. Moreover, if *self* and *other* have the same labels in different order, other gets **transposed** before the action.

iscale_prefactor(*prefactor*)

`self *= prefactor` for scalar *prefactor*.

Note that we allow the type of *self* to change if necessary.

Functions

concatenate(arrays[, axis, copy])	Stack arrays along a given axis, similar as np.concatenate.
detect_grid_outer_legcharge(grid, grid_legs)	Derive a LegCharge for a grid used for *grid_outer()*.
detect_legcharge(flat_array, chargeinfo, ...)	Calculate a missing *LegCharge* by looking for nonzero entries of a flat array.
detect_qtotal(flat_array, legcharges[, cutoff])	Returns the total charge (w.r.t *legs*) of first non-zero sector found in *flat_array*.
diag(s, leg[, dtype, labels])	Returns a square, diagonal matrix of entries *s*.
eig(a[, sort])	Calculate eigenvalues and eigenvectors for a non-hermitian matrix.
eigh(a[, UPLO, sort])	Calculate eigenvalues and eigenvectors for a hermitian matrix.

continues on next page

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eigvals(a[, sort])	Calculate eigenvalues for a hermitian matrix.
eigvalsh(a[, UPLO, sort])	Calculate eigenvalues for a hermitian matrix.
expm(a)	Use scipy.linalg.expm to calculate the matrix exponential of a square matrix.
eye_like(a[, axis, labels])	Return an identity matrix contractible with the leg *axis* of the *Array* *a*.
grid_concat(grid, axes[, copy])	Given an np.array of npc.Arrays, performs a multi-dimensional concatentation along 'axes'.
grid_outer(grid, grid_legs[, qtotal, ...])	Given an np.array of npc.Arrays, return the corresponding higher-dimensional Array.
inner(a, b[, axes, do_conj])	Contract all legs in *a* and *b*, return scalar.
norm(a[, ord, convert_to_float])	Norm of flattened data.
ones(legcharges[, dtype, qtotal, labels])	Short-hand for *Array.from_func()* with function `numpy.ones()`.
outer(a, b)	Forms the outer tensor product, equivalent to `tensordot(a, b, axes=0)`.
pinv(a[, cutoff])	Compute the (Moore-Penrose) pseudo-inverse of a matrix.
qr(a[, mode, inner_labels, cutoff])	Q-R decomposition of a matrix.
speigs(a, charge_sector, k, *args, **kwargs)	Sparse eigenvalue decomposition `w, v` of square *a* in a given charge sector.
svd(a[, full_matrices, compute_uv, cutoff, ...])	Singualar value decomposition of an Array *a*.
tensordot(a, b[, axes])	Similar as `np.tensordot` but for *Array*.
to_iterable_arrays(array_list)	Similar as *to_iterable()*, but also enclose npc Arrays in a list.
trace(a[, leg1, leg2])	Trace of *a*, summing over leg1 and leg2.
zeros(legcharges[, dtype, qtotal, labels])	Create a npc array full of zeros (with no _data).

concatenate

- full name: tenpy.linalg.np_conserved.concatenate
- parent module: *tenpy.linalg.np_conserved*
- type: function

`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

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

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

`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 fo 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

`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 `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 = eig(a)` yields $aV = V diag(w)$.

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 = eigh(a)` yields $a = V diag(w) V^\dagger$. **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 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}*.

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 are 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 are 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 concatentation 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 rank 2 Arrays `A, B, C, D` of shapes `(1, 2), (1, 4), (3, 2), (3, 4)` sharing the legs of equal sizes. Then the following grid will result in a `(1+3, 2+4)` shaped array:

```
>>> g = grid_concat([[A, B], [C, D]], axes=[0, 1])
>>> g.shape
(4, 6)
```

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:

```
>>> 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

`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

- **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.
- **grid_legs** (list of `LegCharge`) – One LegCharge for each dimension of the grid along the grid.
- **qtotal** (*charge*) – The total charge of the Array. By default (`None`), derive it out from a non-trivial entry of the grid.
- **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 `grid.shape + nontrivial_grid_entry.shape`. Constructed such that `res[idx] == grid[idx]` for any index `idx` of the *grid* the *grid* entry is not trivial (`None`).

Return type *Array*

See also:

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 Splus, Sminus, Sz, Id, each with legs [phys.conj(), phys]. Further, you have to define appropriate LegCharges *l_left* and *l_right*. Then one 'matrix' of the MPO for a nearest neighbour Heisenberg Hamiltonian could look like:

```
>>> W_mpo = 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]],
...                     leg_charges=[l_left, l_right])
>>> W_mpo.shape
(5, 5, 2, 2)
```

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

- **b** (*a,*) – 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 $(\sum_i |a_i|^{ord})^{1/ord}$.

ord	norm
None/'fro'	Frobenius norm (same as 2-norm)
np.inf	`max(abs(x))`
-np.inf	`min(abs(x))`
0	`sum(a != 0) == np.count_nonzero(x)`
other	ususal *ord*-norm

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

`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

`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 **b** (*a,*) – The arrays for which to form the product.

Returns

c –

Array of rank `a.rank + b.rank` such that (for `Ra = a.rank; Rb = b.rank`):

```
c[i_1, ..., i_Ra, j_1, ... j_R] = a[i_1, ..., i_Ra] * b[j_1, ..., j_
↪rank_b]
```

Return type *Array*

pinv

- full name: tenpy.linalg.np_conserved.pinv
- parent module: *tenpy.linalg.np_conserved*
- type: function

`tenpy.linalg.np_conserved.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 = svd(a, cutoff=cutoff)` with a *cutoff* > 0, calculate `P = U * diag(1/S) * VH` (with `*` denoting tensordot) and return `P.conj.transpose()`.

Parameters

- **a** ((M, N) *Array*) – Matrix to be pseudo-inverted.
- **cuttof** (*float*) – Cutoff for small singular values, as given to *svd()*. (Note: different convetion 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

`tenpy.linalg.np_conserved.qr`(*a*, *mode='reduced'*, *inner_labels=[None, None]*, *cutoff=None*)

Q-R decomposition of a matrix.

Decomposition such that `A == 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 thatOtherwise such that $q^*_{j,i} q_{j,k} = \delta_{i,k}$
- **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

`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, `tensordot(A, V[i], 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

`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*)

Singualar value decomposition of an Array *a*.

Factorizes `U, S, VH = svd(a)`, such that `a = U*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].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=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; `diag(S)` would need to be a rectangluar `(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. `[None, None]` (Default) is equivalent to `[None, a.qtotal]`. A single *None* entry is replaced the unique charge satisfying the requirement `U.qtotal + VH.qtotal = a.qtotal (modulo qmod)`.
- **inner_labels_LR** (`[{str|None}, {str|None}]`) – The first label corresponds to `U.legs[1]`, the second to `VH.legs[0]`.
- **inner_qconj** (`{+1, -1}`) – Direction of the charges for the new leg. Default +1. The new LegCharge is constructed such that `VH.legs[0].qconj = 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 singluar values of the array. If no *cutoff* is given, it has lenght `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

- **b** (*a,*) – 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 `(range(-axes, 0), range(axes))`. Alternatively, *axes_a* and *axes_b* specifiy 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 tensorproduct 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

`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

`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 **leg2** (*leg1,*) – 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

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.

tenpy.linalg.np_conserved.**QCUTOFF = 2.220446049250313e-15**

A cutoff to ignore machine precision rounding errors when determining charges

tenpy.linalg.np_conserved.**QTYPE = <class 'numpy.int64'>**

the type used for charges

Overview

Classes

Array(legcharges[, dtype, qtotal, labels])	A multidimensional array (=tensor) for using charge conservation.
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.

Array creation

`Array.from_ndarray_trivial`(data_flat[, ...])	convert a flat numpy ndarray to an Array with trivial charge conservation.
`Array.from_ndarray`(data_flat, legcharges[, ...])	convert a flat (numpy) ndarray to an Array.
`Array.from_func`(func, legcharges[, dtype, ...])	Create an Array from a numpy func.
`Array.from_func_square`(func, leg[, dtype, ...])	Create an Array from a (numpy) function.
`zeros`(legcharges[, dtype, qtotal, labels])	Create a npc array full of zeros (with no _data).
`eye_like`(a[, axis, labels])	Return an identity matrix contractible with the leg *axis* of the `Array` *a*.
`diag`(s, leg[, dtype, labels])	Returns a square, diagonal matrix of entries *s*.

Concatenation

`concatenate`(arrays[, axis, copy])	Stack arrays along a given axis, similar as np.concatenate.
`grid_concat`(grid, axes[, copy])	Given an np.array of npc.Arrays, performs a multi-dimensional concatentation along 'axes'.
`grid_outer`(grid, grid_legs[, qtotal, ...])	Given an np.array of npc.Arrays, return the corresponding higher-dimensional Array.

Detecting charges of flat arrays

`detect_qtotal`(flat_array, legcharges[, cutoff])	Returns the total charge (w.r.t *legs*) of first non-zero sector found in *flat_array*.
`detect_legcharge`(flat_array, chargeinfo, ...)	Calculate a missing *LegCharge* by looking for nonzero entries of a flat array.
`detect_grid_outer_legcharge`(grid, grid_legs)	Derive a LegCharge for a grid used for `grid_outer()`.

Contraction of some legs

`tensordot`(a, b[, axes])	Similar as `np.tensordot` but for `Array`.
`outer`(a, b)	Forms the outer tensor product, equivalent to `tensordot(a, b, axes=0)`.
`inner`(a, b[, axes, do_conj])	Contract all legs in *a* and *b*, return scalar.
`trace`(a[, leg1, leg2])	Trace of *a*, summing over leg1 and leg2.

Linear algebra

`svd`(a[, full_matrices, compute_uv, cutoff, ...])	Singualar value decomposition of an Array *a*.
`pinv`(a[, cutoff])	Compute the (Moore-Penrose) pseudo-inverse of a matrix.
`norm`(a[, ord, convert_to_float])	Norm of flattened data.
`qr`(a[, mode, inner_labels, cutoff])	Q-R decomposition of a matrix.
`expm`(a)	Use scipy.linalg.expm to calculate the matrix exponential of a square matrix.

Eigen systems

`eigh`(a[, UPLO, sort])	Calculate eigenvalues and eigenvectors for a hermitian matrix.
`eig`(a[, sort])	Calculate eigenvalues and eigenvectors for a non-hermitian matrix.
`eigvalsh`(a[, UPLO, sort])	Calculate eigenvalues for a hermitian matrix.
`eigvals`(a[, sort])	Calculate eigenvalues for a hermitian matrix.
`speigs`(a, charge_sector, k, *args, **kwargs)	Sparse eigenvalue decomposition `w, v` of square *a* in a given charge sector.

7.8.2 charges

- full name: tenpy.linalg.charges
- parent module: `tenpy.linalg`
- type: module

Classes

`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

ChargeInfo.__init__([mod, names])	Initialize self.
ChargeInfo.add(chinfos)	Create a *ChargeInfo* combining multiple charges.
ChargeInfo.change(chinfo, charge, new_qmod)	Change the *qmod* of a given charge.
ChargeInfo.check_valid(charges)	Check, if *charges* has all entries as expected from self.mod.
ChargeInfo.drop(chinfo[, charge])	Remove a charge from a *ChargeInfo*.
ChargeInfo.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
ChargeInfo.make_valid([charges])	Take charges modulo self.mod.
ChargeInfo.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
ChargeInfo.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.

Class Attributes and Properties

ChargeInfo.mod	Modulo how much each of the charges is taken.
ChargeInfo.qnumber	The number of charges.

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*. For each

charge one entry *m*: the charge is conserved modulo *m*. 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 ValueErrors, if something is wrong.

property qnumber

The number of charges.

property mod

Modulo how much each of the charges is taken.

1 for a $U(1)$ charge, 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

LegCharge

Methods

`LegCharge.__init__`(chargeinfo, slices, charges)	Initialize self.
LegCharge.bunch()	Return a copy with bunched self.charges: form blocks for contiguous equal charges.
LegCharge.charge_sectors()	Return unique rows of self.charges.
LegCharge.conj()	Return a (shallow) copy with opposite `self.qconj`.
LegCharge.copy()	Return a (shallow) copy of self.
LegCharge.extend(extra)	Return a new *LegCharge*, which extends self with futher charges.
LegCharge.flip_charges_qconj()	Return a copy with both negative *qconj* and *charges*.
LegCharge.from_add_charge(legs[, chargeinfo])	Add the (independent) charges of two or more legs to get larger *qnumber*.
LegCharge.from_change_charge(leg, charge, ...)	Remove a charge from a LegCharge.
LegCharge.from_drop_charge(leg[, charge, ...])	Remove a charge from a LegCharge.
LegCharge.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
LegCharge.from_qdict(chargeinfo, qdict[, qconj])	Create a LegCharge from qdict form.
LegCharge.from_qflat(chargeinfo, qflat[, qconj])	Create a LegCharge from qflat form.
LegCharge.from_qind(chargeinfo, slices, charges)	Just a wrapper around self.__init__(), see class docstring for parameters.
LegCharge.from_trivial(ind_len[, ...])	Create trivial (qnumber=0) LegCharge for given len of indices *ind_len*.
LegCharge.get_block_sizes()	Return the sizes of the individual blocks.
LegCharge.get_charge(qindex)	Return charge `self.charges[qindex] * self.qconj` for a given *qindex*.
LegCharge.get_qindex(flat_index)	Find qindex containing a flat index.

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Table 63 – continued from previous page

`LegCharge.get_qindex_of_charges`(charges)	Return the slice selecting the block for given charge values.
`LegCharge.get_slice`(qindex)	Return slice selecting the block for a given *qindex*.
`LegCharge.is_blocked`()	Returns whether self is blocked, i.e.
`LegCharge.is_bunched`()	Checks whether `bunch()` would change something.
`LegCharge.is_sorted`()	Returns whether *self.charges* is sorted lexiographically.
`LegCharge.perm_flat_from_perm_qind`(perm_qind)	Convert a permutation of qind (acting on self) into a flat permutation.
`LegCharge.perm_qind_from_perm_flat`(perm_flat)	Convert flat permutation into qind permutation.
`LegCharge.project`(mask)	Return copy keeping only the indices specified by *mask*.
`LegCharge.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`LegCharge.sort`([bunch])	Return a copy of *self* sorted by charges (but maybe not bunched).
`LegCharge.test_contractible`(other)	Raises a ValueError if charges are incompatible for contraction with other.
`LegCharge.test_equal`(other)	Test if charges are *equal* including *qconj*.
`LegCharge.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.
`LegCharge.to_qdict`()	Return charges in *qdict* form.
`LegCharge.to_qflat`()	Return charges in *qflat* form.

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` correspondes 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).

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)`.

chinfo

The nature of the charge. Can be shared between LegCharges.

Type `ChargeInfo` instance

slices
A block with 'qindex' `qi` correspondes 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, chinfo.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 ouput 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.

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_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_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_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 *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*

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 representing 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 lexiographically.

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 condsidered 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`:

```
self.charges * self.qconj = - other.charges * 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())`.

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_slice(*qindex*)

Return slice selecting the block 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_charge(*qindex*)

Return charge `self.charges[qindex] * 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 permuation such that `sorted_array[..., :] = unsorted_array[..., perm_flat]`, use `perm_flat = unsorted_leg.perm_flat_from_perm_qind(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*) – `idx[:-1]` are the indices of the old qind which are kept, `idx[-1] = 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_new = map_qind[qind_old]`, and `map_qind[qind_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(*extra*)

Return a new *LegCharge*, which extends self with futher 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.

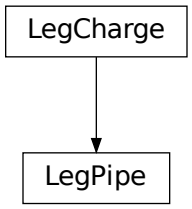
Return type 1D array

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



Methods

LegPipe.__init__(legs[, qconj, sort, bunch])	Initialize self.
LegPipe.bunch(*args, **kwargs)	Convert to LegCharge and call *LegCharge.bunch()*.
LegPipe.charge_sectors()	Return unique rows of self.charges.
LegPipe.conj()	Return a shallow copy with opposite `self.qconj`.
LegPipe.copy()	Return a (shallow) copy of self.
LegPipe.extend(extra)	Return a new *LegCharge*, which extends self with futher charges.
LegPipe.flip_charges_qconj()	Return a copy with both negative *qconj* and *charges*.
LegPipe.from_add_charge(legs[, chargeinfo])	Add the (independent) charges of two or more legs to get larger *qnumber*.
LegPipe.from_change_charge(leg, charge, new_qmod)	Remove a charge from a LegCharge.
LegPipe.from_drop_charge(leg[, charge, ...])	Remove a charge from a LegCharge.

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Table 64 – continued from previous page

`LegPipe.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
`LegPipe.from_qdict`(chargeinfo, qdict[, qconj])	Create a LegCharge from qdict form.
`LegPipe.from_qflat`(chargeinfo, qflat[, qconj])	Create a LegCharge from qflat form.
`LegPipe.from_qind`(chargeinfo, slices, charges)	Just a wrapper around self.__init__(), see class docstring for parameters.
`LegPipe.from_trivial`(ind_len[, chargeinfo, ...])	Create trivial (qnumber=0) LegCharge for given len of indices *ind_len*.
`LegPipe.get_block_sizes`()	Return the sizes of the individual blocks.
`LegPipe.get_charge`(qindex)	Return charge `self.charges[qindex] * self.qconj` for a given *qindex*.
`LegPipe.get_qindex`(flat_index)	Find qindex containing a flat index.
`LegPipe.get_qindex_of_charges`(charges)	Return the slice selecting the block for given charge values.
`LegPipe.get_slice`(qindex)	Return slice selecting the block for a given *qindex*.
`LegPipe.is_blocked`()	Returns whether self is blocked, i.e.
`LegPipe.is_bunched`()	Checks whether `bunch()` would change something.
`LegPipe.is_sorted`()	Returns whether *self.charges* is sorted lexiographically.
`LegPipe.map_incoming_flat`(incoming_indices)	Map (flat) incoming indices to an index in the outgoing pipe.
`LegPipe.outer_conj`()	Like `conj()`, but don't change `qconj` for incoming legs.
`LegPipe.perm_flat_from_perm_qind`(perm_qind)	Convert a permutation of qind (acting on self) into a flat permutation.
`LegPipe.perm_qind_from_perm_flat`(perm_flat)	Convert flat permutation into qind permutation.
`LegPipe.project`(*args, **kwargs)	Convert self to LegCharge and call `LegCharge.project()`.
`LegPipe.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`LegPipe.sort`(*args, **kwargs)	Convert to LegCharge and call `LegCharge.sort()`.
`LegPipe.test_contractible`(other)	Raises a ValueError if charges are incompatible for contraction with other.
`LegPipe.test_equal`(other)	Test if charges are *equal* including *qconj*.
`LegPipe.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.
`LegPipe.to_LegCharge`()	Convert self to a LegCharge, discarding the information how to split the legs.
`LegPipe.to_qdict`()	Return charges in *qdict* form.
`LegPipe.to_qflat`()	Return charges in *qflat* form.

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 perfom 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, $i, j, ... \to k$ 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+3},  I_s + 1, i''_1,   ..., i''_{nlegs} ],
 [ b_{j+3}, b_{j+4},  I_s + 1, i'''_1,  ..., i'''_{nlegs}],
 ...]
```

The charge fusion rule is:

```
self.charges[Qi]*self.qconj == sum([l.charges[qi_l]*l.qconj for l in self.legs]) ␣
↪mod qmod
```

Here the qindex `Qi` of the pipe corresponds to qindices `qi_l` 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 separetely.
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 futher 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 condsidered 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`:

```
self.charges * self.qconj = - other.charges * 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.

7.8.3 svd_robust

- full name: tenpy.linalg.svd_robust
- parent module: *tenpy.linalg*
- type: module

Functions

svd(a[, full_matrices, compute_uv, ...])	Wrapper around `scipy.linalg.svd()` with *gesvd* backup plan.
svd_gesvd(a[, full_matrices, compute_uv, ...])	svd with LAPACK's '#gesvd' (with # = d/z for float/complex).

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

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

- **full_matrices, compute_uv**(*a,*) – 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`:

```
>>> from svd_robust import svd
>>> U, S, VT = svd([[1., 1.], [0., [1.]])
```

7.8.4 random_matrix

- full name: tenpy.linalg.random_matrix
- parent module: *`tenpy.linalg`*
- type: module

Functions

COE(size)	Circular orthogonal ensemble (COE).
CRE(size)	Circular real ensemble (CRE).
CUE(size)	Circular unitary ensemble (CUE).
GOE(size)	Gaussian orthogonal ensemble (GOE).
GUE(size)	Gaussian unitary ensemble (GUE).
O_close_1(size[, a])	return an random orthogonal matrix 'close' to the Identity.
U_close_1(size[, a])	return an random orthogonal matrix 'close' to the identity.
box(size[, W])	return random number uniform in (-W, W].
standard_normal_complex(size)	return `(R + 1.j*I)` for independent R and I from np.random.standard_normal.

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

`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. $p(H) = 1/Zexp(-n/4tr(H^2))$

Return type ndarray

GUE

- full name: tenpy.linalg.random_matrix.GUE
- parent module: *tenpy.linalg.random_matrix*
- type: function

`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. $p(H) = 1/Zexp(-n/4tr(H^2))$.

Return type ndarray

O_close_1

- full name: tenpy.linalg.random_matrix.O_close_1
- parent module: *tenpy.linalg.random_matrix*
- type: function

`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 identiy (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

`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 identiy (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

`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

`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:

ensemble	matrix class drawn from	measure	invariant under	beta
GOE	real, symmetric	`~ exp(-n/4 tr(H^2))`	orthogonal O	1
GUE	hermitian	`~ exp(-n/2 tr(H^2))`	unitary U	2
CRE	O(n)	Haar	orthogonal O	/
COE	U in U(n) with U = U^T	Haar	orthogonal O	1
CUE	U(n)	Haar	unitary U	2
O_close_1	O(n)	?	/	/
U_close_1	U(n)	?	/	/

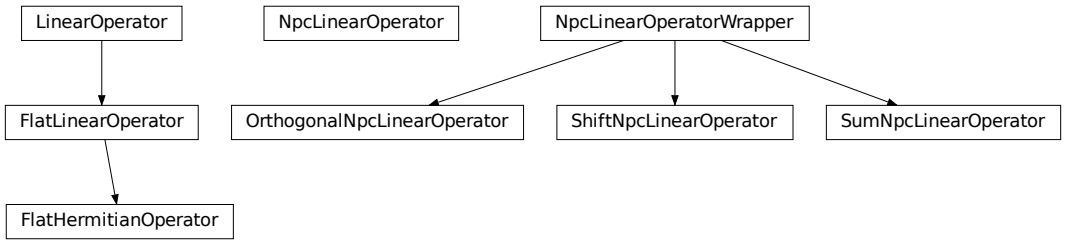
All functions in this module take a tuple `(n, n)` as first argument, such that we can use the function *from_func()* to generate a block diagonal *Array* with the block from the corresponding ensemble, for example:

```
npc.Array.from_func_square(GOE, [leg, leg.conj()])
```

7.8.5 sparse

- full name: tenpy.linalg.sparse
- parent module: *tenpy.linalg*
- type: module

Classes

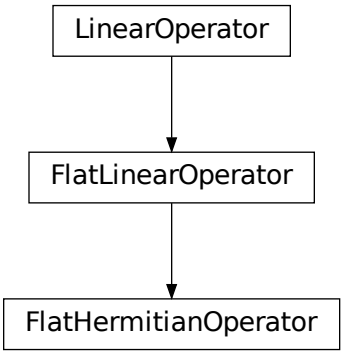


FlatHermitianOperator(npc_matvec, leg, dtype)	Hermitian variant of *FlatLinearOperator*.
FlatLinearOperator(npc_matvec, leg, dtype[, ...])	Square Linear operator acting on numpy arrays based on a *matvec* acting on npc Arrays.
NpcLinearOperator	Prototype for a Linear Operator acting on *Array*.
NpcLinearOperatorWrapper(orig_operator)	Base class for wrapping around another *NpcLinearOperator*.
OrthogonalNpcLinearOperator(orig_operator, ...)	Replace `H -> P H P` with the projector `P = 1 - sum_o |o> <o|`.
ShiftNpcLinearOperator(orig_operator, shift)	Representes `original_operator + shift * identity`.
SumNpcLinearOperator(orig_operator, ...)	Sum of two linear operators.

FlatHermitianOperator

- full name: tenpy.linalg.sparse.FlatHermitianOperator
- parent module: *tenpy.linalg.sparse*
- type: class

Inheritance Diagram



Methods

`FlatHermitianOperator.__init__`(npc_matvec, ...)	Initialize this LinearOperator.
`FlatHermitianOperator.adjoint`()	Hermitian adjoint.
`FlatHermitianOperator.dot`(x)	Matrix-matrix or matrix-vector multiplication.
`FlatHermitianOperator.flat_to_npc`(vec)	Convert flat vector of selected charge sector into npc Array.
`FlatHermitianOperator.from_NpcArray`(mat[, ...])	Create a *FlatLinearOperator* from a square `Array`.
`FlatHermitianOperator.from_guess_with_pipe`(...)	Create a *FlatLinearOperator*` from a *matvec* function acting on multiple legs.
`FlatHermitianOperator.matmat`(X)	Matrix-matrix multiplication.
`FlatHermitianOperator.matvec`(x)	Matrix-vector multiplication.
`FlatHermitianOperator.npc_to_flat`(npc_vec)	Convert npc Array with qtotal = self.charge_sector into ndarray.
`FlatHermitianOperator.rmatmat`(X)	Adjoint matrix-matrix multiplication.
`FlatHermitianOperator.rmatvec`(x)	Adjoint matrix-vector multiplication.
`FlatHermitianOperator.transpose`()	Transpose this linear operator.

Class Attributes and Properties

`FlatHermitianOperator.H`	Hermitian adjoint.
`FlatHermitianOperator.T`	Transpose this linear operator.
`FlatHermitianOperator.charge_sector`	Charge sector of the vector which is acted on.

class tenpy.linalg.sparse.**FlatHermitianOperator**(*npc_matvec*, *leg*, *dtype*, *charge_sector=0*, *vec_label=None*)

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 vector of selected charge sector into npc Array.

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 flat 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 *v0_guess*.

matmat(*X*)

Matrix-matrix multiplication.

Performs the operation y=A*X where A is an MxN linear operator and X dense N*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 MxN 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 with qtotal = self.charge_sector into ndarray.

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 * x where A is an MxN 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 * x where A is an MxN 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()

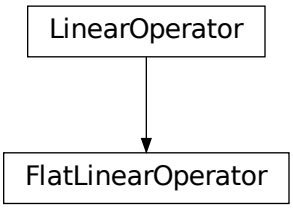
Transpose this linear operator.

Returns a LinearOperator that represents the transpose of this one. Can be abbreviated self.T instead of self.transpose().

FlatLinearOperator

- full name: tenpy.linalg.sparse.FlatLinearOperator
- parent module: *tenpy.linalg.sparse*
- type: class

Inheritance Diagram



Methods

`FlatLinearOperator.__init__`(npc_matvec, leg, ...)	Initialize this LinearOperator.
FlatLinearOperator.adjoint()	Hermitian adjoint.
FlatLinearOperator.dot(x)	Matrix-matrix or matrix-vector multiplication.
FlatLinearOperator.flat_to_npc(vec)	Convert flat vector of selected charge sector into npc Array.
FlatLinearOperator.from_NpcArray(mat[, ...])	Create a *FlatLinearOperator* from a square *Array*.
FlatLinearOperator.from_guess_with_pipe(...)	Create a *FlatLinearOperator*` from a *matvec* function acting on multiple legs.
FlatLinearOperator.matmat(X)	Matrix-matrix multiplication.
FlatLinearOperator.matvec(x)	Matrix-vector multiplication.
FlatLinearOperator.npc_to_flat(npc_vec)	Convert npc Array with qtotal = self.charge_sector into ndarray.
FlatLinearOperator.rmatmat(X)	Adjoint matrix-matrix multiplication.
FlatLinearOperator.rmatvec(x)	Adjoint matrix-vector multiplication.
FlatLinearOperator.transpose()	Transpose this linear operator.

Class Attributes and Properties

`FlatLinearOperator.H`	Hermitian adjoint.
`FlatLinearOperator.T`	Transpose this linear operator.
`FlatLinearOperator.charge_sector`	Charge sector of the vector which is acted on.

class `tenpy.linalg.sparse.`**`FlatLinearOperator`**(*npc_matvec*, *leg*, *dtype*, *charge_sector=0*, *vec_label=None*)

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.conj(), self.leg]` 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 int

_mask
The indices of *leg* corresponding to the *charge_sector* to be diagonalized.

Type ndarray[ndim=1, bool]

_npc_matvec_multileg
Only set if initalized with `from_guess_with_pipe()`. The *npc_matvec* function to be wrapped around. Takes the npc Array in multidimensional form and returns it that way.

Type function | None

_labels_split
Only set if initalized with `from_guess_with_pipe()`. Labels of the guess before combining them into a pipe (stored as *leg*).

Type list of str

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 *v0_guess*.

property charge_sector
Charge sector of the vector which is acted on.

flat_to_npc(*vec*)
Convert flat vector of selected charge sector into npc Array.

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 flat array.

Return type *Array*

npc_to_flat (*npc_vec*)

Convert npc Array with qtotal = self.charge_sector into ndarray.

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

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 MxN linear operator and X dense N*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 MxN 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 MxN 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 * x where A is an MxN 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()

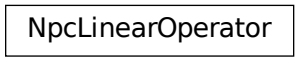
Transpose this linear operator.

Returns a LinearOperator that represents the transpose of this one. Can be abbreviated self.T instead of self.transpose().

NpcLinearOperator

- full name: tenpy.linalg.sparse.NpcLinearOperator
- parent module: *tenpy.linalg.sparse*
- type: class

Inheritance Diagram



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()

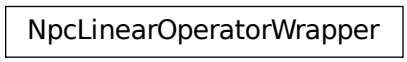
Return the hermitian conjugate of *self*

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



Methods

NpcLinearOperatorWrapper.__init__(orig_operator)	Initialize self.
NpcLinearOperatorWrapper.adjoint()	Return the hermitian conjugate of *self*.
NpcLinearOperatorWrapper.to_matrix()	Contract *self* to a matrix.
NpcLinearOperatorWrapper.unwrapped()	Return to the original NpcLinearOperator.

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*.

Type *NpcLinearOperator*

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()

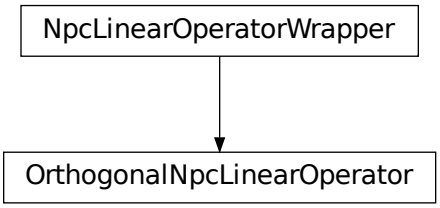
Return the hermitian conjugate of *self*.

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



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 -> P H P` with the projector `P = 1 - sum_o |o> <o|`.

Here, `|o>` are the vectors from `ortho_vecs`.

Parameters

- **`orig_operator`** (`EffectiveH`) – The original *EffectiveH* instance to wrap around.
- **`ortho_vecs`** (list of *`Array`*) – The vectors to orthogonalize against.

`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`()

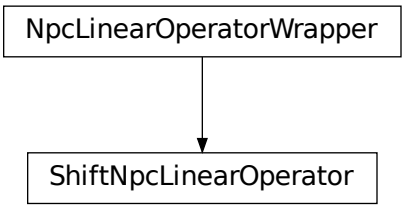
Return to the original NpcLinearOperator.

If multiple levels of wrapping were used, this returns the most unwrapped one.

ShiftNpcLinearOperator

- full name: tenpy.linalg.sparse.ShiftNpcLinearOperator
- parent module: *tenpy.linalg.sparse*
- type: class

Inheritance Diagram



Methods

`ShiftNpcLinearOperator.__init__(...)`	Initialize self.
ShiftNpcLinearOperator.adjoint()	Return the hermitian conjugate of *self*.
`ShiftNpcLinearOperator.matvec`(vec)	
ShiftNpcLinearOperator.to_matrix()	Contract *self* to a matrix.
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`()

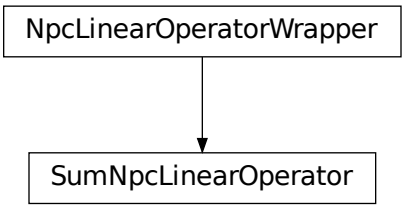
Return to the original NpcLinearOperator.

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



Methods

SumNpcLinearOperator. __init__(orig_operator, ...)	Initialize self.
SumNpcLinearOperator.adjoint()	Return the hermitian conjugate of *self*.
SumNpcLinearOperator.matvec(vec)	
SumNpcLinearOperator.to_matrix()	Contract *self* to a matrix.
SumNpcLinearOperator.unwrapped()	Return to the original NpcLinearOperator.

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*.

unwrapped()

Return to the original NpcLinearOperator.

If multiple levels of wrapping were used, this returns the most unwrapped one.

Module description

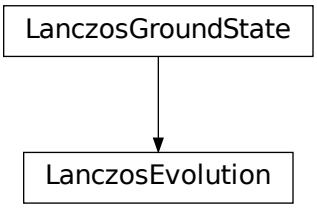
Providing support for sparse algorithms (using matrix-vector products only).

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 strucuture 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.

7.8.6 lanczos

- full name: tenpy.linalg.lanczos
- parent module: `tenpy.linalg`
- type: module

Classes



`LanczosEvolution`(H, psi0, options)	Calculate $exp(deltaH)\|psi0>$ using Lanczos.
`LanczosGroundState`(H, psi0, options[, ...])	Lanczos algorithm working on npc arrays.

Functions

`gram_schmidt`(vecs[, rcond, verbose])	In place Gram-Schmidt Orthogonalization and normalization for npc Arrays.
`lanczos`(H, psi[, options, orthogonal_to])	Simple wrapper calling `LanczosGroundState(H, psi, options, orthogonal_to).run()`
`lanczos_arpack`(H, psi[, options, orthogonal_to])	Use `scipy.sparse.linalg.eigsh()` to find the ground state of H.
`plot_stats`(ax, Es)	Plot the convergence of the energies.

gram_schmidt

- full name: tenpy.linalg.lanczos.gram_schmidt
- parent module: `tenpy.linalg.lanczos`
- type: function

`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

`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 **psi, options, orthogonal_to** (*H,*) – 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 **psi, options, orthogonal_to**(*H,*) – 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.

7.9 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.

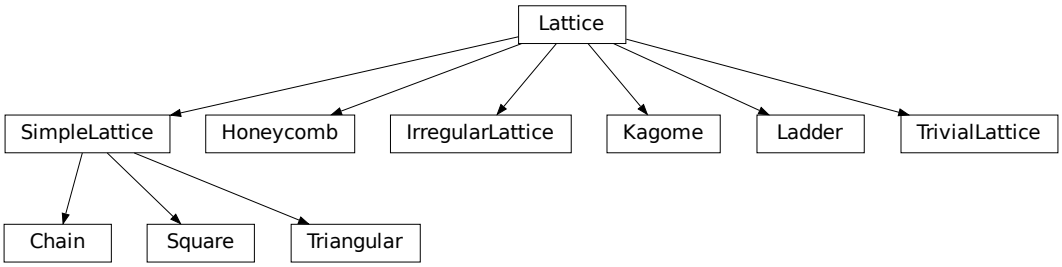
Submodules

lattice	Classes to define the lattice structure of a model.
model	This module contains some base classes for models.

7.9.1 lattice

- full name: tenpy.models.lattice
- parent module: *tenpy.models*
- type: module

Classes

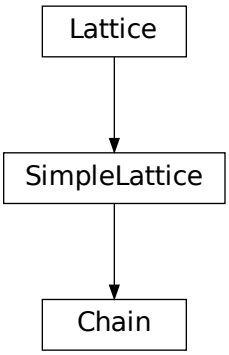


Chain(L, site, **kwargs)	A chain of L equal sites.
Honeycomb(Lx, Ly, sites, **kwargs)	A honeycomb lattice.
IrregularLattice(mps_sites, based_on[, order])	A variant of a regular lattice, where we might have extra sites or sites missing.
Kagome(Lx, Ly, sites, **kwargs)	A Kagome lattice.
Ladder(L, sites, **kwargs)	A ladder coupling two chains.
Lattice(Ls, unit_cell[, order, bc, bc_MPS, . . .])	A general, regular lattice.
SimpleLattice(Ls, site, **kwargs)	A lattice with a unit cell consiting of just a single site.
Square(Lx, Ly, site, **kwargs)	A square lattice.
Triangular(Lx, Ly, site, **kwargs)	A triangular lattice.
TrivialLattice(mps_sites, **kwargs)	Trivial lattice consisting of a single (possibly large) unit cell in 1D.

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, ..., x_{D-1}, u)` to MPS index i.
Chain.mps2lat_idx(i)	Translate MPS index i to lattice indices `(x_0, ..., 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.

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Table 82 – continued from previous page

`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, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
`Chain.plot_bc_identified`(ax[, direction, shift])	Mark two sites indified by periodic boundary conditions.
`Chain.plot_coupling`(ax[, coupling])	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.

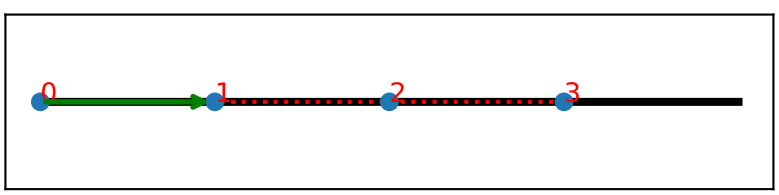
Class Attributes and Properties

`Chain.boundary_conditions`	Human-readable list of boundary conditions from `bc` and `bc_shift`.
`Chain.dim`	
`Chain.nearest_neighbors`	
`Chain.next_nearest_neighbors`	
`Chain.next_next_nearest_neighbors`	
`Chain.order`	Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

class `tenpy.models.lattice.`**`Chain`**(*L*, *site*, ***kwargs*)

Bases: `tenpy.models.lattice.SimpleLattice`

A chain of L equal sites.



Parameters

- **`L`** (`int`) – The lenght 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 initialize

with `[next_]next_]nearest_neighbors`. *positions* can be specified as a single vector.

ordering(*order*)

Provide possible orderings of the *N* lattice sites.

The following orders are defined in this method compared to `Lattice.ordering()`:

order	Resulting order
`'default'`	`0, 1, 2, 3, 4, ... ,L-1`
`'folded'`	`0, L-1, 1, L-2, ... , L//2`. This order might be usefull 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 convetion, 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 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, ..., 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* 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[..., 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.MultiCouplingModel.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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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*

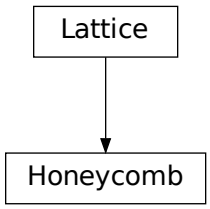
test_sanity()
Sanity check.

Raises ValueErrors, if something is wrong.

Honeycomb

- full name: tenpy.models.lattice.Honeycomb
- parent module: *tenpy.models.lattice*
- type: class

Inheritance Diagram



Methods

`Honeycomb.__init__`(Lx, Ly, sites, **kwargs)	Initialize self.
`Honeycomb.count_neighbors`([u, key])	Count e.g.
`Honeycomb.coupling_shape`(dx)	Calculate correct shape of the *strengths* for a coupling.
`Honeycomb.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`Honeycomb.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.

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Table 84 – continued from previous page

Honeycomb.lat2mps_idx(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
Honeycomb.mps2lat_idx(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
Honeycomb.mps2lat_values(A[, axes, u])	Reshape/reorder *A* to replace an MPS index by lattice indices.
Honeycomb.mps2lat_values_masked(A[, axes, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
Honeycomb.mps_idx_fix_u([u])	return an index array of MPS indices for which the site within the unit cell is *u*.
Honeycomb.mps_lat_idx_fix_u([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
Honeycomb.mps_sites()	Return a list of sites for all MPS indices.
Honeycomb.multi_coupling_shape(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
Honeycomb.number_nearest_neighbors([u])	Deprecated.
Honeycomb.number_next_nearest_neighbors([u])	Deprecated.
Honeycomb.ordering(order)	Provide possible orderings of the *N* lattice sites.
Honeycomb.plot_basis(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
Honeycomb.plot_bc_identified(ax[, ...])	Mark two sites indified by periodic boundary conditions.
Honeycomb.plot_coupling(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.
Honeycomb.plot_order(ax[, order, textkwargs])	Plot a line connecting sites in the specified "order" and text labels enumerating them.
Honeycomb.plot_sites(ax[, markers])	Plot the sites of the lattice with markers.
Honeycomb.position(lat_idx)	return 'space' position of one or multiple sites.
Honeycomb.possible_couplings(u1, u2, dx)	Find possible MPS indices for two-site couplings.
Honeycomb.possible_multi_couplings(ops)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
Honeycomb.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
Honeycomb.site(i)	return *Site* instance corresponding to an MPS index *i*
Honeycomb.test_sanity()	Sanity check.

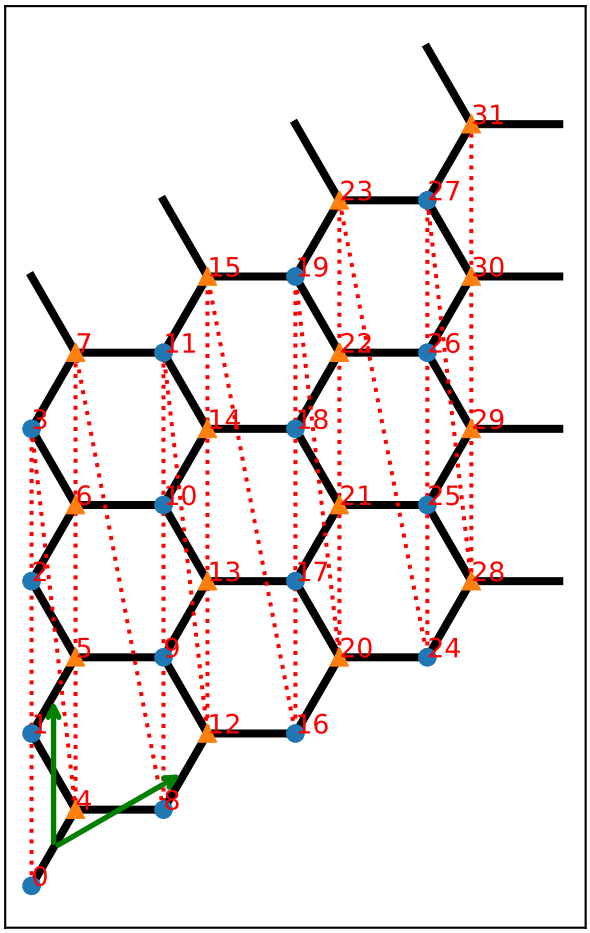
Class Attributes and Properties

Honeycomb.boundary_conditions	Human-readable list of boundary conditions from `bc` and `bc_shift`.
`Honeycomb.dim`	
`Honeycomb.fifth_nearest_neighbors`	
`Honeycomb.fourth_nearest_neighbors`	
`Honeycomb.nearest_neighbors`	
`Honeycomb.next_nearest_neighbors`	
`Honeycomb.next_next_nearest_neighbors`	
Honeycomb.order	Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

class `tenpy.models.lattice.`**`Honeycomb`**(*Lx*, *Ly*, *sites*, ***kwargs*)

Bases: *tenpy.models.lattice.Lattice*

A honeycomb lattice.



Parameters

- **Ly** (*Lx,*) – 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`.

ordering(*order*)

Provide possible orderings of the *N* lattice sites.

The following orders are defined in this method compared to *Lattice.ordering()*:

order	equivalent *priority*	equivalent `snake_winding`
`'default'`	(0, 2, 1)	(False, False, False)
`'snake'`	(0, 2, 1)	(False, True, 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*.

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 convetion, 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 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, ..., 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* accross 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 verions 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 expection 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:

```
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[lat.mps2lat_idx(5)] == A[5]
True
```

If you have a correlation function `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 *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.

```
>>> 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
```

Todo: make sure this function is used for expectation values...

---

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

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.MultiCouplingModel.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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If None, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1) to the site (i0+dx[0], i1+dx[1], ..., u2), taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to ax.plot().

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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*

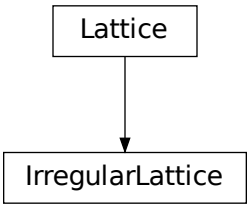
test_sanity()
Sanity check.

Raises ValueErrors, if something is wrong.

IrregularLattice

- full name: tenpy.models.lattice.IrregularLattice
- parent module: *tenpy.models.lattice*
- type: class

Inheritance Diagram



Methods

IrregularLattice.__init__(mps_sites, based_on)	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_add_sites(M)	
IrregularLattice.from_hdf5(hdf5_loader, ...)	Load instance from a HDF5 file.
IrregularLattice.from_mps_sites(mps_sites[, ...])	
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.

continues on next page

Table 86 – continued from previous page

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.
IrregularLattice.number_nearest_neighbors([u])	Deprecated.
IrregularLattice.number_next_nearest_neighbors([u])	Deprecated.
IrregularLattice.ordering(order)	Provide possible orderings of the *N* lattice sites.
IrregularLattice.plot_basis(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
IrregularLattice.plot_bc_identified(ax[, ...])	Mark two sites indified by periodic boundary conditions.
IrregularLattice.plot_coupling(ax[, coupling])	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.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`**(*mps_sites*, *based_on*, *order=None*)

Bases: *tenpy.models.lattice.Lattice*

A variant of a regular lattice, where we might have extra sites or sites missing.

Todo:

- this doesn't fully work yet...

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,...).

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 convetion, 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 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, ..., 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* accross 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 verions 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 expection 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:

```
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[lat.mps2lat_idx(5)] == A[5]
True
```

If you have a correlation function `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 *`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.

```
>>> 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
```

Todo: make sure this function is used for expectation values...

`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

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]`.

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.MultiCouplingModel.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:

order	equivalent *priority*	equivalent `snake_winding`
`'Cstyle'`	(0, 1, . . . , dim-1, dim)	(False, . . . , False, False)
`'default'`		
`'snake'`	(0, 1, . . . , dim-1, dim)	(True, . . . , True, True)
`'snakeCstyle'`		
`'Fstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)
`'snakeFstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)

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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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()

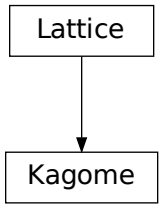
Sanity check.

Raises ValueErrors, if something is wrong.

Kagome

- full name: tenpy.models.lattice.Kagome
- parent module: `tenpy.models.lattice`
- type: class

Inheritance Diagram



Methods

`Kagome.__init__`(Lx, Ly, sites, **kwargs)	Initialize self.
`Kagome.count_neighbors`([u, key])	Count e.g.
`Kagome.coupling_shape`(dx)	Calculate correct shape of the *strengths* for a coupling.
`Kagome.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`Kagome.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
`Kagome.lat2mps_idx`(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
`Kagome.mps2lat_idx`(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
`Kagome.mps2lat_values`(A[, axes, u])	Reshape/reorder *A* to replace an MPS index by lattice indices.
`Kagome.mps2lat_values_masked`(A[, axes, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
`Kagome.mps_idx_fix_u`([u])	return an index array of MPS indices for which the site within the unit cell is *u*.
`Kagome.mps_lat_idx_fix_u`([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
`Kagome.mps_sites`()	Return a list of sites for all MPS indices.
`Kagome.multi_coupling_shape`(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
`Kagome.number_nearest_neighbors`([u])	Deprecated.
`Kagome.number_next_nearest_neighbors`([u])	Deprecated.
`Kagome.ordering`(order)	Provide possible orderings of the *N* lattice sites.
`Kagome.plot_basis`(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
`Kagome.plot_bc_identified`(ax[, direction, shift])	Mark two sites indified by periodic boundary conditions.
`Kagome.plot_coupling`(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.
`Kagome.plot_order`(ax[, order, textkwargs])	Plot a line connecting sites in the specified "order" and text labels enumerating them.
`Kagome.plot_sites`(ax[, markers])	Plot the sites of the lattice with markers.
`Kagome.position`(lat_idx)	return 'space' position of one or multiple sites.

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Table 88 – continued from previous page

Kagome.possible_couplings(u1, u2, dx)	Find possible MPS indices for two-site couplings.
Kagome.possible_multi_couplings(ops)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
Kagome.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
Kagome.site(i)	return *Site* instance corresponding to an MPS index *i*
Kagome.test_sanity()	Sanity check.

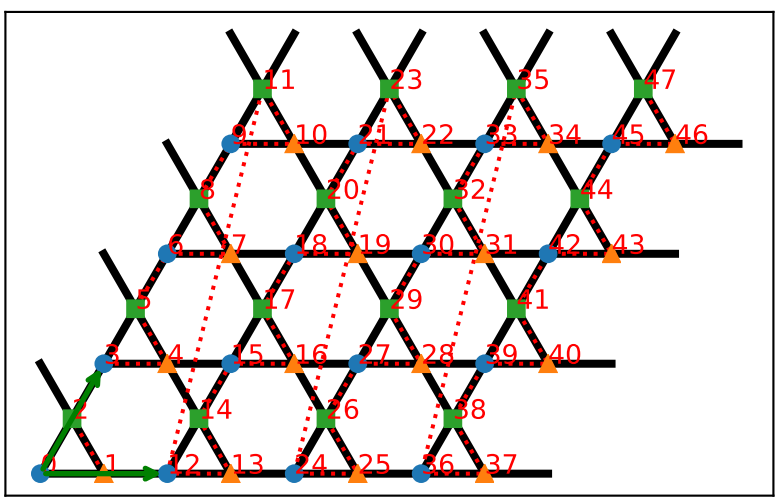
Class Attributes and Properties

Kagome.boundary_conditions	Human-readable list of boundary conditions from `bc` and `bc_shift`.
`Kagome.dim`	
`Kagome.nearest_neighbors`	
`Kagome.next_nearest_neighbors`	
`Kagome.next_next_nearest_neighbors`	
Kagome.order	Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

class `tenpy.models.lattice.`**`Kagome`**(*Lx*, *Ly*, *sites*, ***kwargs*)

Bases: *tenpy.models.lattice.Lattice*

A Kagome lattice.



Parameters

- **`Ly`** (*Lx,*) – 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*, *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 convetion, 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 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, ..., 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* accross 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 verions 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 expection 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:

```
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[lat.mps2lat_idx(5)] == A[5]
True
```

If you have a correlation function `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 `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.

```
>>> 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
```

Todo: make sure this function is used for expectation values...

---

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

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.MultiCouplingModel.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:

order	equivalent *priority*	equivalent `snake_winding`
`'Cstyle'`	(0, 1, . . . , dim-1, dim)	(False, . . . , False, False)
`'default'`		
`'snake'`	(0, 1, . . . , dim-1, dim)	(True, . . . , True, True)
`'snakeCstyle'`		
`'Fstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)
`'snakeFstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)

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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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()

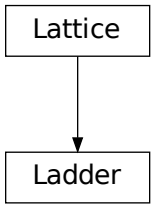
Sanity check.

Raises ValueErrors, if something is wrong.

Ladder

- full name: tenpy.models.lattice.Ladder
- parent module: `tenpy.models.lattice`
- type: class

Inheritance Diagram



Methods

`Ladder.__init__`(L, sites, **kwargs)	Initialize self.
`Ladder.count_neighbors`([u, key])	Count e.g.
`Ladder.coupling_shape`(dx)	Calculate correct shape of the *strengths* for a coupling.
`Ladder.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`Ladder.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
`Ladder.lat2mps_idx`(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
`Ladder.mps2lat_idx`(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
`Ladder.mps2lat_values`(A[, axes, u])	Reshape/reorder *A* to replace an MPS index by lattice indices.
`Ladder.mps2lat_values_masked`(A[, axes, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
`Ladder.mps_idx_fix_u`([u])	return an index array of MPS indices for which the site within the unit cell is *u*.
`Ladder.mps_lat_idx_fix_u`([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
`Ladder.mps_sites`()	Return a list of sites for all MPS indices.
`Ladder.multi_coupling_shape`(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
`Ladder.number_nearest_neighbors`([u])	Deprecated.
`Ladder.number_next_nearest_neighbors`([u])	Deprecated.
`Ladder.ordering`(order)	Provide possible orderings of the *N* lattice sites.
`Ladder.plot_basis`(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
`Ladder.plot_bc_identified`(ax[, direction, shift])	Mark two sites indified by periodic boundary conditions.
`Ladder.plot_coupling`(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.
`Ladder.plot_order`(ax[, order, textkwargs])	Plot a line connecting sites in the specified "order" and text labels enumerating them.
`Ladder.plot_sites`(ax[, markers])	Plot the sites of the lattice with markers.
`Ladder.position`(lat_idx)	return 'space' position of one or multiple sites.

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Table 90 – continued from previous page

`Ladder.possible_couplings`(u1, u2, dx)	Find possible MPS indices for two-site couplings.
`Ladder.possible_multi_couplings`(ops)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
`Ladder.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`Ladder.site`(i)	return `Site` instance corresponding to an MPS index *i*
`Ladder.test_sanity`()	Sanity check.

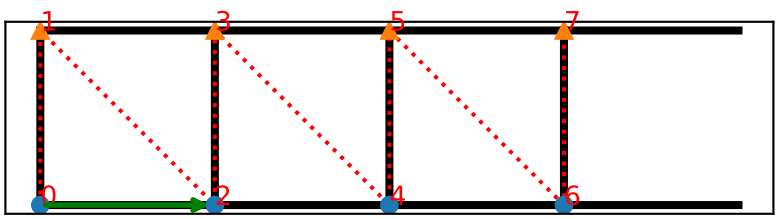
Class Attributes and Properties

`Ladder.boundary_conditions`	Human-readable list of boundary conditions from `bc` and `bc_shift`.
`Ladder.dim`	
`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.

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.

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 convetion, 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 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, ..., 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* accross 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 verions 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 expection 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:

```
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[lat.mps2lat_idx(5)] == A[5]
True
```

If you have a correlation function `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 *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.

```
>>> u = 0
>>> idx_subset = lat.mps_idx_fix_u(u)
>>> A_u = A[idx_subset]
```

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```
>>> 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
```

Todo: make sure this function is used for expectation values...

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

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.MultiCouplingModel.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:

order	equivalent *priority*	equivalent `snake_winding`
`'Cstyle'`	(0, 1, ..., dim-1, dim)	(False, ..., False, False)
`'default'`		
`'snake'`	(0, 1, ..., dim-1, dim)	(True, ..., True, True)
`'snakeCstyle'`		
`'Fstyle'`	(dim-1, ..., 1, 0, dim)	(False, ..., False, False)
`'snakeFstyle'`	(dim-1, ..., 1, 0, dim)	(False, ..., False, False)

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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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()

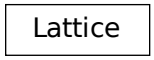
Sanity check.

Raises ValueErrors, if something is wrong.

Lattice

- full name: tenpy.models.lattice.Lattice
- parent module: `tenpy.models.lattice`
- type: class

Inheritance Diagram



Methods

`Lattice.__init__`(Ls, unit_cell[, order, bc, ...])	Initialize self.
`Lattice.count_neighbors`([u, key])	Count e.g.
`Lattice.coupling_shape`(dx)	Calculate correct shape of the *strengths* for a coupling.
`Lattice.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`Lattice.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.

continues on next page

Table 92 – continued from previous page

Lattice.lat2mps_idx(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
Lattice.mps2lat_idx(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
Lattice.mps2lat_values(A[, axes, u])	Reshape/reorder *A* to replace an MPS index by lattice indices.
Lattice.mps2lat_values_masked(A[, axes, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
Lattice.mps_idx_fix_u([u])	return an index array of MPS indices for which the site within the unit cell is *u*.
Lattice.mps_lat_idx_fix_u([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
Lattice.mps_sites()	Return a list of sites for all MPS indices.
Lattice.multi_coupling_shape(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
Lattice.number_nearest_neighbors([u])	Deprecated.
Lattice.number_next_nearest_neighbors([u])	Deprecated.
Lattice.ordering(order)	Provide possible orderings of the *N* lattice sites.
Lattice.plot_basis(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
Lattice.plot_bc_identified(ax[, direction, ...])	Mark two sites indified by periodic boundary conditions.
Lattice.plot_coupling(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.
Lattice.plot_order(ax[, order, textkwargs])	Plot a line connecting sites in the specified "order" and text labels enumerating them.
Lattice.plot_sites(ax[, markers])	Plot the sites of the lattice with markers.
Lattice.position(lat_idx)	return 'space' position of one or multiple sites.
Lattice.possible_couplings(u1, u2, dx)	Find possible MPS indices for two-site couplings.
Lattice.possible_multi_couplings(ops)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
Lattice.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
Lattice.site(i)	return *Site* instance corresponding to an MPS index *i*
Lattice.test_sanity()	Sanity check.

Class Attributes and Properties

Lattice.boundary_conditions	Human-readable list of boundary conditions from `bc` and `bc_shift`.
Lattice.dim	The dimension of the lattice.
`Lattice.nearest_neighbors`	
`Lattice.next_nearest_neighbors`	
`Lattice.next_next_nearest_neighbors`	
Lattice.order	Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

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, ..., x_{dim-1}, u)`, where `0 <= x_l < Ls[l]` pick the position of the unit cell in the lattice and `0 <= u < len(unit_cell)` picks the site within the unit cell. The site is located in 'space' at `sum_l x_l*basis[l] + unit_cell_positions[u]` (see *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, ..., x_{dim-1}, u) = 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, . . . , x_{dim-1},u)`` has MPS index *i*, the site at at `(x_0 + a*Ls[0], x_1 ..., x_{dim-1}, u)` corresponds to MPS index `i + N_sites`. Use *mps2lat_idx()* and *lat2mps_idx()* for conversion of indices. The function *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 *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 `-shift*lattice.basis[0]` (~cylinder axis for `bc_MPS='infinite'`) when going around the boundary along this direction.
- **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`*

bc
Boundary conditions of the couplings in each direction of the lattice, translated into a bool array with the global *bc_choices*.

Type bool ndarray

bc_shift
The shift in x-direction when going around periodic boundaries in other directions.

Type None | ndarray(int)

bc_MPS
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*).

Type 'finite' | 'segment' | 'infinite'

basis
translation vectors shifting the unit cell. The row *i* gives the vector shifting in direction *i*.

Type ndarray (dim, Dim)

unit_cell_positions
for each site in the unit cell a vector giving its position within the unit cell.

Type ndarray, shape (len(unit_cell), Dim)

pairs
See above.

Type dict

_order
The place where *order* is stored.

Type ndarray (N_sites, dim+1)

_strides
necessary for *mps2lat_idx()*

Type ndarray (dim,)

_perm
permutation needed to make *order* lexsorted.

Type ndarray (N,)

_mps2lat_vals_idx
index array for reshape/reordering in `mps2lat_vals()`

Type ndarray *shape*

_mps_fix_u
for each site of the unit cell an index array selecting the mps indices of that site.

Type tuple of ndarray (N_cells,) np.intp

_mps2lat_vals_idx_fix_u
similar as *_mps2lat_vals_idx*, but for a fixed *u* picking a site from the unit cell.

Type tuple of ndarray of shape *Ls*

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:

order	equivalent *priority*	equivalent `snake_winding`
`'Cstyle'`	(0, 1, . . . , dim-1, dim)	(False, . . . , False, False)
`'default'`		
`'snake'`	(0, 1, . . . , dim-1, dim)	(True, . . . , True, True)
`'snakeCstyle'`		
`'Fstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)
`'snakeFstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)

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 convetion, 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* accross 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 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

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]`.

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 verions 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 expection 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:

```
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[lat.mps2lat_idx(5)] == A[5]
True
```

If you have a correlation function `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 *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.

```
>>> 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
```

Todo: make sure this function is used for expectation values...

---

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

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

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.

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

- **u2** (*u1,*) – 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 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*) – Len *dim*. The correct shape for an array specifying the coupling strength. *lat_indices* has only rows within this shape.

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*.

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.MultiCouplingModel.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)

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 keywork *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={}*, ***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_coupling(*ax*, *coupling=None*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_basis(*ax*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***kwargs*)

Mark two sites indified by periodic boundary conditions.

Works only for lattice with a 2-dimensional basis.

Parameters

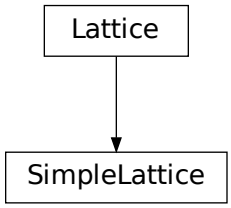
- **ax** (`matplotlib.axes.Axes`) – The axes on which we should plot.

- **direction** (*int*) – The direction of the lattice along which we should mark the idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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`.

SimpleLattice

- full name: tenpy.models.lattice.SimpleLattice
- parent module: *tenpy.models.lattice*
- type: class

Inheritance Diagram



Methods

`SimpleLattice.__init__`(Ls, site, **kwargs)	Initialize self.
SimpleLattice.count_neighbors([u, key])	Count e.g.
SimpleLattice.coupling_shape(dx)	Calculate correct shape of the *strengths* for a coupling.
SimpleLattice.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
SimpleLattice.from_hdf5(hdf5_loader, h5gr, ...)	Load instance from a HDF5 file.
SimpleLattice.lat2mps_idx(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
SimpleLattice.mps2lat_idx(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
SimpleLattice.mps2lat_values(A[, axes, u])	same as *Lattice.mps2lat_values()*, but ignore `u`, setting it to `0`.
SimpleLattice.mps2lat_values_masked(A[, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
SimpleLattice.mps_idx_fix_u([u])	return an index array of MPS indices for which the site within the unit cell is *u*.

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Table 94 – continued from previous page

SimpleLattice.mps_lat_idx_fix_u([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
SimpleLattice.mps_sites()	Return a list of sites for all MPS indices.
SimpleLattice.multi_coupling_shape(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
SimpleLattice.number_nearest_neighbors([D])	Deprecated.
SimpleLattice.number_next_nearest_neighbors([D])	Deprecated.
SimpleLattice.ordering(order)	Provide possible orderings of the *N* lattice sites.
SimpleLattice.plot_basis(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
SimpleLattice.plot_bc_identified(ax[, ...])	Mark two sites indified by periodic boundary conditions.
SimpleLattice.plot_coupling(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.
SimpleLattice.plot_order(ax[, order, textkwargs])	Plot a line connecting sites in the specified "order" and text labels enumerating them.
SimpleLattice.plot_sites(ax[, markers])	Plot the sites of the lattice with markers.
SimpleLattice.position(lat_idx)	return 'space' position of one or multiple sites.
SimpleLattice.possible_couplings(u1, u2, dx)	Find possible MPS indices for two-site couplings.
SimpleLattice.possible_multi_couplings(cons)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
SimpleLattice.save_hdf5(hdf5_saver, h5gr, ...)	Export *self* into a HDF5 file.
SimpleLattice.site(i)	return *Site* instance corresponding to an MPS index *i*
SimpleLattice.test_sanity()	Sanity check.

Class Attributes and Properties

SimpleLattice.boundary_conditions	Human-readable list of boundary conditions from `bc` and `bc_shift`.
SimpleLattice.dim	The dimension of the lattice.
`SimpleLattice.nearest_neighbors`	
`SimpleLattice.next_nearest_neighbors`	
`SimpleLattice.next_next_nearest_neighbors`	
SimpleLattice.order	Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

class `tenpy.models.lattice.`**`SimpleLattice`**(*Ls*, *site*, ***kwargs*)

Bases: *tenpy.models.lattice.Lattice*

A lattice with a unit cell consiting 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.

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 convetion, 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 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, ..., 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* accross the MPS unit cell and "infinite" *bc_MPS*, we shift *x_0* accordingly.

Return type array

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

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.MultiCouplingModel.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:

order	equivalent *priority*	equivalent `snake_winding`
`'Cstyle'`	(0, 1, . . . , dim-1, dim)	(False, . . . , False, False)
`'default'`		
`'snake'`	(0, 1, . . . , dim-1, dim)	(True, . . . , True, True)
`'snakeCstyle'`		
`'Fstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)
`'snakeFstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)

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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1) to the site (i0+dx[0], i1+dx[1], ..., u2), taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to ax.plot().

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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()

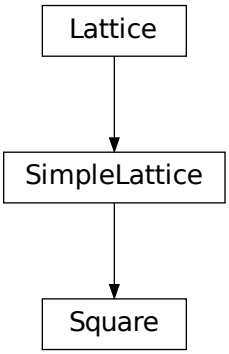
Sanity check.

Raises ValueErrors, if something is wrong.

Square

- full name: tenpy.models.lattice.Square
- parent module: `tenpy.models.lattice`
- type: class

Inheritance Diagram



Methods

`Square.__init__`(Lx, Ly, site, **kwargs)	Initialize self.
`Square.count_neighbors`([u, key])	Count e.g.
`Square.coupling_shape`(dx)	Calculate correct shape of the *strengths* for a coupling.
`Square.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`Square.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
`Square.lat2mps_idx`(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
`Square.mps2lat_idx`(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
`Square.mps2lat_values`(A[, axes, u])	same as *`Lattice.mps2lat_values()`*, but ignore `u`, setting it to `0`.
`Square.mps2lat_values_masked`(A[, axes, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
`Square.mps_idx_fix_u`([u])	return an index array of MPS indices for which the site within the unit cell is *u*.
`Square.mps_lat_idx_fix_u`([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
`Square.mps_sites`()	Return a list of sites for all MPS indices.
`Square.multi_coupling_shape`(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
`Square.number_nearest_neighbors`([u])	Deprecated.
`Square.number_next_nearest_neighbors`([u])	Deprecated.
`Square.ordering`(order)	Provide possible orderings of the *N* lattice sites.
`Square.plot_basis`(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
`Square.plot_bc_identified`(ax[, direction, shift])	Mark two sites indified by periodic boundary conditions.
`Square.plot_coupling`(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.

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Table 96 – continued from previous page

Square.plot_order(ax[, order, textkwargs])	Plot a line connecting sites in the specified "order" and text labels enumerating them.
Square.plot_sites(ax[, markers])	Plot the sites of the lattice with markers.
Square.position(lat_idx)	return 'space' position of one or multiple sites.
Square.possible_couplings(u1, u2, dx)	Find possible MPS indices for two-site couplings.
Square.possible_multi_couplings(ops)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
Square.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
Square.site(i)	return *Site* instance corresponding to an MPS index *i*
Square.test_sanity()	Sanity check.

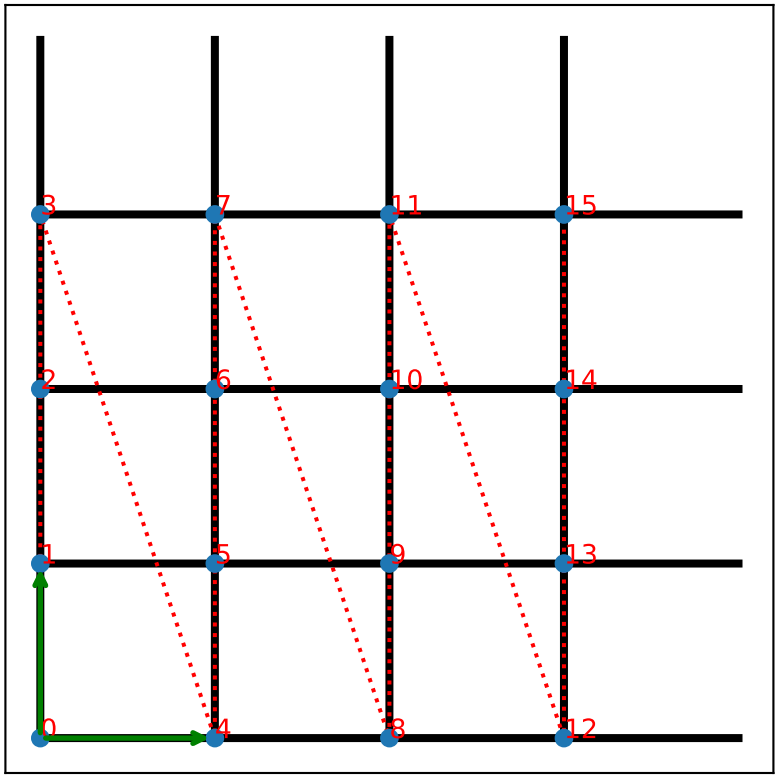
Class Attributes and Properties

Square.boundary_conditions	Human-readable list of boundary conditions from `bc` and `bc_shift`.
`Square.dim`	
`Square.nearest_neighbors`	
`Square.next_nearest_neighbors`	
`Square.next_next_nearest_neighbors`	
Square.order	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.



Parameters

- **Ly** (*Lx,*) – 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.

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 convetion, 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 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, ..., 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* 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[..., 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.MultiCouplingModel.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:

order	equivalent *priority*	equivalent `snake_winding`
`'Cstyle'`	(0, 1, ..., dim-1, dim)	(False, ..., False, False)
`'default'`		
`'snake'`	(0, 1, ..., dim-1, dim)	(True, ..., True, True)
`'snakeCstyle'`		
`'Fstyle'`	(dim-1, ..., 1, 0, dim)	(False, ..., False, False)
`'snakeFstyle'`	(dim-1, ..., 1, 0, dim)	(False, ..., False, False)

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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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*

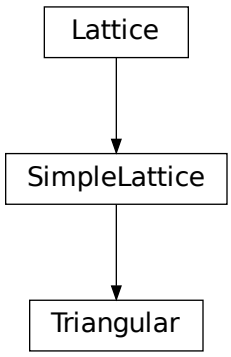
test_sanity()
Sanity check.

Raises ValueErrors, if something is wrong.

Triangular

- full name: tenpy.models.lattice.Triangular
- parent module: `tenpy.models.lattice`
- type: class

Inheritance Diagram



Methods

`Triangular.__init__`(Lx, Ly, site, **kwargs)	Initialize self.
`Triangular.count_neighbors`([u, key])	Count e.g.
`Triangular.coupling_shape`(dx)	Calculate correct shape of the *strengths* for a coupling.
`Triangular.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`Triangular.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
`Triangular.lat2mps_idx`(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
`Triangular.mps2lat_idx`(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
`Triangular.mps2lat_values`(A[, axes, u])	same as *`Lattice.mps2lat_values()`*, but ignore `u`, setting it to `0`.
`Triangular.mps2lat_values_masked`(A[, axes, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
`Triangular.mps_idx_fix_u`([u])	return an index array of MPS indices for which the site within the unit cell is *u*.
`Triangular.mps_lat_idx_fix_u`([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
`Triangular.mps_sites`()	Return a list of sites for all MPS indices.
`Triangular.multi_coupling_shape`(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
`Triangular.number_nearest_neighbors`([u])	Deprecated.
`Triangular.number_next_nearest_neighbors`([u])	Deprecated.
`Triangular.ordering`(order)	Provide possible orderings of the *N* lattice sites.
`Triangular.plot_basis`(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
`Triangular.plot_bc_identified`(ax[, ...])	Mark two sites indified by periodic boundary conditions.
`Triangular.plot_coupling`(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.
`Triangular.plot_order`(ax[, order, textkwargs])	Plot a line connecting sites in the specified "order" and text labels enumerating them.
`Triangular.plot_sites`(ax[, markers])	Plot the sites of the lattice with markers.
`Triangular.position`(lat_idx)	return 'space' position of one or multiple sites.
`Triangular.possible_couplings`(u1, u2, dx)	Find possible MPS indices for two-site couplings.
`Triangular.possible_multi_couplings`(ops)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
`Triangular.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`Triangular.site`(i)	return *`Site`* instance corresponding to an MPS index *i*
`Triangular.test_sanity`()	Sanity check.

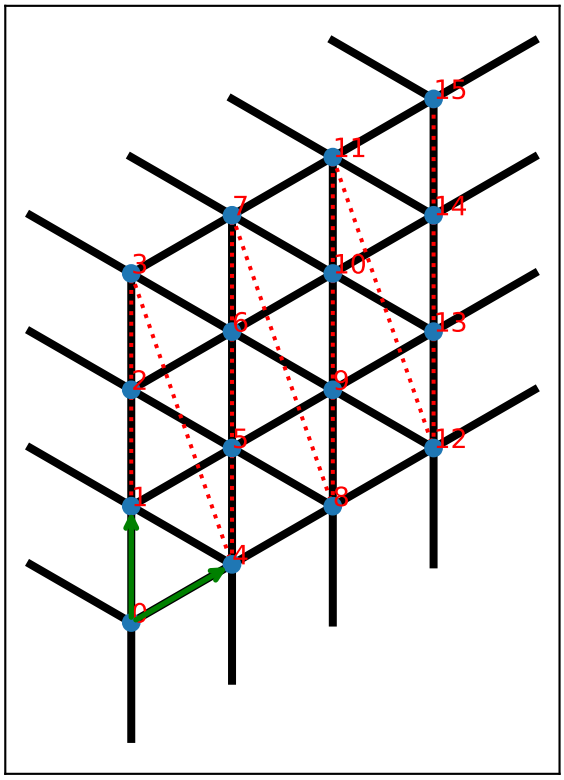
Class Attributes and Properties

Triangular.boundary_conditions	Human-readable list of boundary conditions from `bc` and `bc_shift`.
`Triangular.dim`	
`Triangular.nearest_neighbors`	
`Triangular.next_nearest_neighbors`	
`Triangular.next_next_nearest_neighbors`	
Triangular.order	Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

class `tenpy.models.lattice.`**`Triangular`**(*Lx*, *Ly*, *site*, ***kwargs*)

Bases: *tenpy.models.lattice.SimpleLattice*

A triangular lattice.



Parameters

- **`Ly`** (*Lx,*) – 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_windingi,`

priority), the *snake_winding* and *priority* should only be specified for the spatial directions. Similarly, *positions* can be specified as a single vector.

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 convetion, 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 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, ..., 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* 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[..., 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.MultiCouplingModel.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:

order	equivalent *priority*	equivalent `snake_winding`
`'Cstyle'`	(0, 1, . . . , dim-1, dim)	(False, . . . , False, False)
`'default'`		
`'snake'`	(0, 1, . . . , dim-1, dim)	(True, . . . , True, True)
`'snakeCstyle'`		
`'Fstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)
`'snakeFstyle'`	(dim-1, . . . , 1, 0, dim)	(False, . . . , False, False)

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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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()

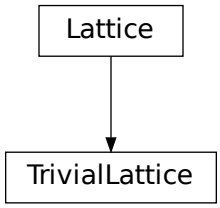
Sanity check.

Raises ValueErrors, if something is wrong.

TrivialLattice

- full name: tenpy.models.lattice.TrivialLattice
- parent module: `tenpy.models.lattice`
- type: class

Inheritance Diagram



Methods

`TrivialLattice.__init__`(mps_sites, **kwargs)	Initialize self.
`TrivialLattice.count_neighbors`([u, key])	Count e.g.
`TrivialLattice.coupling_shape`(dx)	Calculate correct shape of the *strengths* for a coupling.
`TrivialLattice.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`TrivialLattice.from_hdf5`(hdf5_loader, h5gr, ...)	Load instance from a HDF5 file.
`TrivialLattice.lat2mps_idx`(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
`TrivialLattice.mps2lat_idx`(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
`TrivialLattice.mps2lat_values`(A[, axes, u])	Reshape/reorder *A* to replace an MPS index by lattice indices.
`TrivialLattice.mps2lat_values_masked`(A[, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
`TrivialLattice.mps_idx_fix_u`([u])	return an index array of MPS indices for which the site within the unit cell is *u*.
`TrivialLattice.mps_lat_idx_fix_u`([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
`TrivialLattice.mps_sites`()	Return a list of sites for all MPS indices.
`TrivialLattice.multi_coupling_shape`(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
`TrivialLattice.number_nearest_neighbors`([u])	Deprecated.
`TrivialLattice.number_next_nearest_neighbors`([u])	Deprecated.
`TrivialLattice.ordering`(order)	Provide possible orderings of the *N* lattice sites.
`TrivialLattice.plot_basis`(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
`TrivialLattice.plot_bc_identified`(ax[, ...])	Mark two sites indified by periodic boundary conditions.
`TrivialLattice.plot_coupling`(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.
`TrivialLattice.plot_order`(ax[, order, ...])	Plot a line connecting sites in the specified "order" and text labels enumerating them.

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Table 100 – continued from previous page

TrivialLattice.plot_sites(ax[, markers])	Plot the sites of the lattice with markers.
TrivialLattice.position(lat_idx)	return 'space' position of one or multiple sites.
TrivialLattice.possible_couplings(u1, u2, dx)	Find possible MPS indices for two-site couplings.
TrivialLattice.possible_multi_couplings(op)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
TrivialLattice.save_hdf5(hdf5_saver, h5gr, ...)	Export *self* into a HDF5 file.
TrivialLattice.site(i)	return *Site* instance corresponding to an MPS index *i*
TrivialLattice.test_sanity()	Sanity check.

Class Attributes and Properties

TrivialLattice.boundary_conditions	Human-readable list of boundary conditions from `bc` and `bc_shift`.
TrivialLattice.dim	The dimension of the lattice.
`TrivialLattice.nearest_neighbors`	
`TrivialLattice.next_nearest_neighbors`	
`TrivialLattice.next_next_nearest_neighbors`	
TrivialLattice.order	Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

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 usefull if you need a valid *Lattice* given just the *mps_sites()*.

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`.

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 convetion, 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 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, ..., 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* accross 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 verions 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 expection 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:

```
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[lat.mps2lat_idx(5)] == A[5]
True
```

If you have a correlation function `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 *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.

```
>>> 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
```

Todo: make sure this function is used for expectation values...

---

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

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.MultiCouplingModel.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:

order	equivalent *priority*	equivalent `snake_winding`
`'Cstyle'`	(0, 1, ..., dim-1, dim)	(False, ..., False, False)
`'default'`		
`'snake'`	(0, 1, ..., dim-1, dim)	(True, ..., True, True)
`'snakeCstyle'`		
`'Fstyle'`	(dim-1, ..., 1, 0, dim)	(False, ..., False, False)
`'snakeFstyle'`	(dim-1, ..., 1, 0, dim)	(False, ..., False, False)

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*, ***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 specifying the "arrowprops" of `ax.annotate`.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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.

Functions

`get_lattice`(lattice_name)	Given the name of a `Lattice` class, get the lattice class itself.
`get_order`(shape, snake_winding[, priority])	Built the `Lattice.order` in (Snake-) C-Style for a given lattice shape.
`get_order_grouped`(shape, groups)	Variant of `get_order()`, grouping some sites of the unit cell.

get_lattice

- full name: tenpy.models.lattice.get_lattice
- parent module: `tenpy.models.lattice`
- type: function

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

tenpy.models.lattice.**get_order**(*shape*, *snake_winding*, *priority=None*)
Built the `Lattice.order` in (Snake-) C-Style for a given lattice shape.

In this function, the word 'direction' referst 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.

In this function, the word 'direction' referst to a physical direction of the lattice or the index *u* of the unit cell as an "artificial direction". This function is usefull for lattices with a unit cell of more than 2 sites (e.g. Kagome). The argument *group* is a To explain the order, assume we have a 3-site unit cell in a 2D lattice with shape (Lx, Ly, Lu). Calling this function with groups=((1,), (2, 0)) returns an order of the following form:

```
# columns: [x, y, u]
[0, 0, 1]  # first for u = 1 along y
[0, 1, 1]
    :
[0, Ly-1, 1]
[0, 0, 2]  # then for u = 2 and 0
[0, 0, 0]
[0, 1, 2]
[0, 1, 0]
    :
[0, Ly-1, 2]
[0, Ly-1, 0]
# and then repeat the above for increasing `x`.
```

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 Cstyle 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:

Lattice.ordering() method in `Lattice` to obtain the order from parameters.

Lattice.plot_order() visualizes the resulting order in a `Lattice`.

Module description

Classes to define the lattice structure of a model.

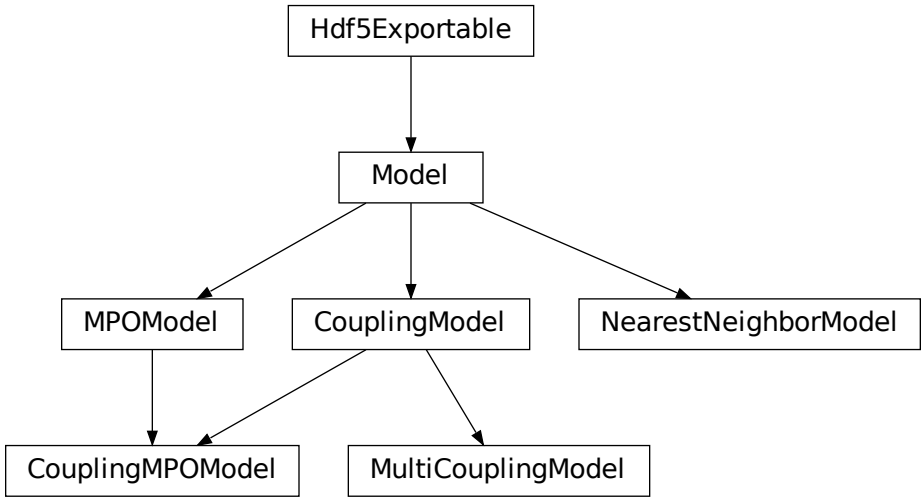
The base class `Lattice` defines the general structure of a lattice, you can subclass this to define you own lattice. The `SimpleLattice` is a slight simplification for lattices with a single-site unit cell. Further, we have some predefined lattices, namely `Chain`, `Ladder` in 1D and `Square`, `Triangular`, `Honeycomb`, and `Kagome` in 2D.

See also the *Models*.

7.9.2 model

- full name: tenpy.models.model
- parent module: `tenpy.models`
- type: module

Classes

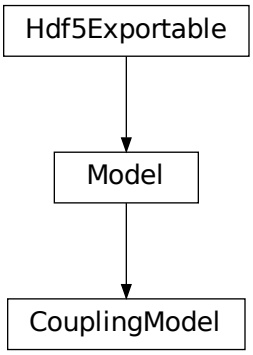


`CouplingMPOModel`(model_params)	Combination of the *CouplingModel* and *MPOModel*.
CouplingModel(lattice[, bc_coupling, . . .])	Base class for a general model of a Hamiltonian consisting of two-site couplings.
MPOModel(lattice, H_MPO)	Base class for a model with an MPO representation of the Hamiltonian.
Model(lattice)	Base class for all models.
MultiCouplingModel(lattice[, bc_coupling, . . .])	Generalizes *CouplingModel* to allow couplings involving more than two sites.
NearestNeighborModel(lattice, H_bond)	Base class for a model of nearest neigbor interactions w.r.t.

CouplingModel

- full name: tenpy.models.model.CouplingModel
- parent module: *tenpy.models.model*
- type: class

Inheritance Diagram



Methods

`CouplingModel.__init__`(lattice[, ...])	Initialize self.
`CouplingModel.add_coupling`(strength, u1, ...)	Add twosite coupling terms to the Hamiltonian, summing over lattice sites.
`CouplingModel.add_coupling_term`(strength, i, ...)	Add a two-site coupling term on given MPS sites.
`CouplingModel.add_local_term`(strength, term)	Add a single term to *self*.
`CouplingModel.add_onsite`(strength, u, opname)	Add onsite terms to `onsite_terms`.
`CouplingModel.add_onsite_term`(strength, i, op)	Add an onsite term on a given MPS site.
`CouplingModel.all_coupling_terms`()	Sum of all `coupling_terms`.
`CouplingModel.all_onsite_terms`()	Sum of all `onsite_terms`.
`CouplingModel.calc_H_MPO`([tol_zero])	Calculate MPO representation of the Hamiltonian.
`CouplingModel.calc_H_bond`([tol_zero])	calculate *H_bond* from `coupling_terms` and `onsite_terms`.
`CouplingModel.calc_H_onsite`([tol_zero])	Calculate *H_onsite* from *self.onsite_terms*.
`CouplingModel.coupling_strength_add_ext_flux`(strength)	Add an external flux to the coupling strength.
`CouplingModel.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`CouplingModel.from_hdf5`(hdf5_loader, h5gr, ...)	Load instance from a HDF5 file.
`CouplingModel.group_sites`([n, grouped_sites])	Modify *self* in place to group sites.
`CouplingModel.save_hdf5`(hdf5_saver, h5gr, ...)	Export *self* into a HDF5 file.
`CouplingModel.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.

class tenpy.models.model.**CouplingModel**(*lattice*, *bc_coupling=None*, *explicit_plus_hc=False*)

Bases: *tenpy.models.model.Model*

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 a *MultiCouplingModel*, values may also be *MultiCouplingTerms*.

Type {'category': *CouplingTerms*}

explicit_plus_hc

If *True*, *self* represents the terms in *onsite_terms* and *coupling_terms* *and* their hermitian conjugate added. The flag will be carried on the MPO, which will have a reduced bond dimension if `self.add_coupling(..., plus_hc=True)` was used. Note that *add_onsite()* and *add_coupling()* respect this flag, ensuring that the *represented* Hamiltonian is indepentent 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 repesented 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 $\sum_{\vec{x}} strength[\vec{x}] * OP$ 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, ..., 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 <= 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(*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 $\sum_{x_0,\ldots,x_{dim-1}} strength[shift(\vec{x})] * OP0 * OP1$, where `OP0 := lat.unit_cell[u0].get_op(op0)` acts on the site `(x_0, ..., x_{dim-1}, u1)`, and `OP1 := lat.unit_cell[u1].get_op(op1)` acts on the site `(x_0+dx[0], ...,`

`x_{dim-1}+dx[dim-1], u1)`. Possible combinations `x_0, ..., 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:

```
>>> 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:

```
>>> self.add_coupling([1.5, 1.], 0, 'Sz', 0, 'Sz', dx)
```

Make sure to use the *plus_hc* argument if necessary, e.g. for hoppings:

```
>>> 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 explictly. 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

```
>>> t = 1.  # hopping strength
>>> 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:

```
>>> 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.␣
↪Cdagger_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.

MultiCouplingModel.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(...)`.

> **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.
- **j** (*i,*) – 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.
- **op2** (*op1,*) – 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*.

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.

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_MPO(*tol_zero=1e-15*)
Calculate MPO representation of the Hamiltonian.

Uses *onsite_terms* and *coupling_terms* to build an MPO graph (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*

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 [Resta1997]. 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]` souch 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.

```
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0,
↪ phi])
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     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 convetion, 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

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'`.

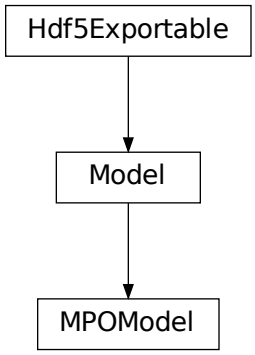
Parameters

- **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



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`()	

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`** (*`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_cojugate(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 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 convetion, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

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_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.:

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

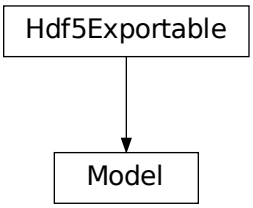
- **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.

- **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



Methods

`Model.__init__`(lattice)	Initialize self.
Model.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
Model.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
Model.group_sites([n, grouped_sites])	Modify *self* in place to group sites.
Model.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.

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_sites* to `factor*N_sites_per_ring`. Since MPS unit cells are repeated in the *x*-direction in our convetion, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

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'`.

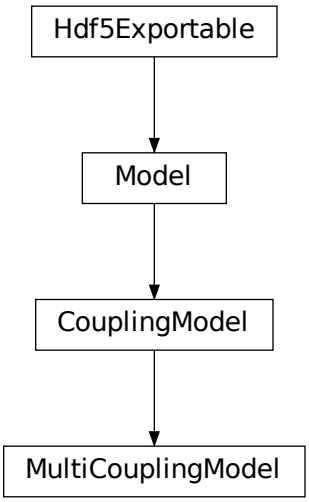
Parameters

- **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



Methods

`MultiCouplingModel.__init__`(lattice[, ...])	Initialize self.
MultiCouplingModel.add_coupling(strength, ...)	Add twosite 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_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`.
MultiCouplingModel.add_onsite_term(strength, ...)	Add an onsite term on a given MPS site.

continues on next page

Table 107 – continued from previous page

MultiCouplingModel.all_coupling_terms()	Sum of all coupling_terms.
MultiCouplingModel.all_onsite_terms()	Sum of all onsite_terms.
MultiCouplingModel.calc_H_MPO([tol_zero])	Calculate MPO representation of the Hamiltonian.
MultiCouplingModel.calc_H_bond([tol_zero])	calculate *H_bond* from coupling_terms and onsite_terms.
MultiCouplingModel.calc_H_onsite([tol_zero])	Calculate *H_onsite* from *self.onsite_terms*.
MultiCouplingModel.coupling_strength_add_ext_flux(...)	Add an external flux to the coupling strength.
MultiCouplingModel.enlarge_mps_unit_cell([...])	Repeat the unit cell for infinite MPS boundary conditions; in place.
MultiCouplingModel.from_hdf5(hdf5_loader, ...)	Load instance from a HDF5 file.
MultiCouplingModel.group_sites([n, ...])	Modify *self* in place to group sites.
MultiCouplingModel.save_hdf5(hdf5_saver, ...)	Export *self* into a HDF5 file.
MultiCouplingModel.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.

class tenpy.models.model.**MultiCouplingModel**(*lattice*, *bc_coupling=None*, *explicit_plus_hc=False*)

Bases: tenpy.models.model.CouplingModel

Generalizes CouplingModel to allow couplings involving more than two sites.

The corresponding couplings can be added with add_multi_coupling() and add_multi_coupling_term() and are saved in coupling_terms, which can now contain instances of MultiCouplingTerms.

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 $sum_{\vec{x}} strength[shift(\vec{x})] * OP_0 * OP_1 * ... * OP_{M-1}$, 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, ...] 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 argment *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:

```
>>> dx_0 = [0] * self.lat.dim  # = [0] for a 1D lattice, [0, 0] in 2D
>>> self.add_coupling(strength, [('A', dx_0, u1), ('B', dx, u2)])
```

To explicitly add the hermitian conjugate, 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:

```
>>> self.add_coupling(np.conj(strength), [(hc('B'), dx, u2), (hc('A'), dx_0,␣
↪u1)])  # h.c.
```

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*, *ijkl*, *ops_ijkl*, *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, ... = ijkl*, 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_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 `"{op0}_i {op1}_j {op2}_k ..."`.
- **plus_hc** (*bool*) – If *True*, the hermitian conjugate of the term is added automatically.

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 $\sum_{x_0,\ldots,x_{dim-1}} strength[shift(\vec{x})] * OP0 * OP1$, where `OP0 := lat.unit_cell[u0].get_op(op0)` acts on the site `(x_0, ..., x_{dim-1}, u1)`, and `OP1 := lat.unit_cell[u1].get_op(op1)` acts on the site `(x_0+dx[0], ..., x_{dim-1}+dx[dim-1], u1)`. Possible combinations `x_0, ..., 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:

```
>>> 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:

```
>>> self.add_coupling([1.5, 1.], 0, 'Sz', 0, 'Sz', dx)
```

Make sure to use the *plus_hc* argument if necessary, e.g. for hoppings:

```
>>> 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 explictly. 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

```
>>> t = 1.  # hopping strength
>>> 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:

```
>>> 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.␣
↪Cdagger_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.

MultiCouplingModel.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(...)`.

> **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.
- **j** (*i,*) – 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.
- **op2** (*op1,*) – 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_local_term(*strength*, *term*, *category=None*, *plus_hc=False*)
Add a single term to *self*.

The repesented 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 $\sum_{\vec{x}} strength[\vec{x}] * OP$ 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, ..., 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 <= 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`.

calc_H_MPO(*tol_zero=1e-15*)

Calculate MPO representation of the Hamiltonian.

Uses `onsite_terms` and `coupling_terms` to build an MPO graph (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_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_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 [Resta1997]. 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]` souch 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.

```
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0,
↪ phi])
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
```

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```
...     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 convetion, 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

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

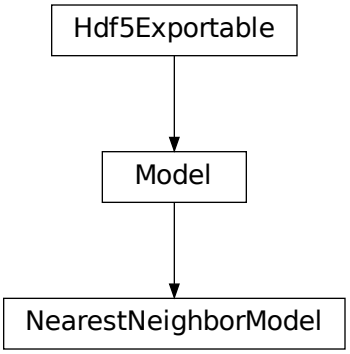
- **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.
- **h5gr** (*:class`Group`*) – HDF5 group which is supposed to represent *self*.
- **subpath** (*str*) – The *name* of *h5gr* with a `'/'` in the end.

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 <psi|H_bond|psi>.
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()	

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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_bond[i]` for MPS indices `i`. `H_bond[i]` acts on sites `(i-1, i)`; we require `len(H_bond) == lat.N_sites`. Legs of each `H_bond[i]` are `['p0', 'p0*', 'p1', 'p1*']`.

H_bond

The Hamiltonian 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*']`. *H_bond* is not affected by the *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})
parameter 'L'=20 for SpinChainNNN2
>>> 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.

```
>>> 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:

```
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
```

---

trivial_like_NNModel()
Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

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

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 convetion, the lattice shape goes from `(Lx, Ly, ..., Lu)` to `(Lx*factor, Ly, ..., Lu)`.

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 intialize 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, namley 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.

For simplicity, the `CouplingModel` is limited to interactions involving only two sites. Yet, we also provide the `MultiCouplingModel` to generate Models for Hamiltonians involving couplings between multiple sites.

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

`tf_ising`	Prototypical example of a quantum model: the transverse field Ising model.
`xxz_chain`	Prototypical example of a 1D quantum model: the spin-1/2 XXZ chain.
`spins`	Nearest-neighbour spin-S models.
`spins_nnn`	Next-Nearest-neighbour spin-S models.

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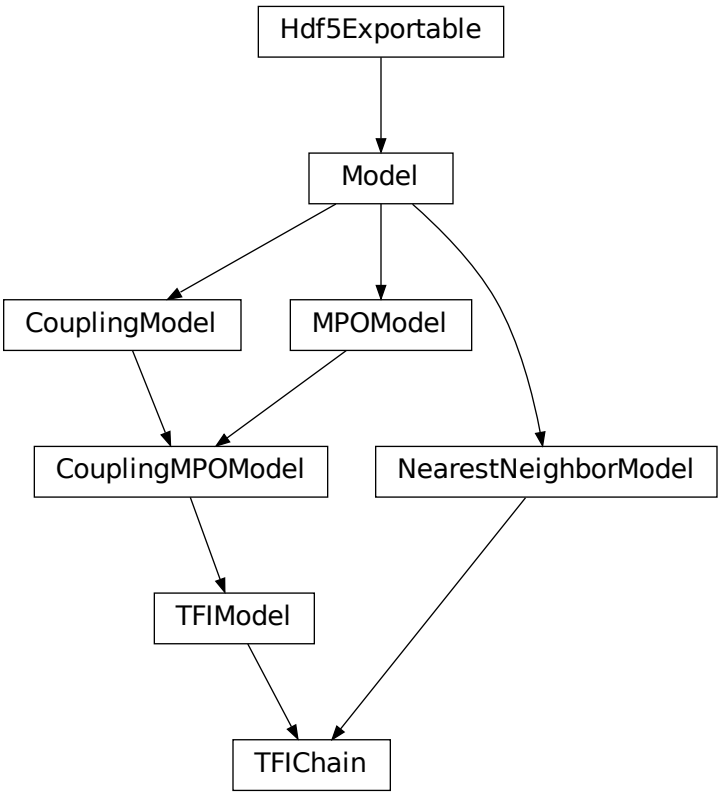
Table 109 – continued from previous page

fermions_spinless	Spinless fermions with hopping and interaction.
hubbard	Bosonic and fermionic Hubbard models.
hofstadter	Cold atomic (Harper-)Hofstadter model on a strip or cylinder.
haldane	Bosonic and fermionic Haldane models.
toric_code	Kitaev's exactly solvable toric code model.

7.9.3 tf_ising

- full name: tenpy.models.tf_ising
- parent module: *tenpy.models*
- type: module

Classes



TFIChain(model_params)	The `TFIModel` on a Chain, suitable for TEBD.

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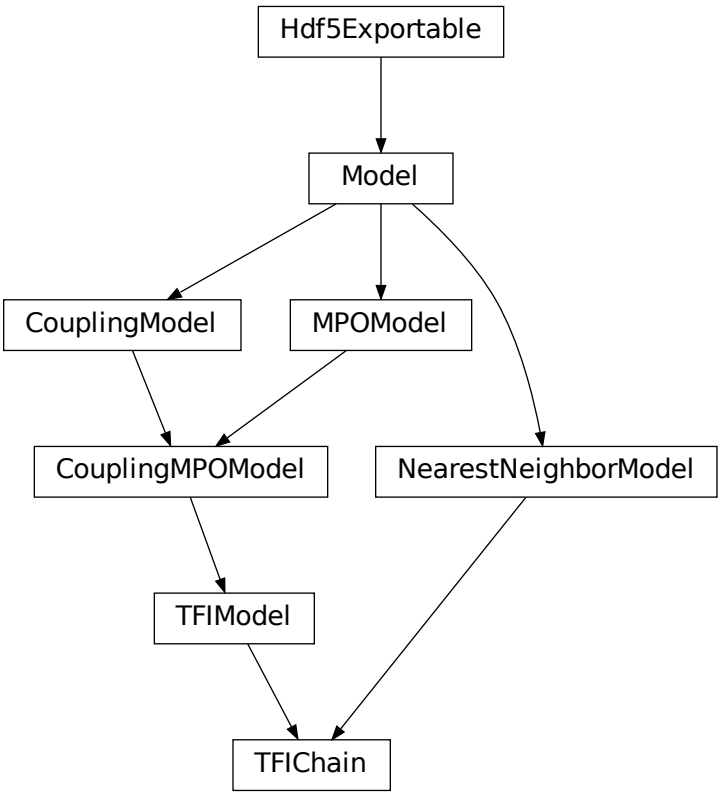
Table 110 – continued from previous page

`TFIModel`(model_params)	Transverse field Ising model on a general lattice.

TFIChain

- full name: tenpy.models.tf_ising.TFIChain
- parent module: *tenpy.models.tf_ising*
- type: class

Inheritance Diagram



Methods

TFIChain.__init__(model_params)	Initialize self.
TFIChain.add_coupling(strength, u1, op1, u2, ...)	Add twosite coupling terms to the Hamiltonian, summing over lattice sites.
TFIChain.add_coupling_term(strength, i, j, ...)	Add a two-site coupling term on given MPS sites.
TFIChain.add_local_term(strength, term[, ...])	Add a single term to *self*.
TFIChain.add_onsite(strength, u, opname[, ...])	Add onsite terms to onsite_terms.
TFIChain.add_onsite_term(strength, i, op[, ...])	Add an onsite term on a given MPS site.
TFIChain.all_coupling_terms()	Sum of all coupling_terms.
TFIChain.all_onsite_terms()	Sum of all onsite_terms.
TFIChain.bond_energies(psi)	Calculate bond energies <psi|H_bond|psi>.
TFIChain.calc_H_MPO([tol_zero])	Calculate MPO representation of the Hamiltonian.
TFIChain.calc_H_MPO_from_bond([tol_zero])	Calculate the MPO Hamiltonian from the bond Hamiltonian.
TFIChain.calc_H_bond([tol_zero])	calculate *H_bond* from coupling_terms and onsite_terms.
TFIChain.calc_H_bond_from_MPO([tol_zero])	Calculate the bond Hamiltonian from the MPO Hamiltonian.
TFIChain.calc_H_onsite([tol_zero])	Calculate *H_onsite* from *self.onsite_terms*.
TFIChain.coupling_strength_add_ext_flux(...)	Add an external flux to the coupling strength.
TFIChain.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
TFIChain.from_MPOModel(mpo_model)	Initialize a NearestNeighborModel from a model class defining an MPO.
TFIChain.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
TFIChain.group_sites([n, grouped_sites])	Modify *self* in place to group sites.
TFIChain.init_lattice(model_params)	Initialize a lattice for the given model parameters.
TFIChain.init_sites(model_params)	Define the local Hilbert space and operators; needs to be implemented in subclasses.
TFIChain.init_terms(model_params)	Add the onsite and coupling terms to the model; subclasses should implement this.
TFIChain.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
TFIChain.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.
TFIChain.trivial_like_NNModel()	Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

class tenpy.models.tf_ising.**TFIChain**(*model_params*)

Bases: tenpy.models.tf_ising.TFIModel, tenpy.models.model.NearestNeighborModel

The TFIModel on a Chain, suitable for TEBD.

See the TFIModel 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 twosite coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form $\sum_{x_0,\ldots,x_{dim-1}} strength[shift(\vec{x})] * OP0 * OP1$, where OP0 := lat.unit_cell[u0].get_op(op0) acts on the site (x_0, ..., x_{dim-1}, u1),

and `OP1 := lat.unit_cell[u1].get_op(op1)` acts on the site `(x_0+dx[0], ..., x_{dim-1}+dx[dim-1], u1)`. Possible combinations `x_0, ..., 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:

```
>>> 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:

```
>>> self.add_coupling([1.5, 1.], 0, 'Sz', 0, 'Sz', dx)
```

Make sure to use the *plus_hc* argument if necessary, e.g. for hoppings:

```
>>> 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 explictly. 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

```
>>> t = 1.  # hopping strength
>>> 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:

```
>>> 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.␣
↪Cdagger_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.

MultiCouplingModel.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(...)`.

> **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.

- **j** (*i,*) – 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.
- **op2** (*op1,*) – 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_local_term(*strength*, *term*, *category=None*, *plus_hc=False*)

Add a single term to *self*.

The repesented 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 $\sum_{\vec{x}} strength[\vec{x}] * OP$ 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, ..., 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 <= 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 MPO graph (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 [Resta1997]. 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]` souch 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.

```
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0,
↪ phi])
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     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 convetion, 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:

```
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20})
parameter 'L'=20 for SpinChainNNN2
>>> 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.

```
>>> 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:

```
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
```

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.

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.

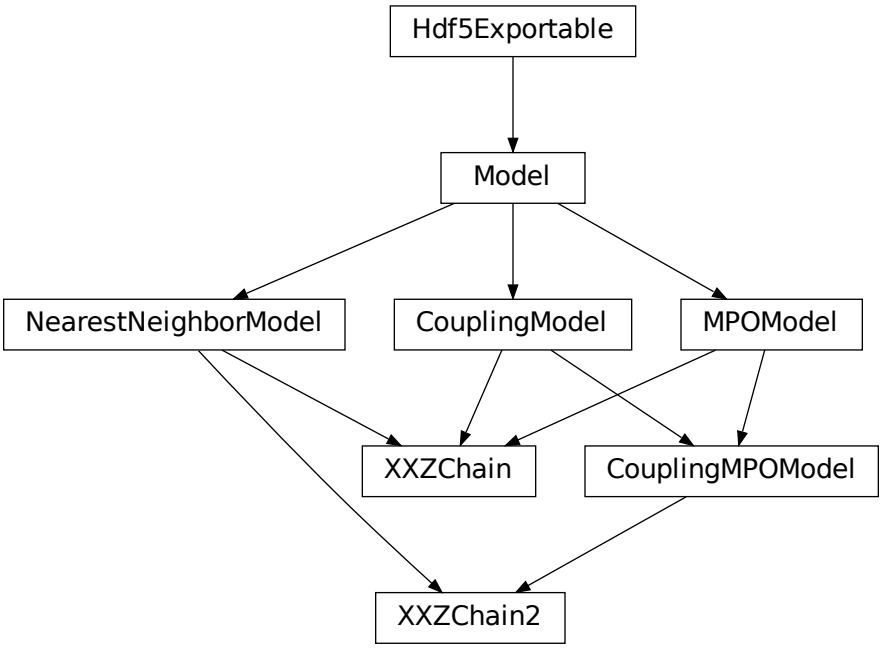
Like the `XXZChain`, the transverse field ising chain *`TFIChain`* is contained in the more general *`SpinChain`*; the idea is more to serve as a pedagogical example for a 'model'.

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

7.9.4 xxz_chain

- full name: tenpy.models.xxz_chain
- parent module: *`tenpy.models`*
- type: module

Classes

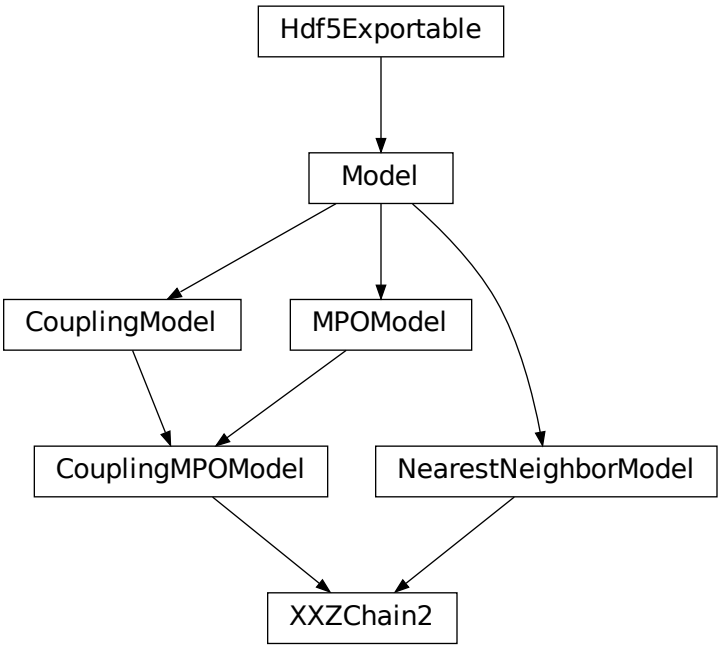


`XXZChain`(model_params)	Spin-1/2 XXZ chain with Sz conservation.
`XXZChain2`(model_params)	Another implementation of the Spin-1/2 XXZ chain with Sz conservation.

XXZChain2

- full name: tenpy.models.xxz_chain.XXZChain2
- parent module: *tenpy.models.xxz_chain*
- type: class

Inheritance Diagram



Methods

`XXZChain2.__init__`(model_params)	Initialize self.
XXZChain2.add_coupling(strength, u1, op1, ...)	Add twosite coupling terms to the Hamiltonian, summing over lattice sites.
XXZChain2.add_coupling_term(strength, i, j, ...)	Add a two-site coupling term on given MPS sites.
XXZChain2.add_local_term(strength, term[, ...])	Add a single term to *self*.
XXZChain2.add_onsite(strength, u, opname[, ...])	Add onsite terms to `onsite_terms`.
XXZChain2.add_onsite_term(strength, i, op[, ...])	Add an onsite term on a given MPS site.

continues on next page

Table 113 – continued from previous page

XXZChain2.all_coupling_terms()	Sum of all `coupling_terms`.
XXZChain2.all_onsite_terms()	Sum of all `onsite_terms`.
XXZChain2.bond_energies(psi)	Calculate bond energies <psi|H_bond|psi>.
XXZChain2.calc_H_MPO([tol_zero])	Calculate MPO representation of the Hamiltonian.
XXZChain2.calc_H_MPO_from_bond([tol_zero])	Calculate the MPO Hamiltonian from the bond Hamiltonian.
XXZChain2.calc_H_bond([tol_zero])	calculate *H_bond* from `coupling_terms` and `onsite_terms`.
XXZChain2.calc_H_bond_from_MPO([tol_zero])	Calculate the bond Hamiltonian from the MPO Hamiltonian.
XXZChain2.calc_H_onsite([tol_zero])	Calculate *H_onsite* from *self.onsite_terms*.
XXZChain2.coupling_strength_add_ext_flux(d, a)	Add an external flux to the coupling strength.
XXZChain2.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
XXZChain2.from_MPOModel(mpo_model)	Initialize a NearestNeighborModel from a model class defining an MPO.
XXZChain2.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
XXZChain2.group_sites([n, grouped_sites])	Modify *self* in place to group sites.
XXZChain2.init_lattice(model_params)	Initialize a lattice for the given model parameters.
XXZChain2.init_sites(model_params)	Define the local Hilbert space and operators; needs to be implemented in subclasses.
XXZChain2.init_terms(model_params)	Add the onsite and coupling terms to the model; subclasses should implement this.
XXZChain2.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
XXZChain2.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.
XXZChain2.trivial_like_NNModel()	Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

class `tenpy.models.xxz_chain.`**`XXZChain2`**(*model_params*)

Bases: `tenpy.models.model.CouplingMPOModel`, *tenpy.models.model.NearestNeighborModel*

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.

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.

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 $\sum_{x_0,\ldots,x_{dim-1}} strength[shift(\vec{x})] * OP0 * OP1$, where `OP0 := lat.unit_cell[u0].get_op(op0)` acts on the site `(x_0, ..., x_{dim-1}, u1)`, and `OP1 := lat.unit_cell[u1].get_op(op1)` acts on the site `(x_0+dx[0], ..., x_{dim-1}+dx[dim-1], u1)`. Possible combinations `x_0, ..., 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:

```
>>> 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:

```
>>> self.add_coupling([1.5, 1.], 0, 'Sz', 0, 'Sz', dx)
```

Make sure to use the *plus_hc* argument if necessary, e.g. for hoppings:

```
>>> 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 explictly. 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

```
>>> t = 1.  # hopping strength
>>> 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:

```
>>> 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.␣
↪Cdagger_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.

MultiCouplingModel.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(...)`.

> **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.
- **j** (*i,*) – 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.
- **op2** (*op1,*) – 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_local_term(*strength*, *term*, *category=None*, *plus_hc=False*)

Add a single term to *self*.

The repesented 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 $\sum_{\vec{x}} strength[\vec{x}] * OP$ 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, ..., 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 <= 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 MPO graph (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 [Resta1997]. 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]` souch 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.

```
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0,
↪ phi])
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     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 convetion, 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:

```
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20})
parameter 'L'=20 for SpinChainNNN2
>>> 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.

```
>>> 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:

```
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
```

---

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!)

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

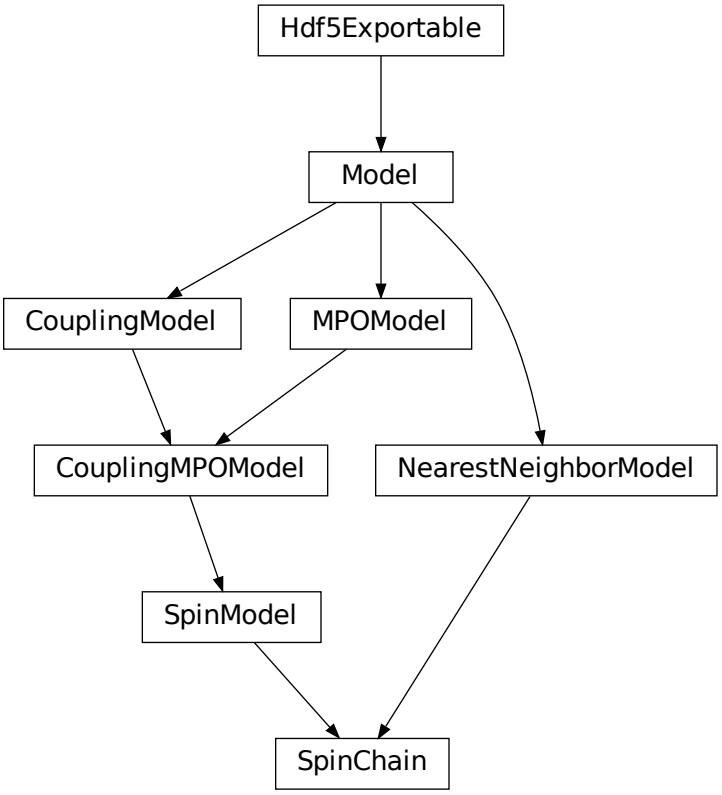
Prototypical example of a 1D quantum model: the spin-1/2 XXZ chain.

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.

7.9.5 spins

- full name: tenpy.models.spins
- parent module: *tenpy.models*
- type: module

Classes

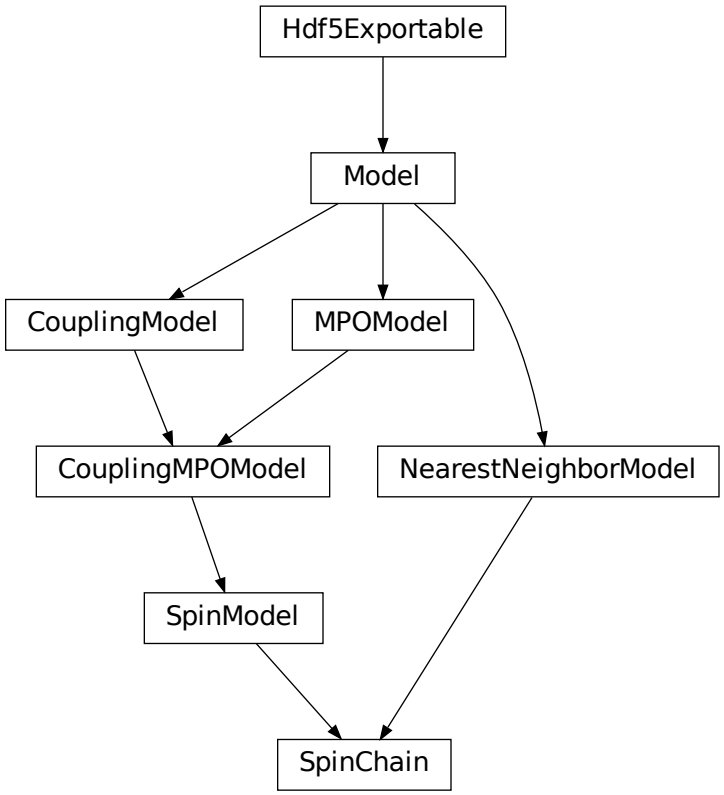


SpinChain(model_params)	The `SpinModel` on a Chain, suitable for TEBD.
`SpinModel`(model_params)	Spin-S sites coupled by nearest neighbour interactions.

SpinChain

- full name: tenpy.models.spins.SpinChain
- parent module: *tenpy.models.spins*
- type: class

Inheritance Diagram



Methods

`SpinChain.__init__`(model_params)	Initialize self.
SpinChain.add_coupling(strength, u1, op1, ...)	Add twosite coupling terms to the Hamiltonian, summing over lattice sites.
SpinChain.add_coupling_term(strength, i, j, ...)	Add a two-site coupling term on given MPS sites.
SpinChain.add_local_term(strength, term[, ...])	Add a single term to *self*.

continues on next page

Table 115 – continued from previous page

SpinChain.add_onsite(strength, u, opname[, ...])	Add onsite terms to onsite_terms.
SpinChain.add_onsite_term(strength, i, op[, ...])	Add an onsite term on a given MPS site.
SpinChain.all_coupling_terms()	Sum of all coupling_terms.
SpinChain.all_onsite_terms()	Sum of all onsite_terms.
SpinChain.bond_energies(psi)	Calculate bond energies <psi|H_bond|psi>.
SpinChain.calc_H_MPO([tol_zero])	Calculate MPO representation of the Hamiltonian.
SpinChain.calc_H_MPO_from_bond([tol_zero])	Calculate the MPO Hamiltonian from the bond Hamiltonian.
SpinChain.calc_H_bond([tol_zero])	calculate *H_bond* from coupling_terms and onsite_terms.
SpinChain.calc_H_bond_from_MPO([tol_zero])	Calculate the bond Hamiltonian from the MPO Hamiltonian.
SpinChain.calc_H_onsite([tol_zero])	Calculate *H_onsite* from *self.onsite_terms*.
SpinChain.coupling_strength_add_ext_flux()	Add an external flux to the coupling strength.
SpinChain.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
SpinChain.from_MPOModel(mpo_model)	Initialize a NearestNeighborModel from a model class defining an MPO.
SpinChain.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
SpinChain.group_sites([n, grouped_sites])	Modify *self* in place to group sites.
SpinChain.init_lattice(model_params)	Initialize a lattice for the given model parameters.
SpinChain.init_sites(model_params)	Define the local Hilbert space and operators; needs to be implemented in subclasses.
SpinChain.init_terms(model_params)	Add the onsite and coupling terms to the model; subclasses should implement this.
SpinChain.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
SpinChain.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.
SpinChain.trivial_like_NNModel()	Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

class tenpy.models.spins.**SpinChain**(*model_params*)

Bases: tenpy.models.spins.SpinModel, *tenpy.models.model.NearestNeighborModel*

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 twosite coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form $\sum_{x_0,\ldots,x_{dim-1}} strength[shift(\vec{x})] * OP0 * OP1$, where OP0 := lat.unit_cell[u0].get_op(op0) acts on the site (x_0, ..., x_{dim-1}, u1), and OP1 := lat.unit_cell[u1].get_op(op1) acts on the site (x_0+dx[0], ..., x_{dim-1}+dx[dim-1], u1). Possible combinations x_0, ..., 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:

```
>>> 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:

```
>>> self.add_coupling([1.5, 1.], 0, 'Sz', 0, 'Sz', dx)
```

Make sure to use the *plus_hc* argument if necessary, e.g. for hoppings:

```
>>> 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 explictly. 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

```
>>> t = 1.  # hopping strength
>>> 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:

```
>>> 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.␣
↪Cdagger_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.

MultiCouplingModel.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(...)`.

> **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.
- **j** (*i,*) – 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.
- **op2** (*op1,*) – 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_local_term(*strength*, *term*, *category=None*, *plus_hc=False*)

Add a single term to *self*.

The repesented 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 $\sum_{\vec{x}} strength[\vec{x}] * OP$ 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, ..., 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 <= 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 MPO graph (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 [Resta1997]. 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]` souch 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.

```
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0,
↪ phi])
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     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 convetion, 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:

```
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20})
parameter 'L'=20 for SpinChainNNN2
>>> 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.

```
>>> 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:

```
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
```

---

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.

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

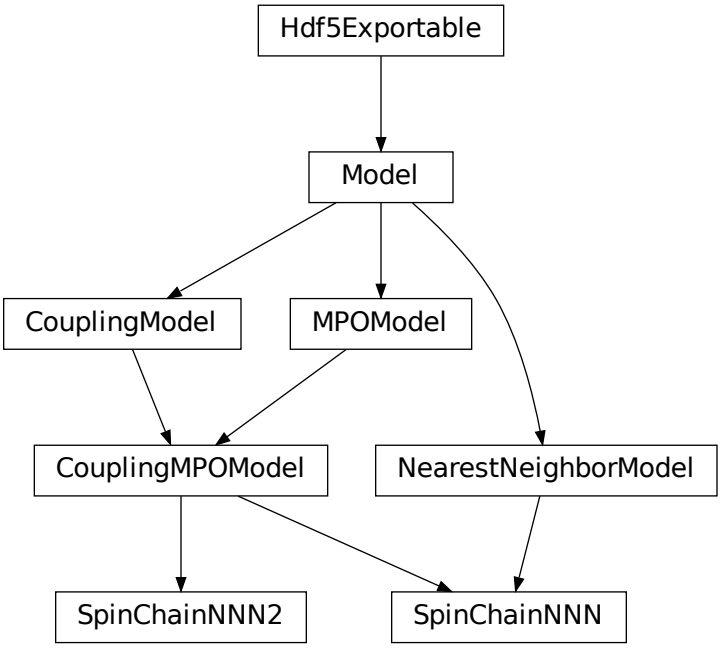
Nearest-neighbour spin-S models.

Uniform lattice of spin-S sites, coupled by nearest-neighbour interactions.

7.9.6 spins_nnn

- full name: tenpy.models.spins_nnn
- parent module: *tenpy.models*
- type: module

Classes



`SpinChainNNN`(model_params)	Spin-S sites coupled by (next-)nearest neighbour interactions on a *GroupedSite*.
`SpinChainNNN2`(model_params)	Spin-S sites coupled by next-nearest neighbour interactions.

Module description

Next-Nearest-neighbour spin-S models.

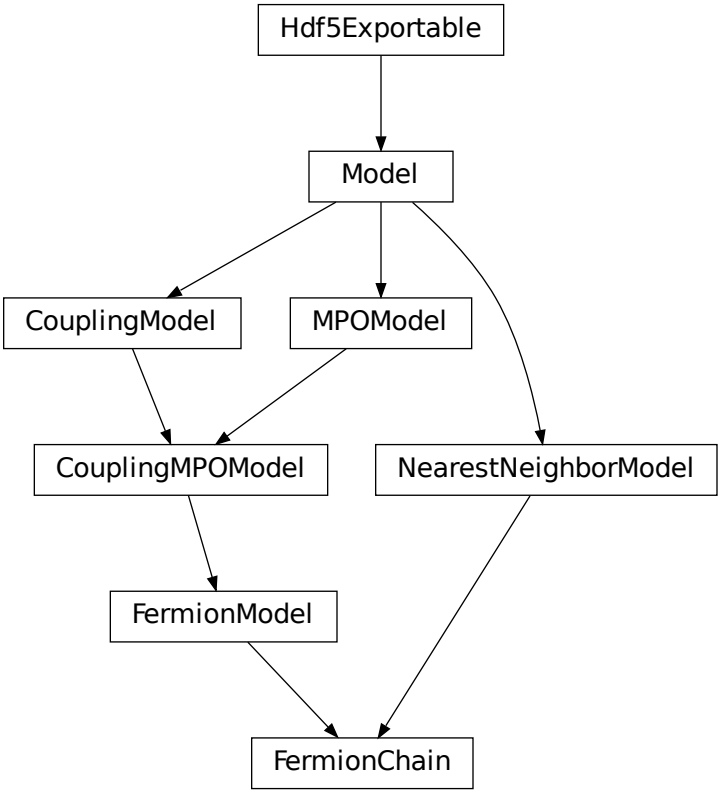
Uniform lattice of spin-S sites, coupled by next-nearest-neighbour interactions. We have two variants implementing the same hamiltonian. The `SpinChainNNN` uses the *`GroupedSite`* to keep it a *`NearestNeighborModel`* suitable for TEBD, while the `SpinChainNNN2` just involves longer-range couplings 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`.

7.9.7 fermions_spinless

- full name: tenpy.models.fermions_spinless
- parent module: *`tenpy.models`*
- type: module

Classes

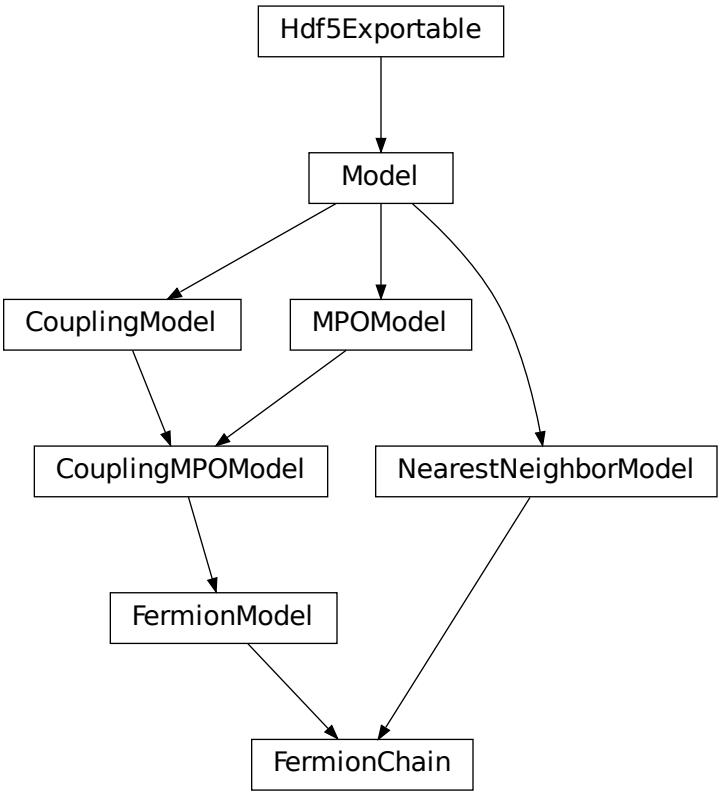


FermionChain(model_params)	The FermionModel on a Chain, suitable for TEBD.
FermionModel(model_params)	Spinless fermions with particle number conservation.

FermionChain

- full name: tenpy.models.fermions_spinless.FermionChain
- parent module: *tenpy.models.fermions_spinless*
- type: class

Inheritance Diagram



Methods

`FermionChain.__init__`(model_params)	Initialize self.
`FermionChain.add_coupling`(strength, u1, op1, ...)	Add twosite coupling terms to the Hamiltonian, summing over lattice sites.
`FermionChain.add_coupling_term`(strength, i, ...)	Add a two-site coupling term on given MPS sites.
`FermionChain.add_local_term`(strength, term)	Add a single term to *self*.
`FermionChain.add_onsite`(strength, u, opname)	Add onsite terms to `onsite_terms`.
`FermionChain.add_onsite_term`(strength, i, op)	Add an onsite term on a given MPS site.
`FermionChain.all_coupling_terms`()	Sum of all `coupling_terms`.
`FermionChain.all_onsite_terms`()	Sum of all `onsite_terms`.
`FermionChain.bond_energies`(psi)	Calculate bond energies <psi|H_bond|psi>.
`FermionChain.calc_H_MPO`([tol_zero])	Calculate MPO representation of the Hamiltonian.
`FermionChain.calc_H_MPO_from_bond`([tol_zero])	Calculate the MPO Hamiltonian from the bond Hamiltonian.
`FermionChain.calc_H_bond`([tol_zero])	calculate *H_bond* from `coupling_terms` and `onsite_terms`.
`FermionChain.calc_H_bond_from_MPO`([tol_zero])	Calculate the bond Hamiltonian from the MPO Hamiltonian.
`FermionChain.calc_H_onsite`([tol_zero])	Calculate *H_onsite* from *self.onsite_terms*.
`FermionChain.coupling_strength_add_ext_flux`(...)	Add an external flux to the coupling strength.
`FermionChain.enlarge_mps_unit_cell`([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
`FermionChain.from_MPOModel`(mpo_model)	Initialize a NearestNeighborModel from a model class defining an MPO.
`FermionChain.from_hdf5`(hdf5_loader, h5gr, ...)	Load instance from a HDF5 file.
`FermionChain.group_sites`([n, grouped_sites])	Modify *self* in place to group sites.
`FermionChain.init_lattice`(model_params)	Initialize a lattice for the given model parameters.
`FermionChain.init_sites`(model_params)	Define the local Hilbert space and operators; needs to be implemented in subclasses.
`FermionChain.init_terms`(model_params)	Add the onsite and coupling terms to the model; subclasses should implement this.
`FermionChain.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`FermionChain.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.
`FermionChain.trivial_like_NNModel`()	Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

class `tenpy.models.fermions_spinless.`**`FermionChain`**(*model_params*)

Bases: `tenpy.models.fermions_spinless.FermionModel`, *`tenpy.models.model.NearestNeighborModel`*

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 twosite coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form $\sum_{x_0,\ldots,x_{dim-1}} strength[shift(\vec{x})] * OP0 * OP1$, where `OP0 := lat.unit_cell[u0].get_op(op0)` acts on the site `(x_0, ..., x_{dim-1}, u1)`, and `OP1 := lat.unit_cell[u1].get_op(op1)` acts on the site `(x_0+dx[0], ..., x_{dim-1}+dx[dim-1], u1)`. Possible combinations `x_0, ..., 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:

```
>>> 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:

```
>>> self.add_coupling([1.5, 1.], 0, 'Sz', 0, 'Sz', dx)
```

Make sure to use the *plus_hc* argument if necessary, e.g. for hoppings:

```
>>> 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 explictly. 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

```
>>> t = 1.  # hopping strength
>>> 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:

```
>>> 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.␣
↪Cdagger_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.

MultiCouplingModel.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(...)`.

> **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.
- **j** (*i,*) – 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.
- **op2** (*op1,*) – 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_local_term(*strength*, *term*, *category=None*, *plus_hc=False*)

Add a single term to *self*.

The repesented 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 $\sum_{\vec{x}} strength[\vec{x}] * OP$ 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, ..., 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 <= 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 MPO graph (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 [Resta1997]. 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]` souch 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.

```
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0,
↪ phi])
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     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 convetion, 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:

```
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20})
parameter 'L'=20 for SpinChainNNN2
>>> 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.

```
>>> 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:

```
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
```

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.

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

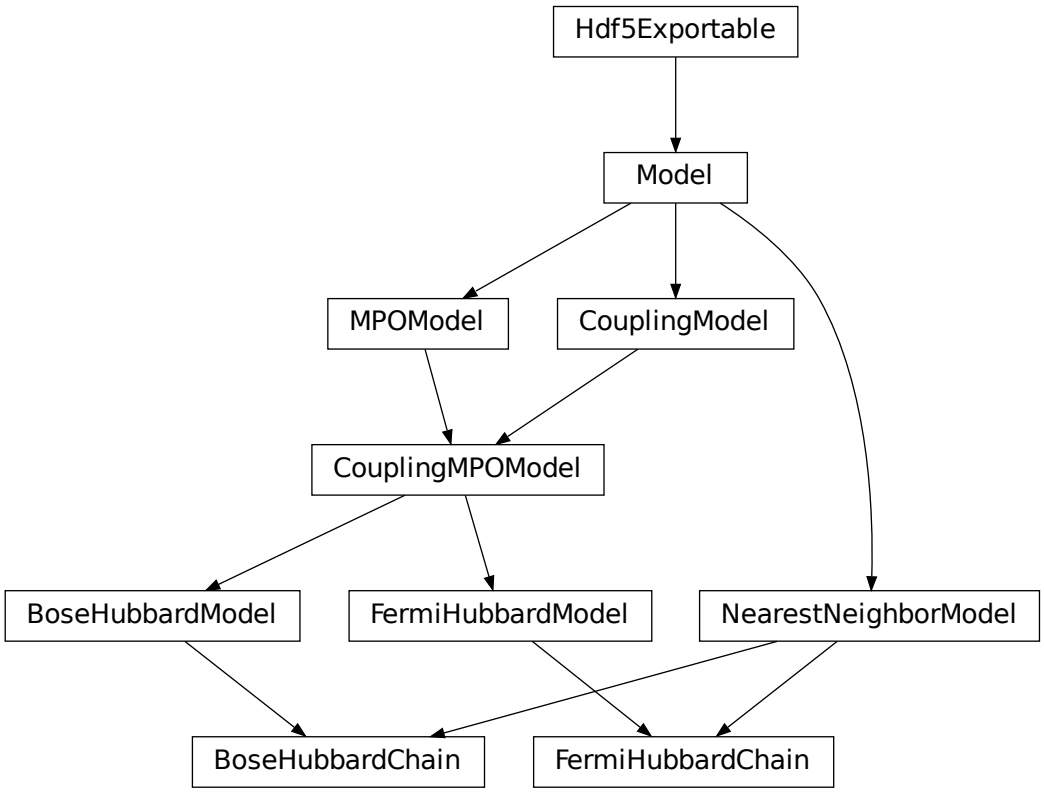
Spinless fermions with hopping and interaction.

Todo: add further terms (e.g. c^dagger c^dagger + h.c.) to the Hamiltonian.

7.9.8 hubbard

- full name: tenpy.models.hubbard
- parent module: *tenpy.models*
- type: module

Classes



BoseHubbardChain(model_params)	The `BoseHubbardModel` on a Chain, suitable for TEBD.

continues on next page

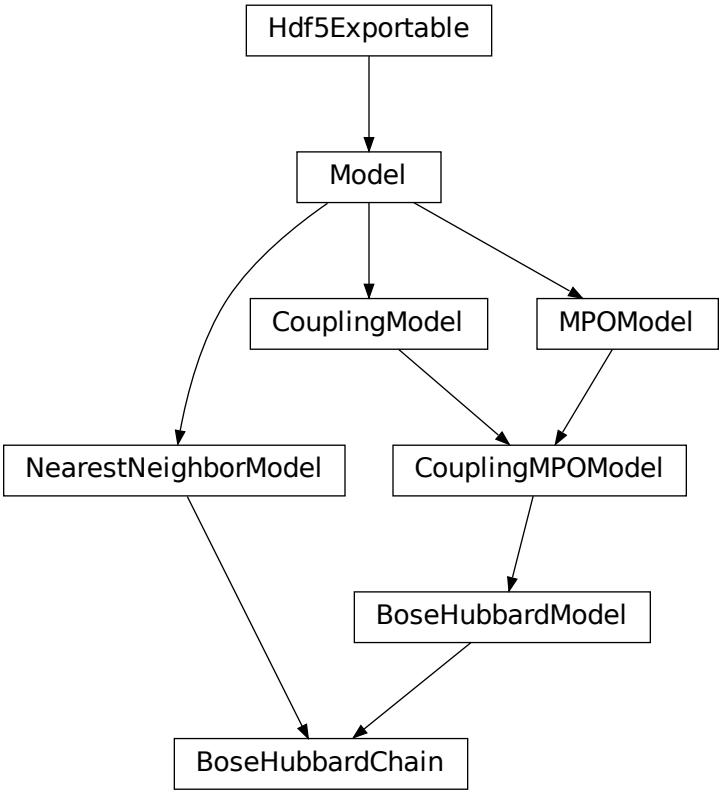
Table 119 – continued from previous page

`BoseHubbardModel`(model_params)	Spinless Bose-Hubbard model.
`FermiHubbardChain`(model_params)	The `FermiHubbardModel` on a Chain, suitable for TEBD.
`FermiHubbardModel`(model_params)	Spin-1/2 Fermi-Hubbard model.

BoseHubbardChain

- full name: tenpy.models.hubbard.BoseHubbardChain
- parent module: *`tenpy.models.hubbard`*
- type: class

Inheritance Diagram



Methods

BoseHubbardChain.__init__(model_params)	Initialize self.
BoseHubbardChain.add_coupling(strength, u1, ...)	Add twosite coupling terms to the Hamiltonian, summing over lattice sites.
BoseHubbardChain.add_coupling_term(strength, ...)	Add a two-site coupling term on given MPS sites.
BoseHubbardChain.add_local_term(strength, term)	Add a single term to *self*.
BoseHubbardChain.add_onsite(strength, u, opname)	Add onsite terms to onsite_terms.
BoseHubbardChain.add_onsite_term(strength, i, op)	Add an onsite term on a given MPS site.
BoseHubbardChain.all_coupling_terms()	Sum of all coupling_terms.
BoseHubbardChain.all_onsite_terms()	Sum of all onsite_terms.
BoseHubbardChain.bond_energies(psi)	Calculate bond energies <psi|H_bond|psi>.
BoseHubbardChain.calc_H_MPO([tol_zero])	Calculate MPO representation of the Hamiltonian.
BoseHubbardChain.calc_H_MPO_from_bond([tol_zero])	Calculate the MPO Hamiltonian from the bond Hamiltonian.
BoseHubbardChain.calc_H_bond([tol_zero])	calculate *H_bond* from coupling_terms and onsite_terms.
BoseHubbardChain.calc_H_bond_from_MPO([tol_zero])	Calculate the bond Hamiltonian from the MPO Hamiltonian.
BoseHubbardChain.calc_H_onsite([tol_zero])	Calculate *H_onsite* from *self.onsite_terms*.
BoseHubbardChain.coupling_strength_add_ext_flux(...)	Add an external flux to the coupling strength.
BoseHubbardChain.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
BoseHubbardChain.from_MPOModel(mpo_model)	Initialize a NearestNeighborModel from a model class defining an MPO.
BoseHubbardChain.from_hdf5(hdf5_loader, ...)	Load instance from a HDF5 file.
BoseHubbardChain.group_sites([n, grouped_sites])	Modify *self* in place to group sites.
BoseHubbardChain.init_lattice(model_params)	Initialize a lattice for the given model parameters.
BoseHubbardChain.init_sites(model_params)	Define the local Hilbert space and operators; needs to be implemented in subclasses.
BoseHubbardChain.init_terms(model_params)	Add the onsite and coupling terms to the model; subclasses should implement this.
BoseHubbardChain.save_hdf5(hdf5_saver, h5gr, ...)	Export *self* into a HDF5 file.
BoseHubbardChain.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.
BoseHubbardChain.trivial_like_NNModel()	Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

class tenpy.models.hubbard.**BoseHubbardChain**(*model_params*)

Bases: tenpy.models.hubbard.BoseHubbardModel, tenpy.models.model.NearestNeighborModel

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_hc=False*)

Add twosite coupling terms to the Hamiltonian, summing over lattice sites.

Represents couplings of the form $\sum_{x_0,\ldots,x_{dim-1}} strength[shift(\vec{x})] * OP0 * OP1$, where `OP0 := lat.unit_cell[u0].get_op(op0)` acts on the site `(x_0, ..., x_{dim-1}, u1)`, and `OP1 := lat.unit_cell[u1].get_op(op1)` acts on the site `(x_0+dx[0], ..., x_{dim-1}+dx[dim-1], u1)`. Possible combinations `x_0, ..., 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:

```
>>> 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:

```
>>> self.add_coupling([1.5, 1.], 0, 'Sz', 0, 'Sz', dx)
```

Make sure to use the *plus_hc* argument if necessary, e.g. for hoppings:

```
>>> 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 explictly. 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

```
>>> t = 1.  # hopping strength
>>> 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:

```
>>> 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.␣
↪Cdagger_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.

`MultiCouplingModel.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(...)`.

> **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.
- **j** (*i,*) – 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.
- **op2** (*op1,*) – 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_local_term(*strength*, *term*, *category=None*, *plus_hc=False*)

Add a single term to *self*.

The repesented 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 $\sum_{\vec{x}} strength[\vec{x}] * OP$ 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, ..., 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 <= 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 MPO graph (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 [Resta1997]. 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]` souch 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.

```
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0,
↪ phi])
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     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 convetion, 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:

```
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20})
parameter 'L'=20 for SpinChainNNN2
>>> 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.

```
>>> 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:

```
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
```

---

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.

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.

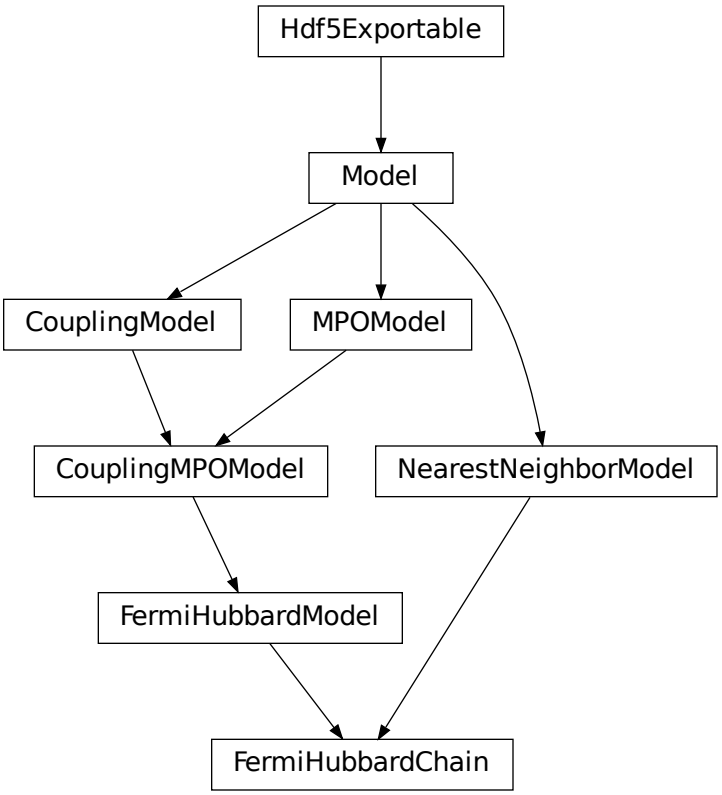
test_sanity()
Sanity check, raises ValueErrors, if something is wrong.

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

Inheritance Diagram



Methods

FermiHubbardChain.__init__(model_params)	Initialize self.
FermiHubbardChain.add_coupling(strength, u1, ...)	Add twosite coupling terms to the Hamiltonian, summing over lattice sites.
FermiHubbardChain.add_coupling_term(...[, ...])	Add a two-site coupling term on given MPS sites.
FermiHubbardChain.add_local_term(strength, term)	Add a single term to *self*.
FermiHubbardChain.add_onsite(strength, u, opname)	Add onsite terms to onsite_terms.
FermiHubbardChain.add_onsite_term(strength, ...)	Add an onsite term on a given MPS site.
FermiHubbardChain.all_coupling_terms()	Sum of all coupling_terms.
FermiHubbardChain.all_onsite_terms()	Sum of all onsite_terms.
FermiHubbardChain.bond_energies(psi)	Calculate bond energies <psi|H_bond|psi>.
FermiHubbardChain.calc_H_MPO([tol_zero])	Calculate MPO representation of the Hamiltonian.
FermiHubbardChain.calc_H_MPO_from_bond([...])	Calculate the MPO Hamiltonian from the bond Hamiltonian.
FermiHubbardChain.calc_H_bond([tol_zero])	calculate *H_bond* from coupling_terms and onsite_terms.
FermiHubbardChain.calc_H_bond_from_MPO([...])	Calculate the bond Hamiltonian from the MPO Hamiltonian.
FermiHubbardChain.calc_H_onsite([tol_zero])	Calculate *H_onsite* from *self.onsite_terms*.
FermiHubbardChain.coupling_strength_add_ext_flux(...)	Add an external flux to the coupling strength.
FermiHubbardChain.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
FermiHubbardChain.from_MPOModel(mpo_model)	Initialize a NearestNeighborModel from a model class defining an MPO.
FermiHubbardChain.from_hdf5(hdf5_loader, ...)	Load instance from a HDF5 file.
FermiHubbardChain.group_sites([n, grouped_sites])	Modify *self* in place to group sites.
FermiHubbardChain.init_lattice(model_params)	Initialize a lattice for the given model parameters.
FermiHubbardChain.init_sites(model_params)	Define the local Hilbert space and operators; needs to be implemented in subclasses.
FermiHubbardChain.init_terms(model_params)	Add the onsite and coupling terms to the model; subclasses should implement this.
FermiHubbardChain.save_hdf5(hdf5_saver, ...)	Export *self* into a HDF5 file.
FermiHubbardChain.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.
FermiHubbardChain.trivial_like_NNModel()	Return a NearestNeighborModel with same lattice, but trivial (H=0) bonds.

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*, *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 $\sum_{x_0,\ldots,x_{dim-1}} strength[shift(\vec{x})] * OP0 * OP1$, where `OP0 := lat.unit_cell[u0].get_op(op0)` acts on the site `(x_0, ..., x_{dim-1}, u1)`, and `OP1 := lat.unit_cell[u1].get_op(op1)` acts on the site `(x_0+dx[0], ..., x_{dim-1}+dx[dim-1], u1)`. Possible combinations `x_0, ..., 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:

```
>>> 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:

```
>>> self.add_coupling([1.5, 1.], 0, 'Sz', 0, 'Sz', dx)
```

Make sure to use the *plus_hc* argument if necessary, e.g. for hoppings:

```
>>> 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 explictly. 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

```
>>> t = 1.  # hopping strength
>>> 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:

```
>>> 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.␣
↪Cdagger_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.

MultiCouplingModel.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(...)`.

> **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.
- **j** (*i,*) – 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.
- **op2** (*op1,*) – 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_local_term(*strength*, *term*, *category=None*, *plus_hc=False*)

Add a single term to *self*.

The repesented 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 $\sum_{\vec{x}} strength[\vec{x}] * OP$ 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, ..., 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 <= 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 MPO graph (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 [Resta1997]. 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]` souch 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.

```
>>> strength = 1. # hopping strength without external flux
>>> phi = np.pi/4 # determines the external flux strength
>>> strength_with_flux = self.coupling_strength_add_ext_flux(strength, dx, [0,
↪ phi])
>>> for u1, u2, dx in self.lat.pairs['nearest_neighbors']:
...     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 convetion, 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:

```
>>> from tenpy.models.spins_nnn import SpinChainNNN2
>>> nnn_chain = SpinChainNNN2({'L': 20})
parameter 'L'=20 for SpinChainNNN2
>>> 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.

```
>>> 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:

```
>>> nnn_chain_for_tebd = NearestNeighborModel.from_MPOModel(nnn_chain)
```

---

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.

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.

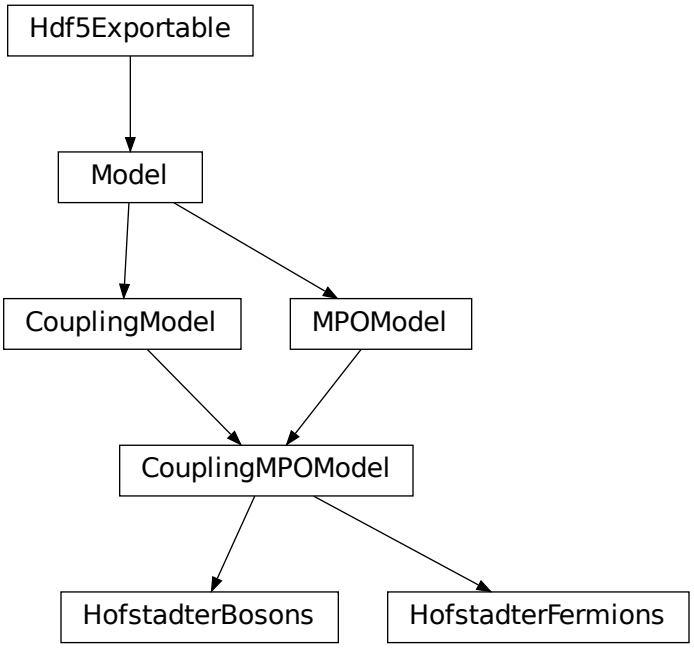
Module description

Bosonic and fermionic Hubbard models.

7.9.9 hofstadter

- full name: tenpy.models.hofstadter
- parent module: *tenpy.models*
- type: module

Classes



`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 :math`(mathtt{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 :math`(1, mathtt{my})`. For flux densities :math`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 axactly 3 flux quanta.
- 'symmetric': symmetric gauge. The magnetic unit cell will have shape $(\mathtt{mx}, \mathtt{my})$, 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.
- **my** (*mx,*) – Dimensions of the magnetic unit cell in terms of lattice sites. `None` defaults to the minimal choice compatible with *gauge* and *phi_pq*.
- **Jy** (*Jx,*) – 'Bare' hopping amplitudes (without phase). Without any flux we have `hop_x = -Jx` and `hop_y = -Jy`.
- **phi_pq** (*tuple (int, int)*) – Magnetic flux as a fraction p/q, defined as (p, q)

Returns **hop_x, hop_y** – Hopping amplitudes to be used as prefactors for $c^\dagger_{x,y} c_{x+1,y}$ (*hop_x*) and $c^\dagger_{x,y} c_{x,y+1}$ (*hop_x*), respectively, with the necessary phases for the gauge.

Return type float | array

Module description

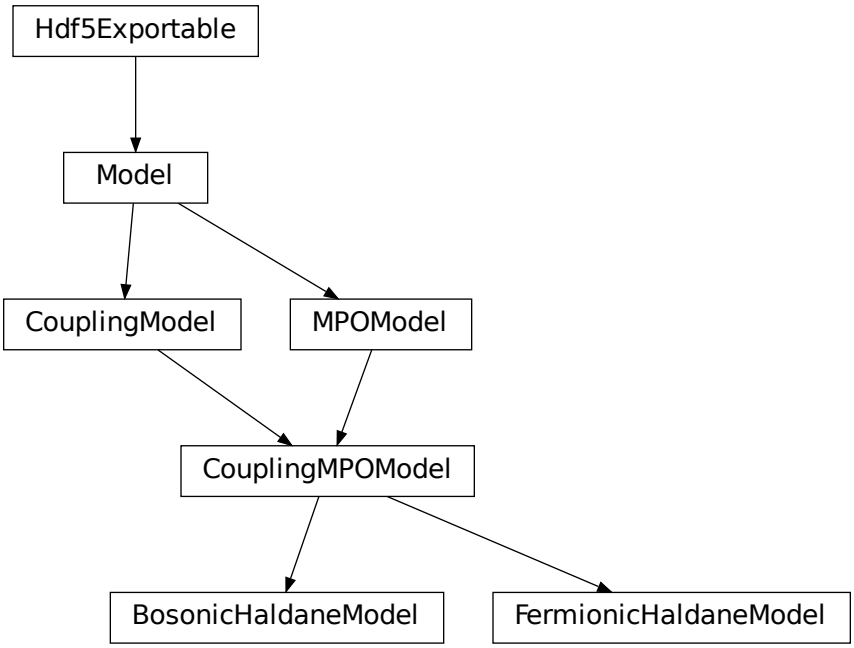
Cold atomic (Harper-)Hofstadter model on a strip or cylinder.

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.

7.9.10 haldane

- full name: tenpy.models.haldane
- parent module: *tenpy.models*
- type: module

Classes



`BosonicHaldaneModel`(model_params)	Hardcore bosonic Haldane model.
`FermionicHaldaneModel`(model_params)	Spinless fermionic Haldane model.

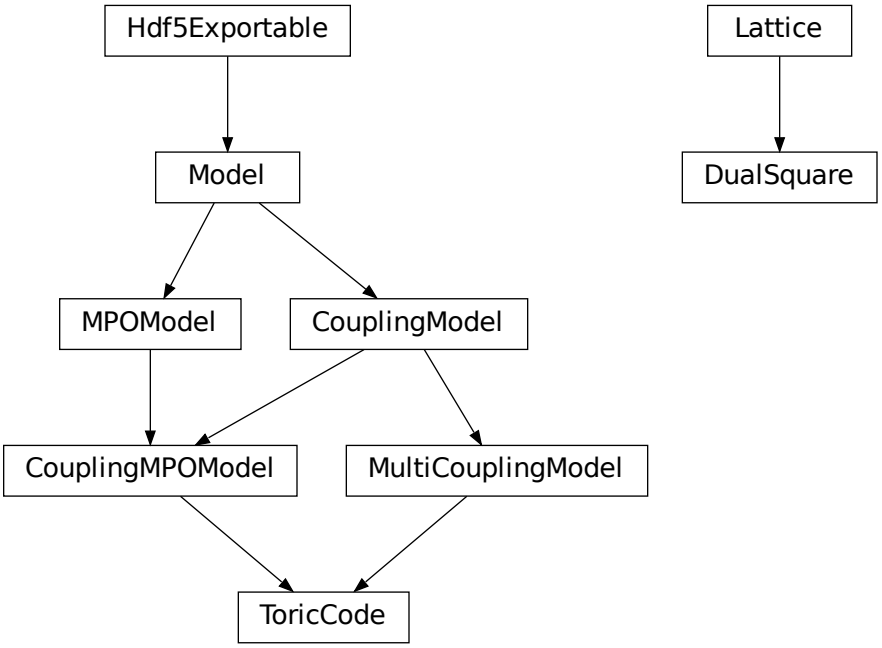
Module description

Bosonic and fermionic Haldane models.

7.9.11 toric_code

- full name: tenpy.models.toric_code
- parent module: *tenpy.models*
- type: module

Classes

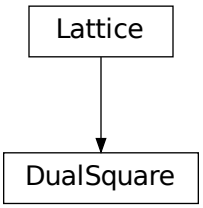


DualSquare(Lx, Ly, sites, **kwargs)	The dual lattice of the square lattice (again square).
ToricCode(model_params)	Toric code model.

DualSquare

- full name: tenpy.models.toric_code.DualSquare
- parent module: *tenpy.models.toric_code*
- type: class

Inheritance Diagram



Methods

`DualSquare.__init__`(Lx, Ly, sites, **kwargs)	Initialize self.
DualSquare.count_neighbors([u, key])	Count e.g.
DualSquare.coupling_shape(dx)	Calculate correct shape of the *strengths* for a coupling.
DualSquare.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
DualSquare.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
DualSquare.lat2mps_idx(lat_idx)	Translate lattice indices `(x_0, ..., x_{D-1}, u)` to MPS index *i*.
DualSquare.mps2lat_idx(i)	Translate MPS index *i* to lattice indices `(x_0, ..., x_{dim-1}, u)`.
DualSquare.mps2lat_values(A[, axes, u])	Reshape/reorder *A* to replace an MPS index by lattice indices.
DualSquare.mps2lat_values_masked(A[, axes, ...])	Reshape/reorder an array *A* to replace an MPS index by lattice indices.
DualSquare.mps_idx_fix_u([u])	return an index array of MPS indices for which the site within the unit cell is *u*.
DualSquare.mps_lat_idx_fix_u([u])	Similar as `mps_idx_fix_u()`, but return also the corresponding lattice indices.
DualSquare.mps_sites()	Return a list of sites for all MPS indices.
DualSquare.multi_coupling_shape(dx)	Calculate correct shape of the *strengths* for a multi_coupling.
DualSquare.number_nearest_neighbors([u])	Deprecated.
DualSquare.number_next_nearest_neighbors([u])	Deprecated.
DualSquare.ordering(order)	Provide possible orderings of the *N* lattice sites.

continues on next page

Table 126 – continued from previous page

DualSquare.plot_basis(ax, **kwargs)	Plot arrows indicating the basis vectors of the lattice.
DualSquare.plot_bc_identified(ax[, ...])	Mark two sites indified by periodic boundary conditions.
DualSquare.plot_coupling(ax[, coupling])	Plot lines connecting nearest neighbors of the lattice.
DualSquare.plot_order(ax[, order, textkwargs])	Plot a line connecting sites in the specified "order" and text labels enumerating them.
DualSquare.plot_sites(ax[, markers])	Plot the sites of the lattice with markers.
DualSquare.position(lat_idx)	return 'space' position of one or multiple sites.
DualSquare.possible_couplings(u1, u2, dx)	Find possible MPS indices for two-site couplings.
DualSquare.possible_multi_couplings(ops)	Generalization of `possible_couplings()` to couplings with more than 2 sites.
DualSquare.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
DualSquare.site(i)	return *Site* instance corresponding to an MPS index *i*
DualSquare.test_sanity()	Sanity check.

Class Attributes and Properties

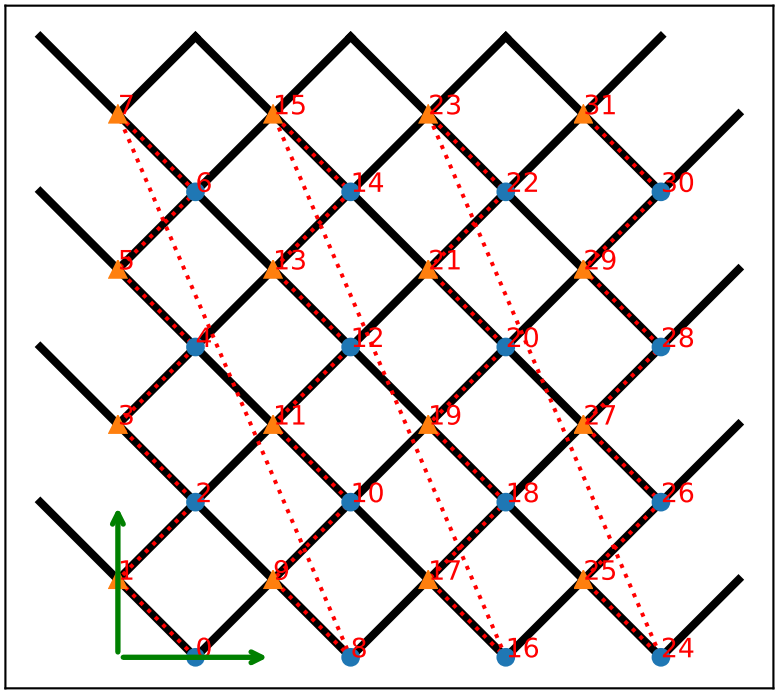
DualSquare.boundary_conditions	Human-readable list of boundary conditions from `bc` and `bc_shift`.
DualSquare.dim	The dimension of the lattice.
`DualSquare.nearest_neighbors`	
`DualSquare.next_nearest_neighbors`	
`DualSquare.next_next_nearest_neighbors`	
DualSquare.order	Defines an ordering of the lattice sites, thus mapping the lattice to a 1D chain.

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

- **Ly** (*Lx,*) – 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 convetion, 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 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, ..., 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* accross 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 verions 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 expection 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:

```
>>> print(lat.shape, A.shape)
(10, 3, 2) (60,)
>>> A_res = lat.mps2lat_values(A)
>>> A_res.shape
(10, 3, 2)
>>> A_res[lat.mps2lat_idx(5)] == A[5]
True
```

If you have a correlation function `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 `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.

```
>>> 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
```

Todo: make sure this function is used for expectation values...

---

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

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.MultiCouplingModel.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*, ***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 specifying the "arrowprops" of ax.annotate.

plot_bc_identified(*ax*, *direction=- 1*, *shift=None*, ***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 idenitified sites. If `None`, mark it along all directions with periodic boundary conditions.
- **shift** (*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*, ***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, ..., u1)` to the site `(i0+dx[0], i1+dx[1], ..., u2)`, taking into account the boundary conditions.
- ****kwargs** – Further keyword arguments given to `ax.plot()`.

plot_order(*ax*, *order=None*, *textkwargs={}*, ***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 keywork *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

- **u2** (*u1,*) – 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 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*) – 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.

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…

7.10 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 (parital) contraction of tensors. For example an MPS represents the contraction along the 'virtual' legs/bonds of its B.

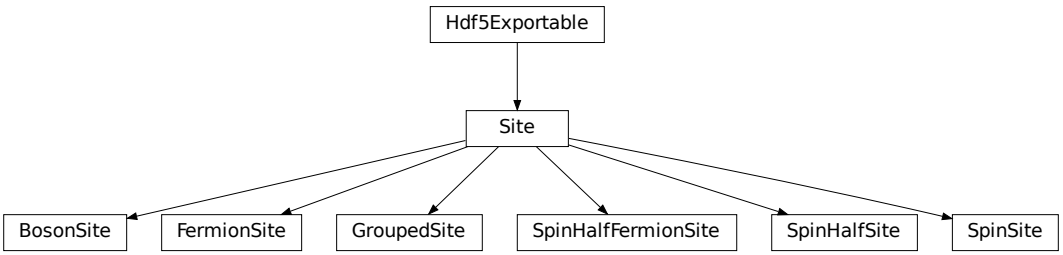
Submodules

site	Defines a class describing the local physical Hilbert space.
mps	This module contains a base class for a Matrix Product State (MPS).
mpo	Matrix product operator (MPO).
terms	Classes to store a collection of operator names and sites they act on, together with prefactors.
purification_mps	This module contains an MPS class representing an density matrix by purification.

7.10.1 site

- full name: tenpy.networks.site
- parent module: *tenpy.networks*
- type: module

Classes

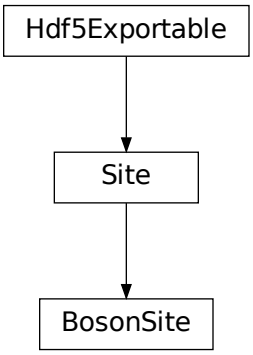


`BosonSite`([Nmax, conserve, filling])	Create a `Site` for up to *Nmax* bosons.
`FermionSite`([conserve, filling])	Create a `Site` for spin-less fermions.
`GroupedSite`(sites[, labels, charges])	Group two or more `Site` into a larger one.
`Site`(leg[, state_labels])	Collects necessary information about 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



Methods

`BosonSite.__init__`([Nmax, conserve, filling])	Initialize self.
`BosonSite.add_op`(name, op[, need_JW, hc])	Add one on-site operators.
`BosonSite.change_charge`([new_leg_charge, ...])	Change the charges of the site (in place).
`BosonSite.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
`BosonSite.get_hc_op_name`(name)	Return the hermitian conjugate of a given operator.
`BosonSite.get_op`(name)	Return operator of given name.
`BosonSite.multiply_op_names`(names)	Multiply operator names together.
`BosonSite.op_needs_JW`(name)	Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.
`BosonSite.remove_op`(name)	Remove an added operator.
`BosonSite.rename_op`(old_name, new_name)	Rename an added operator.
`BosonSite.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`BosonSite.state_index`(label)	Return index of a basis state from its label.
`BosonSite.state_indices`(labels)	Same as `state_index()`, but for multiple labels.
`BosonSite.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.
`BosonSite.valid_opname`(name)	Check whether 'name' labels a valid onsite-operator.

Class Attributes and Properties

`BosonSite.dim`	Dimension of the local Hilbert space.
`BosonSite.onsite_ops`	Dictionary of on-site operators for iteration.

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, ...`.)

operator	description
`Id, JW`	Identity $\mathbb{1}$
`B`	Annihilation operator b
`Bd`	Creation operator $b^\dagger$
`N`	Number operator $n = b^\dagger b$
`NN`	n^2
`dN`	$\delta n := n - filling$
`dNdN`	$(\delta n)^2$
`P`	Parity $Id - 2(n \mod 2)$.

conserve	qmod	*excluded* onsite operators
`'N'`	[1]	–
`'parity'`	[2]	–
`None`	[]	–

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

`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 permuation 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

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*) – eather 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.

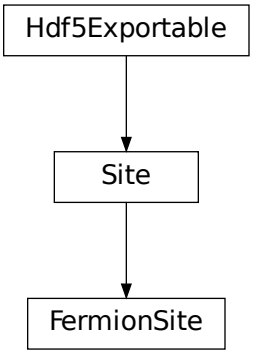
Returns **valid** – `True` if *name* is a valid argument to *get_op()*.

Return type bool

FermionSite

- full name: tenpy.networks.site.FermionSite
- parent module: *tenpy.networks.site*
- type: class

Inheritance Diagram



Methods

FermionSite.__init__([conserve, filling])	Initialize self.
FermionSite.add_op(name, op[, need_JW, hc])	Add one on-site operators.
FermionSite.change_charge([new_leg_charge, ...])	Change the charges of the site (in place).
FermionSite.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
FermionSite.get_hc_op_name(name)	Return the hermitian conjugate of a given operator.
FermionSite.get_op(name)	Return operator of given name.
FermionSite.multiply_op_names(names)	Multiply operator names together.

continues on next page

Table 132 – continued from previous page

`FermionSite.op_needs_JW`(name)	Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.
`FermionSite.remove_op`(name)	Remove an added operator.
`FermionSite.rename_op`(old_name, new_name)	Rename an added operator.
`FermionSite.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`FermionSite.state_index`(label)	Return index of a basis state from its label.
`FermionSite.state_indices`(labels)	Same as `state_index()`, but for multiple labels.
`FermionSite.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.
`FermionSite.valid_opname`(name)	Check whether 'name' labels a valid onsite-operator.

Class Attributes and Properties

`FermionSite.dim`	Dimension of the local Hilbert space.
`FermionSite.onsite_ops`	Dictionary of on-site operators for iteration.

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*.

operator	description
`Id`	Identity $\mathbb{1}$
`JW`	Sign for the Jordan-Wigner string.
`C`	Annihilation operator c (up to 'JW'-string left of it)
`Cd`	Creation operator $c^\dagger$ (up to 'JW'-string left of it)
`N`	Number operator $n = c^\dagger c$
`dN`	$\delta n := n - filling$
`dNdN`	$(\delta n)^2$

conserve	qmod	*exluded* onsite operators
`'N'`	[1]	–
`'parity'`	[2]	–
`None`	[]	–

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 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 permuation 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

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*) – eather 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.

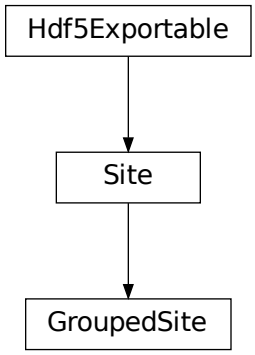
Returns **valid** – `True` if *name* is a valid argument to *get_op()*.

Return type bool

GroupedSite

- full name: tenpy.networks.site.GroupedSite
- parent module: *tenpy.networks.site*
- type: class

Inheritance Diagram



Methods

`GroupedSite.__init__`(sites[, labels, charges])	Initialize self.
`GroupedSite.add_op`(name, op[, need_JW, hc])	Add one on-site operators.
`GroupedSite.change_charge`([new_leg_charge, ...])	Change the charges of the site (in place).
`GroupedSite.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
`GroupedSite.get_hc_op_name`(name)	Return the hermitian conjugate of a given operator.
`GroupedSite.get_op`(name)	Return operator of given name.
`GroupedSite.kroneckerproduct`(ops)	Return the Kronecker product $op0 \otimes op1$ of local operators.
`GroupedSite.multiply_op_names`(names)	Multiply operator names together.
`GroupedSite.op_needs_JW`(name)	Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.
`GroupedSite.remove_op`(name)	Remove an added operator.
`GroupedSite.rename_op`(old_name, new_name)	Rename an added operator.
`GroupedSite.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`GroupedSite.state_index`(label)	Return index of a basis state from its label.
`GroupedSite.state_indices`(labels)	Same as `state_index()`, but for multiple labels.
`GroupedSite.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.
`GroupedSite.valid_opname`(name)	Check whether 'name' labels a valid onsite-operator.

Class Attributes and Properties

`GroupedSite.dim`	Dimension of the local Hilbert space.
`GroupedSite.onsite_ops`	Dictionary of on-site operators for iteration.

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 onsite oerators 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.

n_sites

The number of sites grouped together, i.e. len(sites).

Type int

sites

The sites grouped together into self.

Type list of *Site*

labels

The labels using which the single-site operators are added during construction.

Type list of str

kroneckerproduct(*ops*)

Return the Kronecker product $op0 \otimes op1$ 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 $ops[0] \otimes ops[1] \otimes \cdots$, 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 permuation applied to the physical leg, which gets used to adjust state_labels and perm. If you sorted the previ-

ous 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

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*) – eather 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.

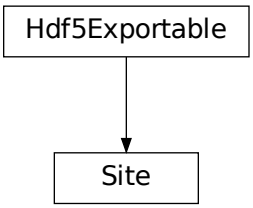
Returns **valid** – `True` if *name* is a valid argument to *get_op()*.

Return type bool

Site

- full name: tenpy.networks.site.Site
- parent module: *tenpy.networks.site*
- type: class

Inheritance Diagram



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.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.

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` is the Sz operator for the `SpinSite`. Alternatively, operators can be obained with `get_op()`. The operator names `Id` and `JW` are reserved for the identy 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 `state_labels` and `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=op` given to `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 `LegCharge`

`state_labels`

(Optional) labels for the local basis states.

Type {str: int}

`opnames`

Labels of all onsite operators (i.e. `self.op` exists if `'op'` in `self.opnames`). Note that `get_op()` allows arbitrary concatenations of them.

Type set

`need_JW_string`

Labels of all onsite operators that need a Jordan-Wigner string. Used in `op_needs_JW()` to determine whether an operator anticommutes or commutes with operators on other sites.

Type 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 S_z operator. All onsite operators have labels `'p', 'p*'`.

Type `Array`

perm
Index permutation of the physical leg compared to *conserve=None*, i.e. `OP_conserved = OP_nonconserved[np.ix_(perm, perm)]` and `perm[state_labels_conserved["some_state"]] == state_labels_nonconserved["some_state"]`.

Type 1D array

JW_exponent
Exponents of the `'JW'` operator, such that `self.JW.to_ndarray() = np.diag(np.exp(1.j*np.pi* JW_exponent))`

Type 1D array

hc_ops
Mapping from operator names to their hermitian conjugates. Use *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 `Sx = (Sp + Sm)/2` violates Sz conservation and is thus not a valid on-site operator.

```
>>> chinfo = npc.ChargeInfo([1], ['Sz'])
>>> ch = npc.LegCharge.from_qflat(chinfo, [1, -1])
>>> Sp = [[0, 1.], [0, 0]]
>>> Sm = [[0, 0], [1., 0]]
>>> Sz = [[0.5, 0], [0, -0.5]]
>>> site = Site(ch, ['up', 'down'], Splus=Sp, Sminus=Sm, Sz=Sz)
>>> print(site.Splus.to_ndarray())
array([[ 0.,  1.],
       [ 0.,  0.]])
>>> print(site.get_op('Sminus').to_ndarray())
array([[ 0.,  0.],
       [ 1.,  0.]])
>>> print(site.get_op('Splus Sminus').to_ndarray())
array([[ 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 permuation 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*'`.
- **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 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 an added operator.

Parameters **name** (*str*) – The name of the operator to be removed.

state_index(*label*)
Return index of a basis state from its label.

Parameters **label** (*int | string*) – eather 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.

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*)
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*)

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

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

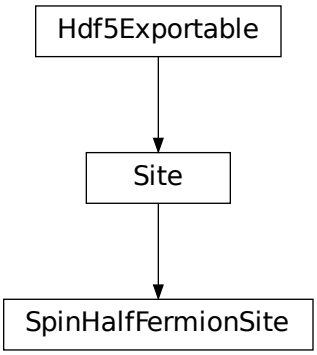
- **hdf5_saver** (*Hdf5Saver*) – Instance of the saving engine.

- **h5gr** (*:class`Group`*) – HDF5 group which is supposed to represent *self*.
- **subpath** (*str*) – The *name* of *h5gr* with a '/' in the end.

SpinHalfFermionSite

- full name: tenpy.networks.site.SpinHalfFermionSite
- parent module: *tenpy.networks.site*
- type: class

Inheritance Diagram



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.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.

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Table 138 – continued from previous page

`SpinHalfFermionSite.rename_op`(old_name, new_name)	Rename an added operator.
`SpinHalfFermionSite.save_hdf5`(hdf5_saver, ...)	Export *self* into a HDF5 file.
`SpinHalfFermionSite.state_index`(label)	Return index of a basis state from its label.
`SpinHalfFermionSite.state_indices`(labels)	Same as `state_index()`, but for multiple labels.
`SpinHalfFermionSite.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.
`SpinHalfFermionSite.valid_opname`(name)	Check whether 'name' labels a valid onsite-operator.

Class Attributes and Properties

`SpinHalfFermionSite.dim`	Dimension of the local Hilbert space.
`SpinHalfFermionSite.onsite_ops`	Dictionary of on-site operators for iteration.

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!

operator	description
`Id`	Identity $\mathbb{1}$
`JW`	Sign for the Jordan-Wigner string $(-1)^{n_\uparrow + n_\downarrow}$
`JWu`	Partial sign for the Jordan-Wigner string $(-1)^{n_\uparrow}$
`JWd`	Partial sign for the Jordan-Wigner string $(-1)^{n_\downarrow}$
`Cu`	Annihilation operator spin-up $c_\uparrow$ (up to 'JW'-string on sites left of it).
`Cdu`	Creation operator spin-up $c_\uparrow^\dagger$ (up to 'JW'-string on sites left of it).
`Cd`	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`.
`Cdd`	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`.
`Nu`	Number operator $n_\uparrow = c_\uparrow^\dagger c_\uparrow$
`Nd`	Number operator $n_\downarrow = c_\downarrow^\dagger c_\downarrow$
`NuNd`	Dotted number operators $n_\uparrow n_\downarrow$
`Ntot`	Total number operator $n_t = n_\uparrow + n_\downarrow$
`dN`	Total number operator compared to the filling $\Delta n = n_t - filling$
`Sx, Sy, Sz`	Spin operators $S^{x,y,z}$, in particular $S^z = \frac{1}{2}(n_\uparrow - n_\downarrow)$
`Sp, Sm`	Spin flips $S^\pm = S^x \pm iS^y$, e.g. $S^+ = c_\uparrow^\dagger c_\downarrow$

The spin operators are defined as $S^\gamma = (c_\uparrow^\dagger, c_\downarrow^\dagger)\sigma^\gamma(c_\uparrow, c_\downarrow)^T$, where σ^γ are spin-1/2 matrices (i.e. half the pauli matrices).

cons_N	*cons_Sz*	qmod	*excluded* onsite operators
`'N'`	`'Sz'`	[1, 1]	`Sx, Sy`
`'N'`	`'parity'`	[1, 2]	–
`'N'`	`None`	[1]	–
`'parity'`	`'Sz'`	[2, 1]	`Sx, Sy`
`'parity'`	`'parity'`	[2, 2]	–
`'parity'`	`None`	[2]	–
`None`	`'Sz'`	[1]	`Sx, Sy`
`None`	`'parity'`	[2]	–
`None`	`None`	[]	–

Todo: Check if Jordan-Wigner strings for 4x4 operators are correct.

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 `[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 permuation 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

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*) – eather 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.

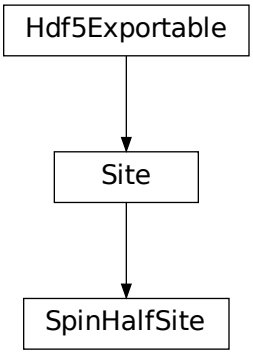
Returns **valid** – `True` if *name* is a valid argument to *get_op()*.

Return type bool

SpinHalfSite

- full name: tenpy.networks.site.SpinHalfSite
- parent module: *tenpy.networks.site*
- type: class

Inheritance Diagram



Methods

`SpinHalfSite.__init__`([conserve])	Initialize self.
SpinHalfSite.add_op(name, op[, need_JW, hc])	Add one on-site operators.
SpinHalfSite.change_charge([new_leg_charge, ...])	Change the charges of the site (in place).
SpinHalfSite.from_hdf5(hdf5_loader, h5gr, ...)	Load instance from a HDF5 file.
SpinHalfSite.get_hc_op_name(name)	Return the hermitian conjugate of a given operator.
SpinHalfSite.get_op(name)	Return operator of given name.
SpinHalfSite.multiply_op_names(names)	Multiply operator names together.
SpinHalfSite.op_needs_JW(name)	Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.
SpinHalfSite.remove_op(name)	Remove an added operator.
SpinHalfSite.rename_op(old_name, new_name)	Rename an added operator.
SpinHalfSite.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
SpinHalfSite.state_index(label)	Return index of a basis state from its label.
SpinHalfSite.state_indices(labels)	Same as `state_index()`, but for multiple labels.

continues on next page

Table 140 – continued from previous page

`SpinHalfSite.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.
`SpinHalfSite.valid_opname`(name)	Check whether 'name' labels a valid onsite-operator.

Class Attributes and Properties

`SpinHalfSite.dim`	Dimension of the local Hilbert space.
`SpinHalfSite.onsite_ops`	Dictionary of on-site operators for iteration.

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. `Sz = [[0.5, 0.], [0., -0.5]]`, `Sx = 0.5*sigma_x` for the Pauli matrix *sigma_x*.

operator	description
`Id, JW`	Identity $\mathbb{1}$
`Sx, Sy, Sz`	Spin components $S^{x,y,z}$, equal to half the Pauli matrices.
`Sigmax, Sigmay, Sigmaz`	Pauli matrices $\sigma^{x,y,z}$
`Sp, Sm`	Spin flips $S^{\pm} = S^x \pm iS^y$

conserve	qmod	*excluded* onsite operators
`'Sz'`	[1]	`Sx, Sy, Sigmax, Sigmay`
`'parity'`	[2]	–
`None`	[]	–

Parameters **`conserve`** (`str`) – Defines what is conserved, see table above.

`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 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 permuation 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

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*) – eather 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.

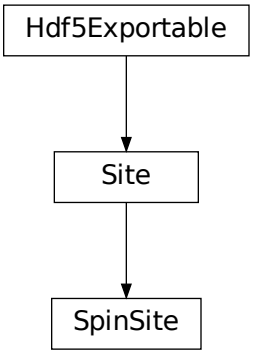
Returns **valid** – `True` if *name* is a valid argument to *get_op()*.

Return type bool

SpinSite

- full name: tenpy.networks.site.SpinSite
- parent module: *tenpy.networks.site*
- type: class

Inheritance Diagram



Methods

`SpinSite.__init__`([S, conserve])	Initialize self.
SpinSite.add_op(name, op[, need_JW, hc])	Add one on-site operators.
SpinSite.change_charge([new_leg_charge, permute])	Change the charges of the site (in place).
SpinSite.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
SpinSite.get_hc_op_name(name)	Return the hermitian conjugate of a given operator.
SpinSite.get_op(name)	Return operator of given name.
SpinSite.multiply_op_names(names)	Multiply operator names together.
SpinSite.op_needs_JW(name)	Whether an (composite) onsite operator is fermionic and needs a Jordan-Wigner string.
SpinSite.remove_op(name)	Remove an added operator.
SpinSite.rename_op(old_name, new_name)	Rename an added operator.
SpinSite.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
SpinSite.state_index(label)	Return index of a basis state from its label.
SpinSite.state_indices(labels)	Same as `state_index()`, but for multiple labels.
SpinSite.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.
SpinSite.valid_opname(name)	Check whether 'name' labels a valid onsite-operator.

Class Attributes and Properties

`SpinSite.dim`	Dimension of the local Hilbert space.
`SpinSite.onsite_ops`	Dictionary of on-site operators for iteration.

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. `Sz = [[0.5, 0.], [0., -0.5]]`, `Sx = 0.5*sigma_x` for the Pauli matrix *sigma_x*.

operator	description
`Id, JW`	Identity $\mathbb{1}$
`Sx, Sy, Sz`	Spin components $S^{x,y,z}$, equal to half the Pauli matrices.
`Sp, Sm`	Spin flips $S^{\pm} = S^x \pm iS^y$

conserve	qmod	*excluded* onsite operators
`'Sz'`	[1]	`Sx, Sy`
`'parity'`	[2]	–
`None`	[]	–

Parameters **`conserve`** (`str`) – Defines what is conserved, see table above.

`S`

The 2S+1 states range from m = -S, -S+1, … +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 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 permuation 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

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*) – eather 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

group_sites(sites[, n, labels, charges])	Given a list of sites, group each *n* sites together.
multi_sites_combine_charges(sites[, ...])	Adjust the charges of the given sites (in place) such that they can be used together.

group_sites

- full name: tenpy.networks.site.group_sites
- parent module: *tenpy.networks.site*
- type: function

`tenpy.networks.site.`**`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*.
- **charges** (*labels,*) – 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

`tenpy.networks.site.`**`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.

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

```
>>> 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 [[-1]
1  [ 1]]
2
>>> multi_sites_combine_charges([ferm, spin], same_charges=[[(0, 'Sz'), (1, 0)]])
[array([0, 1, 2, 3]), array([0, 1])]
>>> # no permutations where needed
>>> ferm.leg.chinfo is spin.leg.chinfo
True
>> ferm.leg.chinfo.names
['N', 'Sz']
>>> print(spin.leg)
+1
0 [[ 0 -1]
1  [ 0  1]]
2
```

Module description

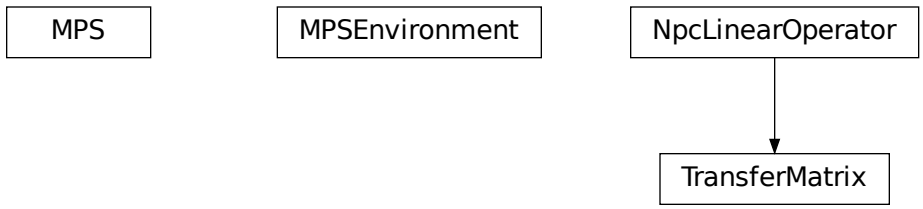
Defines a class describing the local physical Hilbert space.

The `Site` is the prototype, read it's docstring.

7.10.2 mps

- full name: tenpy.networks.mps
- parent module: `tenpy.networks`
- type: module

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 $< bra\|Op\|ket >$ for local operators Op.
TransferMatrix(bra, ket[, shift_bra, ...])	Transfer matrix of two MPS (bra & ket).

MPS

- full name: tenpy.networks.mps.MPS
- parent module: *tenpy.networks.mps*
- type: class

Inheritance Diagram

Methods

MPS.__init__(sites, Bs, SVs[, bc, form, norm])	Initialize self.
MPS.add(other, alpha, beta[, cutoff])	Return an MPS which represents alpha|self> + beta |others>.
MPS.apply_local_op(i, op[, unitary, ...])	Apply a local (one or multi-site) operator to *self*.
MPS.average_charge([bond])	Return the average charge for the block on the left of a given bond.
MPS.canonical_form([renormalize])	Bring self into canonical 'B' form, (re-)calculate singular values.
MPS.canonical_form_finite([renormalize, cutoff])	Bring a finite (or segment) MPS into canonical form (in place).
MPS.canonical_form_infinite([renormalize, ...])	Bring an infinite MPS into canonical form (in place).
MPS.charge_variance([bond])	Return the charge variance on the left of a given bond.
MPS.compute_K(perm[, swap_op, trunc_par, ...])	Compute the momentum quantum numbers of the entanglement spectrum for 2D states.
MPS.convert_form([new_form])	Tranform self into different canonical form (by scaling the legs with singular values).
MPS.copy()	Returns a copy of *self*.
MPS.correlation_function(ops1, ops2[, ...])	Correlation function <psi|op1_i op2_j|psi>/<psi|psi> of single site operators.
MPS.correlation_length([target, tol_ev0, ...])	Calculate the correlation length by diagonalizing the transfer matrix.

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Table 146 – continued from previous page

MPS.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
MPS.entanglement_entropy([n, bonds, ...])	Calculate the (half-chain) entanglement entropy for all nontrivial bonds.
MPS.entanglement_entropy_segment([segment, ...])	Calculate entanglement entropy for general geometry of the bipartition.
MPS.entanglement_spectrum([by_charge])	return entanglement energy spectrum.
MPS.expectation_value(ops[, sites, axes])	Expectation value `<psi|ops|psi>/<psi|psi>` of (n-site) operator(s).
MPS.expectation_value_multi_sites(operators, i0)	Expectation value `<psi|op0_{i0}op1_{i0+1}...opN_{i0+N}|psi>/<psi|psi>`.
MPS.expectation_value_term(term[, autoJW])	Expectation value `<psi|op_{i0}op_{i1}...op_{iN}|psi>/<psi|psi>`.
MPS.expectation_value_terms_sum(term_list[, ...])	Calculate expectation values for a bunch of terms and sum them up.
MPS.from_Bflat(sites, Bflat[, SVs, bc, ...])	Construct a matrix product state from a set of numpy arrays *Bflat* and singular vals.
MPS.from_full(sites, psi[, form, cutoff, ...])	Construct an MPS from a single tensor *psi* with one leg per physical site.
MPS.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
MPS.from_lat_product_state(lat, p_state, ...)	Construct an MPS from a product state given in lattice coordinates.
MPS.from_product_state(sites, p_state[, bc, ...])	Construct a matrix product state from a given product state.
MPS.from_singlets(site, L, pairs[, up, ...])	Create an MPS of entangled singlets.
MPS.gauge_total_charge([qtotal, vL_leg, vR_leg])	Gauge the legcharges of the virtual bonds such that the MPS has a total *qtotal*.
MPS.get_B(i[, form, copy, cutoff, label_p])	Return (view of) *B* at site *i* in canonical form.
MPS.get_SL(i)	Return singular values on the left of site *i*
MPS.get_SR(i)	Return singular values on the right of site *i*
MPS.get_grouped_mps(blocklen)	contract blocklen subsequent tensors into a single one and return result as a new MPS.
MPS.get_op(op_list, i)	Given a list of operators, select the one corresponding to site *i*.
MPS.get_rho_segment(segment)	Return reduced density matrix for a segment.
MPS.get_theta(i[, n, cutoff, formL, formR])	Calculates the *n*-site wavefunction on `sites[i:i+n]`.
MPS.get_total_charge([only_physical_legs])	Calculate and return the *qtotal* of the whole MPS (when contracted).
MPS.group_sites([n, grouped_sites])	Modify *self* inplace to group sites.
MPS.group_split([trunc_par])	Modify *self* inplace to split previously grouped sites.
MPS.increase_L([new_L])	Modify *self* inplace to enlarge the MPS unit cell; in place.
MPS.mutinf_two_site([max_range, n])	Calculate the two-site mutual information $I(i:j)$.
MPS.norm_test()	Check that self is in canonical form.
MPS.overlap(other[, charge_sector, ignore_form])	Compute overlap `<self|other>`.
MPS.permute_sites(perm[, swap_op, ...])	Applies the permutation perm to the state (inplace).
MPS.probability_per_charge([bond])	Return probabilites of charge value on the left of a given bond.
MPS.roll_mps_unit_cell([shift])	Shift the section we define as unit cellof an infinite MPS; in place.

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Table 146 – continued from previous page

`MPS.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`MPS.set_B`(i, B[, form])	Set *B* at site *i*.
`MPS.set_SL`(i, S)	Set singular values on the left of site *i*
`MPS.set_SR`(i, S)	Set singular values on the right of site *i*
`MPS.swap_sites`(i[, swap_op, trunc_par])	Swap the two neighboring sites *i* and *i+1* (inplace).
`MPS.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.

Class Attributes and Properties

`MPS.L`	Number of physical sites; for an iMPS the len of the MPS unit cell.
`MPS.chi`	Dimensions of the (nontrivial) virtual bonds.
`MPS.dim`	List of local physical dimensions.
`MPS.finite`	Distinguish MPS vs iMPS.
`MPS.nontrivial_bonds`	Slice of the non-trivial bond indices, depending on `self.bc`.

class `tenpy.networks.mps.`**`MPS`**(*sites*, *Bs*, *SVs*, *bc='finite'*, *form='B'*, *norm=1.0*)

Bases: `object`

A Matrix Product State, finite (MPS) or infinite (iMPS).

Parameters

- **sites** (list of `Site`) – Defines the local Hilbert space for each site.
- **Bs** (list of `Array`) – The 'matrices' of the MPS. Labels are `vL, vR, p` (in any order).
- **SVs** (`list of 1D array`) – The singular values on *each* bond. Should always have length *L+1*. Entries out of `nontrivial_bonds` are ignored.
- **bc** (`'finite' | 'segment' | 'infinite'`) – Boundary conditions as described in the tabel of the module doc-string.
- **form** ((list of) {`'B' | 'A' | 'C' | 'G' | 'Th' | None` | tuple(float, float)}) – The form of the stored 'matrices', see table in module doc-string. A single choice holds for all of the entries.

sites

Defines the local Hilbert space for each site.

Type list of `Site`

bc

Boundary conditions as described in above table.

Type {'finite', 'segment', 'infinite'}

form

Describes the canonical form on each site. `None` means non-canonical form. For `form = (nuL, nuR)`, the stored `_B[i]` are `s**form[0] -- Gamma -- s**form[1]` (in Vidal's notation).

Type list of {`None` | tuple(float, float)}

chinfo

The nature of the charge.

Type `ChargeInfo`

dtype
The data type of the `_B`.

Type type

norm
The norm of the state, i.e. `sqrt(<psi|psi>)`. Ignored for (normalized) *expectation_value()*, but important for *overlap()*.

Type float

grouped
Number of sites grouped together, see *group_sites()*.

Type int

_B
The 'matrices' of the MPS. Labels are `vL, vR, p` (in any order). We recommend using *get_B()* and *set_B()*, which will take care of the different canonical forms.

Type list of `npc.Array`

_S
The singular values on each virtual bond, length `L+1`. May be `None` if the MPS is not in canonical form. Otherwise, `_S[i]` is to the left of `_B[i]`. We recommend using *get_SL()*, *get_SR()*, *set_SL()*, *set_SR()*, which takes proper care of the boundary conditions.

Type list of (`None` | 1D array)

_valid_forms
Class attribute. Mapping for canonical forms to a tuple `(nuL, nuR)` indicating that `self._Bs[i] = s[i]**nuL -- Gamma[i] -- s[i]**nuR` is saved.

Type dict

_valid_bc
Class attribute. Possible valid boundary conditions.

Type tuple of str

_transfermatrix_keep
How many states to keep at least when diagonalizing a *TransferMatrix*. Important if the state develops a near-degeneracy.

Type int

_p_label, _B_labels
Class attribute. *_p_label* defines the physical legs of the B-tensors, *_B_labels* lists all the labels of the B tensors. Used by methods like *get_theta()* to avoid the necessity of re-implementations for derived classes like the `Purification_MPS` if just the number of physical legs changed.

Type list of str

test_sanity()
Sanity check, raises ValueErrors, if something is wrong.

copy()
Returns a copy of *self*.

The copy still shares the sites, chinfo, and LegCharges of the B tensors, but the values of B and S are deeply copied.

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 `sites`, `chinfo` (under these names), `_B` as `"tensors"`, `_S` as `"singular_values"`, `bc` as `"boundary_condition"`, and `form` converted to a single array of shape (L, 2) as `"canonical_form"`, Moreover, it saves `norm`, `L`, `grouped` and `_transfermatrix_keep` (as "transfermatrix_keep") as HDF5 attributes, as well as the maximum of `chi` under the name "max_bond_dimension".

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_lat_product_state(*lat*, *p_state*, ***kwargs*)

Construct an MPS from a product state given in lattice coordinates.

This is a wrapper around `from_product_state()`. The purpuse is to make the *p_state* argument independent of the *order* of the *Lattice*, and specify it in terms of lattice indices instead.

Parameters

- **lat** (`Lattice`) – The underlying lattice defining the geometry and Hilbert Space.
- **p_state** (*array_like of {int | str | 1D array}*) – Defines the product state to be represented. Should be of dimension *lat.dim`+1, entries are indexed by lattice indices. Entries of the array as for the `p_state* argument of `from_product_state()`. It gets tiled to the shape `lat.shape`, if it is smaller.
- ****kwargs** – Other keyword arguments as definied in `from_product_state()`. *bc* is set by default from `lat.bc_MPS`.

Returns **product_mps** – An MPS representing the specified product state.

Return type `MPS`

Examples

Let's first consider a `Ladder` composed of a `SpinHalfSite` and a `FermionSite`.

```
>>> spin_half = tenpy.networks.site.SpinHalfSite()
>>> fermion = tenpy.networks.site.FermionSite()
>>> ladder_i = tenpy.models.lattice.Ladder(2, [spin_half, fermion], bc_MPS=
↪"infinite")
```

To initialize a state of up-spins on the spin sites and half-filled ferions, you can use:

```
>>> p_state = [["up", "empty"], ["up", "full"]]
>>> psi = tenpy.networks.MPS.from_lat_product_state(ladder_i, p_state)
```

Note that the same *p_state* works for a finite lattice of even length, say `L=10`, as well. We then just "tile" in x-direction, i.e., repeat the specified state 5 times:

```
>>> ladder_f = tenpy.models.lattice.Ladder(10, [spin_half, fermion], bc_MPS=
↪"finite")
>>> psi = tenpy.networks.MPS.from_lat_product_state(ladder_f, p_state)
```

You can also easily half-fill a *Honeycomb*, for example with only the *A* sites occupied, or as stripe parallel to the x-direction (*stripe_x*, alternating along *y* axis), or as stripes parallel to the y-direction (*stripe_y*, alternating along *x* axis).

```
>>> honeycomb = tenpy.models.lattice.Honeycomb([4, 4], [fermion, fermion], bc_
↪MPS="finite")
>>> p_state_only_A = [[["empty", "full"]]]
>>> psi_only_A = tenpy.networks.MPS.from_lat_product_state(honeycomb, p_state_
↪only_A)
>>> p_state_stripe_x = [[["empty", "empty"],
...                      ["full", "full"]]]
>>> psi_stripe_x = tenpy.networks.MPS.from_lat_product_state(honeycomb, p_
↪state_stripe_x)
>>> p_state_stripe_y = [[["empty", "empty"]],
...                      [["full", "full"]]]
>>> psi_stripe_y = tenpy.networks.MPS.from_lat_product_state(honeycomb, p_
↪state_stripe_y)
```

---

classmethod from_product_state(*sites*, *p_state*, *bc='finite'*, *dtype=<class 'numpy.float64'>*, *permute=True*, *form='B'*, *chargeL=None*)

Construct a matrix product state from a given product state.

Parameters

- **sites** (list of *Site*) – The sites defining the local Hilbert space.
- **p_state** (*list of {int | str | 1D array}*) – Defines the product state to be represented; one entry for each *site* of the MPS. An entry of *str* type is translated to an *int* with the help of *state_labels()*. An entry of *int* type represents the physical index of the state to be used. An entry which is a 1D array defines the complete wavefunction on that site; this allows to make a (local) superposition.
- **bc** (*{'infinite', 'finite', 'segmemt'}*) – MPS boundary conditions. See docstring of *MPS*.
- **dtype** (*type or string*) – The data type of the array entries.
- **permute** (*bool*) – The `Site` might permute the local basis states if charge conservation gets enabled. If *permute* is True (default), we permute the given *p_state* locally according to each site's `perm`. The *p_state* entries should then always be given as if *conserve=None* in the Site.
- **form** ((list of) {`'B' | 'A' | 'C' | 'G' | None` | tuple(float, float)}) – Defines the canonical form. See module doc-string. A single choice holds for all of the entries.
- **chargeL** (*charges*) – Leg charges at bond 0, which are purely conventional.

Returns **product_mps** – An MPS representing the specified product state.

Return type *MPS*

Examples

Example to get a Neel state for a `TIChain`:

```
>>> M = TFIChain({'L': 10})
>>> p_state = ["up", "down"] * (L//2)  # repeats entries L/2 times
>>> psi = MPS.from_product_state(M.lat.mps_sites(), p_state, bc=M.lat.bc_MPS)
```

The meaning of the labels `"up"`,`"down"` is defined by the `Site`, in this example a *SpinHalfSite*.

Extending the example, we can replace the spin in the center with one with arbitrary angles `theta, phi` in the bloch sphere:

```
>>> M = TFIChain({'L': 8, 'conserve': None})
>>> p_state = ["up", "down"] * (L//2)  # repeats entries L/2 times
>>> bloch_sphere_state = np.array([np.cos(theta/2), np.exp(1.j*phi)*np.
↪sin(theta/2)])
>>> p_state[L//2] = bloch_sphere_state   # replace one spin in center
>>> psi = MPS.from_product_state(M.lat.mps_sites(), p_state, bc=M.lat.bc_MPS,␣
↪dtype=np.complex)
```

Note that for the more general *SpinChain*, the order of the two entries for the `bloch_sphere_state` would be *exactly the opposite* (when we keep the the north-pole of the bloch sphere being the up-state). The reason is that the *SpinChain* uses the general *SpinSite*, where the states are orderd ascending from `'down'` to `'up'`. The *SpinHalfSite* on the other hand uses the order `'up', 'down'` where that the Pauli matrices look as usual.

Moreover, note that you can not write this bloch state (for `theta != 0, pi`) when conserving symmetries, as the two physical basis states correspond to different symmetry sectors.

---

classmethod from_Bflat(*sites*, *Bflat*, *SVs=None*, *bc='finite'*, *dtype=None*, *permute=True*, *form='B'*, *legL=None*)

Construct a matrix product state from a set of numpy arrays *Bflat* and singular vals.

Parameters

- **sites** (list of *Site*) – The sites defining the local Hilbert space.
- **Bflat** (*iterable of numpy ndarrays*) – The matrix defining the MPS on each site, with legs `'p', 'vL', 'vR'` (physical, virtual left/right).
- **SVs** (list of 1D array | `None`) – The singular values on *each* bond. Should always have length *L+1*. By default (`None`), set all singular values to the same value. Entries out of *nontrivial_bonds* are ignored.
- **bc** (*{'infinite', 'finite', 'segmemt'}*) – MPS boundary conditions. See docstring of *MPS*.
- **dtype** (*type or string*) – The data type of the array entries. Defaults to the common dtype of *Bflat*.
- **permute** (*bool*) – The `Site` might permute the local basis states if charge conservation gets enabled. If *permute* is True (default), we permute the given *Bflat* locally according to each site's `perm`. The *p_state* argument should then always be given as if *conserve=None* in the Site.

- **form** ((list of) {'B' | 'A' | 'C' | 'G' | None | tuple(float, float)}) – Defines the canonical form of *Bflat*. See module doc-string. A single choice holds for all of the entries.
- **leg_L** (LegCharge | None) – Leg charges at bond 0, which are purely conventional. If None, use trivial charges.

Returns **mps** – An MPS with the matrices *Bflat* converted to npc arrays.

Return type *MPS*

classmethod from_full(*sites*, *psi*, *form=None*, *cutoff=1e-16*, *normalize=True*, *bc='finite'*, *outer_S=None*)

Construct an MPS from a single tensor *psi* with one leg per physical site.

Performs a sequence of SVDs of psi to split off the *B* matrices and obtain the singular values, the result will be in canonical form. Obviously, this is only well-defined for *finite* or *segment* boundary conditions.

Parameters

- **sites** (list of *Site*) – The sites defining the local Hilbert space.
- **psi** (*Array*) – The full wave function to be represented as an MPS. Should have labels 'p0', 'p1', ..., 'p{L-1}'. Additionally, it may have (or must have for 'segment' *bc*) the legs 'vL', 'vR', which are trivial for 'finite' *bc*.
- **form** ('B' | 'A' | 'C' | 'G' | None) – The canonical form of the resulting MPS, see module doc-string. None defaults to 'A' form on the first site and 'B' form on all following sites.
- **cutoff** (*float*) – Cutoff of singular values used in the SVDs.
- **normalize** (*bool*) – Whether the resulting MPS should have 'norm' 1.
- **bc** (*'finite' | 'segment'*) – Boundary conditions.
- **outer_S** (*None | (array, array)*) – For 'semgent' *bc* the singular values on the left and right of the considered segment, *None* for 'finite' boundary conditions.

Returns **psi_mps** – MPS representation of *psi*, in canonical form and possibly normalized.

Return type *MPS*

classmethod from_singlets(*site*, *L*, *pairs*, *up='up'*, *down='down'*, *lonely=[]*, *lonely_state='up'*, *bc='finite'*)

Create an MPS of entangled singlets.

Parameters

- **site** (*Site*) – The *site* defining the local Hilbert space, taken uniformly for all sites.
- **L** (*int*) – The number of sites.
- **pairs** (*list of (int, int)*) – Pairs of sites to be entangled; the returned MPS will have a singlet for each pair in *pairs*.
- **down** (*up,*) – A singlet is defined as (|up down> - |down up>)/2**0.5, up and down give state indices or labels defined on the corresponding site.
- **lonely** (*list of int*) – Sites which are not included into a singlet pair.
- **lonely_state** (*int | str*) – The state for the lonely sites.
- **bc** (*{'infinite', 'finite', 'segmemt'}*) – MPS boundary conditions. See docstring of *MPS*.

Returns **singlet_mps** – An MPS representing singlets on the specified pairs of sites.

Return type *MPS*

property L
Number of physical sites; for an iMPS the len of the MPS unit cell.

property dim
List of local physical dimensions.

property finite
Distinguish MPS vs iMPS.

True for an MPS (`bc='finite', 'segment'`), False for an iMPS (`bc='infinite'`).

property chi
Dimensions of the (nontrivial) virtual bonds.

property nontrivial_bonds
Slice of the non-trivial bond indices, depending on `self.bc`.

get_B(*i*, *form='B'*, *copy=False*, *cutoff=1e-16*, *label_p=None*)
Return (view of) *B* at site *i* in canonical form.

Parameters

- **i** (*int*) – Index choosing the site.
- **form** (`'B' | 'A' | 'C' | 'G' | 'Th' | None` | tuple(float, float)) – The (canonical) form of the returned B. For `None`, return the matrix in whatever form it is. If any of the tuple entry is None, also don't scale on the corresponding axis.
- **copy** (*bool*) – Whether to return a copy even if *form* matches the current form.
- **cutoff** (*float*) – During DMRG with a mixer, *S* may be a matrix for which we need the inverse. This is calculated as the Penrose pseudo-inverse, which uses a cutoff for the singular values.
- **label_p** (*None | str*) – Ignored by default (`None`). Otherwise replace the physical label `'p'` with `'p'+label_p'`. (For derived classes with more than one "physical" leg, replace all the physical leg labels accordingly.)

Returns **B** – The MPS 'matrix' *B* at site *i* with leg labels `'vL', 'p', 'vR'`. May be a view of the matrix (if `copy=False`), or a copy (if the form changed or `copy=True`).

Return type *Array*

:raises ValueError : if self is not in canoncial form and *form* is not None.:

set_B(*i*, *B*, *form='B'*)
Set *B* at site *i*.

Parameters

- **i** (*int*) – Index choosing the site.
- **B** (*Array*) – The 'matrix' at site *i*. No copy is made! Should have leg labels `'vL', 'p', 'vR'` (not necessarily in that order).
- **form** (`'B' | 'A' | 'C' | 'G' | 'Th' | None` | tuple(float, float)) – The (canonical) form of the *B* to set. `None` stands for non-canonical form.

get_SL(*i*)
Return singular values on the left of site *i*

get_SR(*i*)
Return singular values on the right of site *i*

set_SL(*i*, *S*)
Set singular values on the left of site *i*

set_SR(*i*, *S*)
Set singular values on the right of site *i*

get_op(*op_list*, *i*)
Given a list of operators, select the one corresponding to site *i*.

Parameters

- **op_list** (*(list of) {str | npc.array}*) – List of operators from which we choose. We assume that `op_list[j]` acts on site `j`. If the length is shorter than *L*, we repeat it periodically. Strings are translated using *get_op()* of site *i*.
- **i** (*int*) – Index of the site on which the operator acts.

Returns **op** – One of the entries in *op_list*, not copied.

Return type npc.array

get_theta(*i*, *n=2*, *cutoff=1e-16*, *formL=1.0*, *formR=1.0*)
Calculates the *n*-site wavefunction on `sites[i:i+n]`.

Parameters

- **i** (*int*) – Site index.
- **n** (*int*) – Number of sites. The result lives on `sites[i:i+n]`.
- **cutoff** (*float*) – During DMRG with a mixer, *S* may be a matrix for which we need the inverse. This is calculated as the Penrose pseudo-inverse, which uses a cutoff for the singular values.
- **formL** (*float*) – Exponent for the singular values to the left.
- **formR** (*float*) – Exponent for the singular values to the right.

Returns **theta** – The n-site wave function with leg labels `vL, p0, p1, .... p{n-1}, vR`. In Vidal's notation (with s=lambda, G=Gamma): `theta = s**form_L G_i s G_{i+1} s ... G_{i+n-1} s**form_R`.

Return type *Array*

convert_form(*new_form='B'*)
Tranform self into different canonical form (by scaling the legs with singular values).

Parameters **new_form** ((list of) {`'B' | 'A' | 'C' | 'G' | 'Th' | None` | tuple(float, float)}) – The form the stored 'matrices'. The table in module doc-string. A single choice holds for all of the entries.

:raises ValueError : if trying to convert from a `None` form. Use *canonical_form()* instead!:

increase_L(*new_L=None*)
Modify *self* inplace to enlarge the MPS unit cell; in place.

Deprecated since version 0.5.1: This method will be removed in version 1.0.0. Use the equivalent `psi.enlarge_mps_unit_cell(new_L//psi.L)` instead of `psi.increase_L(new_L)`.

Parameters **new_L** (*int*) – New number of sites. Needs to be an integer multiple of *L*. Defaults to `2*self.L`.

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 unit cell will be increased from *L* to `factor*L`.

roll_mps_unit_cell (*shift=1*)

Shift the section we define as unit cellof an infinite MPS; in place.

Suppose we have a unit cell with tensors `[A, B, C, D]` (repeated on both sites). With `shift = 1`, the new unit cell will be `[D, A, B, C]`, whereas `shift = -1` will give `[B, C, D, A]`.

Parameters **shift** (*int*) – By how many sites to move the tensors to the right.

group_sites (*n=2*, *grouped_sites=None*)

Modify *self* inplace 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).

Parameters

- **n** (*int*) – Number of sites to be grouped together.
- **grouped_sites** (None | list of *GroupedSite*) – The sites grouped together.

See also:

group_split() Reverts the grouping.

group_split (*trunc_par=None*)

Modify *self* inplace to split previously grouped sites.

Parameters **trunc_par** (*dict*) – Parameters for truncation, see `truncate()`. Defaults to `{'chi_max': max(self.chi)}`.

Returns **trunc_err** – The error introduced by the truncation for the splitting.

Return type *TruncationError*

See also:

group_sites() Should have been used before to combine sites.

get_grouped_mps (*blocklen*)

contract blocklen subsequent tensors into a single one and return result as a new MPS.

blocklen = number of subsequent sites to be combined.

Returns

Return type new MPS object with bunched sites.

get_total_charge (*only_physical_legs=False*)

Calculate and return the *qtotal* of the whole MPS (when contracted).

Parameters **only_physical_legs** (*bool*) – For `'finite'` boundary conditions, the total charge can be gauged away by changing the LegCharge of the trivial legs on the left and right of the MPS. This option allows to project out the trivial legs to get the actual "physical" total charge.

Returns **qtotal** – The sum of the *qtotal* of the individual *B* tensors.

Return type charges

gauge_total_charge (*qtotal=None*, *vL_leg=None*, *vR_leg=None*)

Gauge the legcharges of the virtual bonds such that the MPS has a total *qtotal*.

Parameters

- **qtotal** (*(list of) charges*) – If a single set of charges is given, it is the desired total charge of the MPS (which `get_total_charge()` will return afterwards). By default (`None`), use 0 charges, unless vL_leg and vR_leg are specified, in which case we adjust the total charge to match these legs.
- **vL_leg** (*None | LegCharge*) – Desired new virtual leg on the very left. Needs to have the same block strucuture as current leg, but can have shifted charge entries.
- **vR_leg** (*None | LegCharge*) – Desired new virtual leg on the very right. Needs to have the same block strucuture as current leg, but can have shifted charge entries. Should be *vL_leg.conj()* for infinite MPS, if *qtotal* is not given.

entanglement_entropy(*n=1*, *bonds=None*, *for_matrix_S=False*)

Calculate the (half-chain) entanglement entropy for all nontrivial bonds.

Consider a bipartition of the sytem into $A = \{j : j <= i_b\}$ and $B = \{j : j > i_b\}$ and the reduced density matrix $\rho_A = tr_B(\rho)$. The von-Neumann entanglement entropy is defined as $S(A, n = 1) = -tr(\rho_A \log(\rho_A)) = S(B, n = 1)$. The generalization for `n != 1, n>0` are the Renyi entropies: $S(A, n) = \frac{1}{1-n} \log(tr(\rho_A^2)) = S(B, n = 1)$

This function calculates the entropy for a cut at different bonds *i*, for which the the eigenvalues of the reduced density matrix ρ_A and ρ_B is given by the squared schmidt values *S* of the bond.

Parameters

- **n** (*int/float*) – Selects which entropy to calculate; *n=1* (default) is the ususal von-Neumann entanglement entropy.
- **bonds** (`None` | (iterable of) int) – Selects the bonds at which the entropy should be calculated. `None` defaults to `range(0, L+1)[self.nontrivial_bonds]`.
- **for_matrix_S** (*bool*) – Switch calculate the entanglement entropy even if the *_S* are matrices. Since $O(\chi^3)$ is expensive compared to the ususal $O(\chi)$, we raise an error by default.

Returns entropies – Entanglement entropies for half-cuts. *entropies[j]* contains the entropy for a cut at bond `bonds[j]` (i.e. left to site `bonds[j]`).

Return type 1D ndarray

entanglement_entropy_segment(*segment=[0]*, *first_site=None*, *n=1*)

Calculate entanglement entropy for general geometry of the bipartition.

This function is similar as `entanglement_entropy()`, but for more general geometry of the region *A* to be a segment of a *few* sites.

This is acchieved by explicitly calculating the reduced density matrix of *A* and thus works only for small segments.

Parameters

- **segment** (*list of int*) – Given a first site *i*, the region `A_i` is defined to be `[i+j for j in segment]`.
- **first_site** (`None` | (iterable of) int) – Calculate the entropy for segments starting at these sites. `None` defaults to `range(L-segment[-1])` for finite or *range(L)* for infinite boundary conditions.
- **n** (*int | float*) – Selects which entropy to calculate; *n=1* (default) is the ususal von-Neumann entanglement entropy, otherwise the *n*-th Renyi entropy.

Returns entropies – `entropies[i]` contains the entropy for the the region `A_i` defined above.

Return type 1D ndarray

entanglement_spectrum(*by_charge=False*)

return entanglement energy spectrum.

Parameters by_charge (*bool*) – Wheter we should sort the spectrum on each bond by the possible charges.

Returns ent_spectrum – For each (non-trivial) bond the entanglement spectrum. If *by_charge* is `False`, return (for each bond) a sorted 1D ndarray with the convention $S_i^2 = e^{-\xi_i}$, where S_i labels a Schmidt value and ξ_i labels the entanglement 'energy' in the returned spectrum. If *by_charge* is True, return a a list of tuples `(charge, sub_spectrum)` for each possible charge on that bond.

Return type list

get_rho_segment(*segment*)

Return reduced density matrix for a segment.

Note that the dimension of rho_A scales exponentially in the length of the segment.

Parameters segment (*iterable of int*) – Sites for which the reduced density matrix is to be calculated. Assumed to be sorted.

Returns rho – Reduced density matrix of the segment sites. Labels `'p0', 'p1', ..., 'pk', 'p0*', 'p1*', ..., 'pk*'` with `k=len(segment)`.

Return type *Array*

probability_per_charge(*bond=0*)

Return probabilites of charge value on the left of a given bond.

For example for particle number conservation, define $N_b = sum_{i<b} n_i$ for a given bond b. This function returns the possible values of *N_b* as rows of *charge_values*, and for each row the probabilty that this combination occurs in the given state.

Parameters bond (*int*) – The bond to be considered. The returned charges are summed on the left of this bond.

Returns

- **charge_values** (*2D array*) – Columns correspond to the different charges in *self.chinfo*. Rows are the different charge fluctuations at this bond
- **probabilities** (*1D array*) – For each row of *charge_values* the probablity for these values of charge fluctuations.

average_charge(*bond=0*)

Return the average charge for the block on the left of a given bond.

For example for particle number conservation, define $N_b = sum_{i<b} n_i$ for a given bond b. Then this function returns $< \psi | N_b | \psi >$.

Parameters bond (*int*) – The bond to be considered. The returned charges are summed over the sites left of *bond*.

Returns average_charge – For each type of charge in *chinfo* the average value when summing the charge values over sites left of the given bond.

Return type 1D array

charge_variance(*bond=0*)

Return the charge variance on the left of a given bond.

For example for particle number conservation, define $N_b = sum_{i<b} n_i$ for a given bond b. Then this function returns $< \psi | N_b^2 | \psi > - (< \psi | N_b | \psi >)^2$.

Parameters **bond** (*int*) – The bond to be considered. The returned charges are summed over the sites left of *bond*.

Returns **average_charge** – For each type of charge in *chinfo* the variance of of the charge values left of the given bond.

Return type 1D array

mutinf_two_site(*max_range=None*, *n=1*)

Calculate the two-site mutual information $I(i:j)$.

Calculates $I(i:j) = S(i) + S(j) - S(i,j)$, where $S(i)$ is the single site entropy on site i and $S(i,j)$ the two-site entropy on sites i, j.

Parameters

- **max_range** (*int*) – Maximal distance `|i-j|` for which the mutual information should be calculated. `None` defaults to *L-1*.
- **n** (*float*) – Selects the entropy to use, see *entropy()*.

Returns

- **coords** (*2D array*) – Coordinates for the mutinf array.
- **mutinf** (*1D array*) – `mutinf[k]` is the mutual information $I(i:j)$ between the sites `i, j = coords[k]`.

overlap(*other*, *charge_sector=None*, *ignore_form=False*, ***kwargs*)

Compute overlap `<self|other>`.

Parameters

- **other** (*MPS*) – An MPS with the same physical sites.
- **charge_sector** (None | charges | `0`) – Selects the charge sector in which the dominant eigenvector of the TransferMatrix is. `None` stands for *all* sectors, `0` stands for the sector of zero charges. If a sector is given, it *assumes* the dominant eigenvector is in that charge sector.
- **ignore_form** (*bool*) – If `False` (default), take into account the canonical form *form* at each site. If `True`, we ignore the canonical form (i.e., whether the MPS is in left, right, mixed or no canonical form) and just contract all the *_B* as they are. (This can give different results!)
- ****kwargs** – Further keyword arguments given to *TransferMatrix.eigenvectors()*; only used for infinite boundary conditions.

Returns **overlap** – The contraction `<self|other> * self.norm * other.norm` (i.e., taking into account the *norm* of both MPS). For an infinite MPS, `<self|other>` is the overlap per unit cell, i.e., the largest eigenvalue of the TransferMatrix.

Return type dtype.type

expectation_value(*ops*, *sites=None*, *axes=None*)

Expectation value `<psi|ops|psi>/<psi|psi>` of (n-site) operator(s).

Given the MPS in canonical form, it calculates n-site expectation values. For example the contraction for a two-site ($n = 2$) operator on site i would look like:

```
|           .--S--B[i]--B[i+1]--.
|           |     |     |       |
|           |     |-----|       |
|           |     | op  |       |
|           |     |-----|       |
|           |     |     |       |
|           .--S--B*[i]-B*[i+1]-.
```

Parameters

- **ops** ((list of) { *Array* | str }) – The operators, for wich the expectation value should be taken, All operators should all have the same number of legs (namely *2 n*). If less than *self.L* operators are given, we repeat them periodically. Strings (like `'Id', 'Sz'`) are translated into single-site operators defined by *sites*.
- **sites** (*None | list of int*) – 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 operators ($n = 1$), or `(['p0', 'p1', ... 'p{n-1}'], ['p0*', 'p1*', .... 'p{n-1}*'])` for $n > 1$.

Returns **exp_vals** – Expectation values, `exp_vals[i] = <psi|ops[i]|psi>`, where `ops[i]` acts on site(s) `j, j+1, ..., j+{n-1}` with `j=sites[i]`.

Return type 1D ndarray

Examples

One site examples (n=1):

```
>>> psi.expectation_value('Sz')
[Sz0, Sz1, ..., Sz{L-1}]
>>> psi.expectation_value(['Sz', 'Sx'])
[Sz0, Sx1, Sz2, Sx3, ... ]
>>> psi.expectation_value('Sz', sites=[0, 3, 4])
[Sz0, Sz3, Sz4]
```

Two site example (n=2), assuming homogeneous sites:

```
>>> SzSx = npc.outer(psi.sites[0].Sz.replace_labels(['p', 'p*'], ['p0', 'p0*
↪']),
                     psi.sites[1].Sx.replace_labels(['p', 'p*'], ['p1', 'p1*
↪']))
>>> psi.expectation_value(SzSx)
[Sz0Sx1, Sz1Sx2, Sz2Sx3, ... ]   # with len L-1 for finite bc, or L for␣
↪infinite
```

Example measuring <psi|SzSx|psi2> on each second site, for inhomogeneous sites:

```
>>> SzSx_list = [npc.outer(psi.sites[i].Sz.replace_labels(['p', 'p*'], ['p0',
↪'p0*']),
                           psi.sites[i+1].Sx.replace_labels(['p', 'p*'], ['p1
↪', 'p1*']))
                 for i in range(0, psi.L-1, 2)]
```

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```
>>> psi.expectation_value(SzSx_list, range(0, psi.L-1, 2))
[Sz0Sx1, Sz2Sx3, Sz4Sx5, ...]
```

---

expectation_value_term(*term*, *autoJW=True*)

Expectation value `<psi|op_{i0}op_{i1}...op_{iN}|psi>/<psi|psi>`.

Calculates the expectation value of a tensor product of single-site operators acting on different sites *i0*, *i1*, ... (not necessarily next to each other). In other words, evaluate the expectation value of a term `op0_i0 op1_i1 op2_i2 ....`

For example the contraction of three one-site operators on sites *i0*, *i1=i0+1*, *i2=i0+3* would look like:

```
|          .--S--B[i0]---B[i0+1]--B[i0+2]--B[i0+3]--.
|          |     |        |        |        |        |
|          |    op1      op2       |       op3       |
|          |     |        |        |        |        |
|          .--S--B*[i0]--B*[i0+1]-B*[i0+2]-B*[i0+3]-.
```

Parameters

- **term** (*list of (str, int)*) – List of tuples `op, i` where *i* is the MPS index of the site the operator named *op* acts on. The order inside *term* determines the order in which they act (in the mathematical convention: the last operator in *term* is right-most, so it acts first on a Ket).
- **autoJW** (*bool*) – If True (default), automatically insert Jordan Wigner strings for Fermions as needed.

Returns **exp_val** – The expectation value of the tensorproduct of the given onsite operators, `<psi|op_i0 op_i1 ... op_iN |psi>/<psi|psi>`, where `|psi>` is the represented MPS.

Return type float/complex

See also:

correlation_function() efficient way to evaluate many correlation functions.

Examples

```
>>> a = psi.expectation_value_term([('Sx', 2), ('Sz', 4)])
>>> b = psi.expectation_value_term([('Sz', 4), ('Sx', 2)])
>>> c = psi.expectation_value_multi_sites(['Sz', 'Id', 'Sz'], i0=2)
>>> assert a == b == c
```

---

expectation_value_multi_sites(*operators*, *i0*)

Expectation value `<psi|op0_{i0}op1_{i0+1}...opN_{i0+N}|psi>/<psi|psi>`.

Calculates the expectation value of a tensor product of single-site operators acting on different sites next to each other. In other words, evaluate the expectation value of a term `op0_i0 op1_{i0+1} op2_{i0+2} ....`

> **Warning:** This function does *not* automatically add Jordan-Wigner strings! For correct handling of fermions, use `expectation_value_term()` instead.

Parameters

- **operators** (List of { `Array` | str }) – List of one-site operators. This method calculates the expectation value of the n-sites operator given by their tensor product.
- **i0** (`int`) – The left most index on which an operator acts, i.e., `operators[i]` acts on site `i + i0`.

Returns exp_val – The expectation value of the tensorproduct of the given onsite operators, `<psi|operators[0]_{i0} operators[1]_{i0+1} ... |psi>/<psi|psi>`, where `|psi>` is the represented MPS.

Return type float/complex

expectation_value_terms_sum(*term_list*, *prefactors=None*)

Calculate expectation values for a bunch of terms and sum them up.

This is equivalent to the following expression:

```
sum([self.expectation_value_term(term)*strength for term, strength in term_
↪list])
```

However, for effiency, the term_list is converted to an MPO and the expectation value of the MPO is evaluated.

> **Note:** Due to the way MPO expectation values are evaluated for infinite systems, it works only if all terms in the *term_list* start within the MPS unit cell.

Deprecated since version 0.4.0: *prefactor* will be removed in version 1.0.0. Instead, directly give just `TermList(term_list, prefactors)` as argument.

Parameters

- **term_list** (`TermList`) – The terms and prefactors (*strength*) to be summed up.
- **prefactors** – Instead of specifying a `TermList`, one can also specify the term_list and strength separately. This is deprecated.

Returns

- **terms_sum** (*list of (complex) float*) – Equivalent to the expression `sum([self.expectation_value_term(term)*strength for term, strength in term_list])`.
- *_mpo* – Intermediate results: the generated MPO. For a finite MPS, `terms_sum = _mpo.expectation_value(self)`, for an infinite MPS `terms_sum = _mpo.expectation_value(self) * self.L`

See also:

`expectation_value_term()` evaluates a single *term*.

`tenpy.networks.mpo.MPO.expectation_value()` expectation value density of an MPO.

correlation_function(*ops1*, *ops2*, *sites1=None*, *sites2=None*, *opstr=None*, *str_on_first=True*, *hermitian=False*, *autoJW=True*)

Correlation function `<psi|op1_i op2_j|psi>/<psi|psi>` of single site operators.

Given the MPS in canonical form, it calculates 2-site correlation functions. For examples the contraction for a two-site operator on site *i* would look like:

```
|           .--S--B[i]--B[i+1]--...--B[j]---.
|           |     |     |             |     |
|           |     |     |             op2   |
|           |     op1   |             |     |
|           |     |     |             |     |
|           .--S--B*[i]-B*[i+1]-...--B*[j]--.
```

Onsite terms are taken in the order `<psi | op1 op2 | psi>`.

If *opstr* is given and `str_on_first=True`, it calculates:

```
|            for i < j                                for i > j
|
|           .--S--B[i]---B[i+1]--...- B[j]---.     .--S--B[j]---B[j+1]--...-␣
↪B[i]---.
|           |     |      |             |      |     |     |      |             |␣
↪     |
|           |     opstr  opstr        op2    |     |     op2    |             |␣
↪     |
|           |     |      |             |      |     |     |      |             |␣
↪     |
|           |     op1    |             |      |     |     opstr  opstr       ␣
↪op1    |
|           |     |      |             |      |     |     |      |             |␣
↪     |
|           .--S--B*[i]--B*[i+1]-...- B*[j]--.     .--S--B*[j]--B*[j+1]-...-␣
↪B*[i]--.
```

For `i==j`, no *opstr* is included. For `str_on_first=False`, the *opstr* on site `min(i, j)` is always left out.

Strings (like `'Id', 'Sz'`) in the arguments are translated into single-site operators defined by the *Site* on which they act. Each operator should have the two legs `'p', 'p*'`.

Parameters

- **ops1** ((list of) { *Array* | str }) – First operator of the correlation function (acting after ops2). If a list is given, `ops1[i]` acts on site *i* of the MPS.
- **ops2** ((list of) { *Array* | str }) – Second operator of the correlation function (acting before ops1). If a list is given, `ops2[j]` acts on site *j* of the MPS.
- **sites1** (*None | int | list of int*) – List of site indices *i*; a single *int* is translated to `range(0, sites1)`. `None` defaults to all sites `range(0, L)`. Is sorted before use, i.e. the order is ignored.
- **sites2** (*None | int | list of int*) – List of site indices; a single *int* is translated to `range(0, sites2)`. `None` defaults to all sites `range(0, L)`. Is sorted before use, i.e. the order is ignored.
- **opstr** (None | (list of) { *Array* | str }) – Ignored by default (`None`). Operator(s) to be inserted between `ops1` and `ops2`. If less than *L* operators are given, we repeat them periodically. If given as a list, `opstr[r]` is inserted at site *r* (independent of *sites1* and *sites2*).

- **str_on_first** (*bool*) – Whether the *opstr* is included on the site `min(i, j)`. Note the order, which is chosen that way to handle fermionic Jordan-Wigner strings correctly. (In other words: choose `str_on_first=True` for fermions!)
- **hermitian** (*bool*) – Optimization flag: if `sites1 == sites2` and `Ops1[i]^\dagger == Ops2[i]` (which is not checked explicitly!), the resulting `C[x, y]` will be hermitian. We can use that to avoid calculations, so `hermitian=True` will run faster.
- **autoJW** (*bool*) – *Ignored* if *opstr* is given. If *True*, auto-determine if a Jordan-Wigner string is needed. Works only if exclusively strings were used for *op1* and *op2*.

Returns

C – The correlation function `C[x, y] = <psi|ops1[i] ops2[j]|psi>`, where `ops1[i]` acts on site `i=sites1[x]` and `ops2[j]` on site `j=sites2[y]`. If *opstr* is given, it gives (for `str_on_first=True`):

- For `i < j`: `C[x, y] = <psi|ops1[i] prod_{i <= r < j} opstr[r] ops2[j]|psi>`.
- For `i > j`: `C[x, y] = <psi|prod_{j <= r < i} opstr[r] ops1[i] ops2[j]|psi>`.
- For `i = j`: `C[x, y] = <psi|ops1[i] ops2[j]|psi>`.

The condition `<= r` is replaced by a strict `< r`, if `str_on_first=False`.

Return type 2D ndarray

Examples

For a spin chain:

```
>>> psi.correlation_function("A", "B")
[[A0B0,     A0B1, ..., A0B{L-1}],
 [A1B0,     A1B1, ..., A1B{L-1}],
 ...,
 [A{L-1}B0, ALB1, ..., A{L-1}B{L-1}],
]
```

To evaluate the correlation function for a single *i*, you can use `sites1=[i]`:

```
>>> psi.correlation_function("A", "B", [3])
[[A3B0,     A3B1, ..., A3B{L-1}]]
```

For fermions, it auto-determines that/whether a Jordan Wigner string is needed:

```
>>> CdC = psi.correlation_function("Cd", "C")  # optionally: use␣
↪`hermitian=True`
>>> psi.correlation_function("C", "Cd")[1, 2] == -CdC[1, 2]
True
>>> np.all(np.diag(CdC) == psi.expectation_value("Cd C"))  # "Cd C" is␣
↪equivalent to "N"
True
```

See also:

expectation_value_term() best for a single combination of *i* and *j*.

norm_test()

Check that self is in canonical form.

Returns

norm_error – For each site the norm error to the left and right. The error `norm_error[i, 0]` is defined as the norm-difference between the following networks:

```
|   --theta[i]---.        --s[i]--.
|       |        |    vs          |
|   --theta*[i]--.        --s[i]--.
```

Similarly, `norm_errror[i, 1]` is the norm-difference of:

```
|   .--theta[i]---          .--s[i+1]--
|   |    |           vs     |
|   .--theta*[i]--          .--s[i+1]--
```

Return type array, shape (L, 2)

canonical_form(*renormalize=True*)

Bring self into canonical 'B' form, (re-)calculate singular values.

Simply calls *canonical_form_finite()* or *canonical_form_infinite()*.

canonical_form_finite(*renormalize=True*, *cutoff=0.0*)

Bring a finite (or segment) MPS into canonical form (in place).

If any site is in *form* `None`, it does *not* use any of the singular values *S* (for 'finite' boundary conditions, or only the very left *S* for 'segment' b.c.). If all sites have a *form*, it respects the *form* to ensure that one *S* is included per bond. The final state is always in right-canonical 'B' form.

Performs one sweep left to right doing QR decompositions, and one sweep right to left doing SVDs calculating the singular values.

Parameters

- **renormalize** (*bool*) – Whether a change in the norm should be discarded or used to update *norm*.
- **cutoff** (*float | None*) – Cutoff of singular values used in the SVDs.

Returns **U_L, V_R** – Only returned for `'segment'` boundary conditions. The unitaries defining the new left and right Schmidt states in terms of the old ones, with legs `'vL', 'vR'`.

Return type *Array*

canonical_form_infinite(*renormalize=True*, *tol_xi=1000000.0*)

Bring an infinite MPS into canonical form (in place).

If any site is in *form* `None`, it does *not* use any of the singular values *S*. If all sites have a *form*, it respects the *form* to ensure that one *S* is included per bond. The final state is always in right-canonical 'B' form.

Proceeds in three steps, namely 1) diagonalize right and left transfermatrix on a given bond to bring that bond into canonical form, and then 2) sweep right to left, and 3) left to right to bringing other bonds into canonical form.

Parameters

- **renormalize** (*bool*) – Whether a change in the norm should be discarded or used to update *norm*.
- **tol_xi** (*float*) – Raise an error if the correlation length is larger than that (which indicates a degenerate "cat" state, e.g., for spontaneous symmetry breaking).

correlation_length (*target=1*, *tol_ev0=1e-08*, *charge_sector=0*)

Calculate the correlation length by diagonalizing the transfer matrix.

Assumes that *self* is in canonical form.

Works only for infinite MPS, where the transfer matrix is a useful concept. Assuming a single-site unit cell, any correlation function splits into $C(A_i, B_j) = A'_i T^{j-i-1} B'_j$ with some parts left and right and the $j-i-1$-th power of the transfer matrix in between. The largest eigenvalue is 1 (if self is properly normalized) and gives the dominant contribution of $A'_i E_1 * 1^{j-i-1} * E_1^T B'_j =< A >< B >$, and the second largest one gives a contribution $\propto \lambda_2^{j-i-1}$. Thus $\lambda_2 = \exp(-\frac{1}{\xi})$.

More general for a *L*-site unit cell we get $\lambda_2 = \exp(-\frac{L}{\xi})$, where the *xi* is given in units of 1 lattice spacing in the MPS.

> **Warning:** For a higher-dimensional lattice (which the MPS class doesn't know about), the correct unit is the lattice spacing in x-direction, and the correct formula is $\lambda_2 = \exp(-\frac{L_x}{\xi})$, where *L_x* is the number of lattice spacings in the infinite direction within the MPS unit cell, e.g. the number of "rings" of a cylinder in the MPS unit cell. To get to these units, divide the returned *xi* by the number of sites within a "ring", for a lattice given in `N_sites_per_ring`.

Parameters

- **target** (*int*) – We look for the *target* + 1 largest eigenvalues.
- **tol_ev0** (*float*) – Print warning if largest eigenvalue deviates from 1 by more than *tol_ev0*.
- **charge_sector** (None | charges | `0`) – Selects the charge sector in which the dominant eigenvector of the TransferMatrix is. `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.

Returns **xi** – If *target`=1, return just the correlation length, otherwise an array of the `target* largest correlation lengths. It is measured in units of a single lattice spacing in the MPS language, see the warning above.

Return type float | 1D array

add (*other*, *alpha*, *beta*, *cutoff=1e-15*)

Return an MPS which represents `alpha|self> + beta |others>`.

Works only for 'finite', 'segment' boundary conditions. For 'segment' boundary conditions, the virtual legs on the very left/right are assumed to correspond to each other (i.e. self and other have the same state outside of the considered segment). Takes into account *norm*.

Parameters

- **other** (*MPS*) – Another MPS of the same length to be added with self.
- **beta** (*alpha,*) – Prefactors for self and other. We calculate `alpha * |self> + beta * |other>`
- **cutoff** (*float | None*) – Cutoff of singular values used in the SVDs.

Returns

- **sum** (*MPS*) – An MPS representing `alpha|self> + beta |other>`. Has same total charge as *self*.

- **U_L, V_R** (*Array*) – Only returned for `'segment'` boundary conditions. The unitaries defining the new left and right Schmidt states in terms of the old ones, with legs `'vL', 'vR'`.

apply_local_op(*i*, *op*, *unitary=None*, *renormalize=False*, *cutoff=1e-13*)

Apply a local (one or multi-site) operator to *self*.

Note that this destroys the canonical form if the local operator is non-unitary. Therefore, this function calls *canonical_form()* if necessary.

Parameters

- **i** (*int*) – (Left-most) index of the site(s) on which the operator should act.
- **op** (*str | npc.Array*) – A physical operator acting on site *i*, with legs `'p', 'p*'` for a single-site operator or with legs `['p0', 'p1', ...], ['p0*', 'p1*', ...]` for an operator acting on *n*>=2 sites. Strings (like `'Id', 'Sz'`) are translated into single-site operators defined by *sites*.
- **unitary** (*None | bool*) – Whether *op* is unitary, i.e., whether the canonical form is preserved (`True`) or whether we should call *canonical_form()* (`False`). `None` checks whether `norm(op dagger(op) - identity)` is smaller than *cutoff*.
- **renormalize** (*bool*) – Whether the final state should keep track of the norm (False, default) or be renormalized to have norm 1 (True).
- **cutoff** (*float*) – Cutoff for singular values if *op* acts on more than one site (see *from_full()*). (And used as cutoff for a unspecified *unitary*.)

swap_sites(*i*, *swap_op='auto'*, *trunc_par={}*)

Swap the two neighboring sites *i* and *i+1* (inplace).

Exchange two neighboring sites: form theta, 'swap' the physical legs and split with an svd. While the 'swap' is just a transposition/relabeling for bosons, one needs to be careful about the sign for fermions.

Parameters

- **i** (*int*) – Swap the two sites at positions *i* and *i+1*.
- **swap_op** (`None` | `'auto'` | *Array*) – The operator used to swap the phyiscal legs of the two-site wave function *theta*. For `None`, just transpose/relabel the legs, for `'auto'` also take care of fermionic signs. Alternative give an npc *Array* which represents the full operator used for the swap. Should have legs `['p0', 'p1', 'p0*', 'p1*']` whith `'p0', 'p1*'` contractible.
- **trunc_par** (*dict*) – Parameters for truncation, see `truncate()`. *chi_max* defaults to `max(self.chi)`.

Returns **trunc_err** – The error of the represented state introduced by the truncation after the swap.

Return type *TruncationError*

permute_sites(*perm*, *swap_op='auto'*, *trunc_par={}*, *verbose=0*)

Applies the permutation perm to the state (inplace).

Parameters

- **perm** (*ndarray[ndim=1, int]*) – The applied permutation, such that `psi.permute_sites(perm)[i] = psi[perm[i]]` (where `[i]` indicates the *i*-th site).
- **swap_op** (`None` | `'auto'` | *Array*) – The operator used to swap the phyiscal legs of a two-site wave function *theta*, see *swap_sites()*.

- **trunc_par** (*dict*) – Parameters for truncation, see `truncate()`. *chi_max* defaults to `max(self.chi)`.
- **verbose** (*float*) – Level of verbosity, print status messages if verbose > 0.

Returns **trunc_err** – The error of the represented state introduced by the truncation after the swaps.

Return type *TruncationError*

compute_K(*perm*, *swap_op='auto'*, *trunc_par=None*, *canonicalize=1e-06*, *verbose=0*)

Compute the momentum quantum numbers of the entanglement spectrum for 2D states.

Works for an infinite MPS living on a cylinder, infinitely long in *x* direction and with periodic boundary conditions in *y* directions. If the state is invariant under 'rotations' around the cylinder axis, one can find the momentum quantum numbers of it. (The rotation is nothing more than a translation in *y*.) This function permutes some sites (on a copy of *self*) to enact the rotation, and then finds the dominant eigenvector of the mixed transfer matrix to get the quantum numbers, along the lines of [PollmannTurner2012], see also (the appendix and Fig. 11 in the arXiv version of) [CincioVidal2013].

Parameters

- **perm** (1D ndarray | *Lattice*) – Permuation to be applied to the physical indices, see *permute_sites()*. If a lattice is given, we use it to read out the lattice structure and shift each site by one lattice-vector in y-direction (assuming periodic boundary conditions). (If you have a *CouplingModel*, give its *lat* attribute for this argument)
- **swap_op** (`None` | `'auto'` | *Array*) – The operator used to swap the phyiscal legs of a two-site wave function *theta*, see *swap_sites()*.
- **trunc_par** (*dict*) – Parameters for truncation, see `truncate()`. If not set, *chi_max* defaults to `max(self.chi)`.
- **canonicalize** (*float*) – Check that *self* is in canonical form; call *canonical_form()* if *norm_test()* yields `np.linalg.norm(self.norm_test()) > canonicalize`.
- **verbose** (*float*) – Level of verbosity, print status messages if verbose > 0.

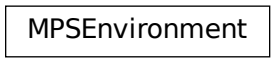
Returns

- **U** (*Array*) – Unitary representation of the applied permutation on left Schmidt states.
- **W** (*ndarray*) – 1D array of the form `S**2 exp(i K)`, where *S* are the Schmidt values on the left bond. You can use `np.abs()` and `np.angle()` to extract the Schmidt values *S* and momenta *K* from *W*.
- **q** (*LegCharge*) – LegCharge corresponding to *W*.
- **ov** (*complex*) – The eigenvalue of the mixed transfer matrix <*psi*|*T*|*psi*> per *L* sites. An absolute value different smaller than 1 indicates that the state is not invariant under the permutation or that the truncation error *trunc_err* was too large!
- **trunc_err** (*TruncationError*) – The error of the represented state introduced by the truncation after swaps when performing the truncation.

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 storde part scrictly to the right of site *i*.
MPSEnvironment.expectation_value(ops[, ...])	Expectation value <bra|ops|ket> of (n-site) operator(s).
MPSEnvironment.full_contraction(i0)	Calculate the overlap by a full contraction of the network.
MPSEnvironment.get_LP(i[, store])	Calculate LP at given site from nearest available one (including *i*).
MPSEnvironment.get_LP_age(i)	Return number of physical sites in the contractions of get_LP(i).
MPSEnvironment.get_RP(i[, store])	Calculate RP at given site from nearest available one (including *i*).
MPSEnvironment.get_RP_age(i)	Return number of physical sites in the contractions of get_RP(i).
MPSEnvironment.get_initialization_data()	Return data for (re-)initialization.
MPSEnvironment.init_LP(i)	Build initial left part LP.
MPSEnvironment.init_RP(i)	Build initial right part RP for an MPS/MPOEnvironment.
MPSEnvironment.set_LP(i, LP, age)	Store part to the left of site *i*.
MPSEnvironment.set_RP(i, RP, age)	Store part to the right of site *i*.
MPSEnvironment.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.

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:

```
|      .-----M[0]--- ... --M[1]---M[2]--- ... ->--.
|      |     |              |      |               |
|      |     |              |------|               |
|      LP[0] |              |  Op  |              RP[-1]
|      |     |              |------|               |
|      |     |              |      |               |
|      .-----N[0]*-- ... --N[1]*--N[2]*-- ... -<--.
```

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*):

```
|     .-->- 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 invovled 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 invovled 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** (*int*) – Build `LP` left of site *i*.

Returns **init_LP** – Identity contractible with the *vL* leg of `ket.get_B(i)`, labels `'vR*'`, `'vR'`.

Return type *Array*

init_RP(*i*)
Build initial right part `RP` for an MPS/MPOEnvironment.

Parameters **i** (*int*) – Build `RP` right of site *i*.

Returns **init_RP** – Identity contractible with the *vR* leg of `ket.get_B(i)`, labels `'vL*'`, `'vL'`.

Return type *Array*

get_LP(*i*, *store=True*)
Calculate LP at given site from nearest available one (including *i*).

The returned `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]    |              |
|      |        |              |
|      .-------N[0]*-- ... --N[i-1]*--<-    'vR*'
```

Parameters

- **i** (*int*) – The returned *LP* will contain the contraction *strictly* left of site *i*.
- **store** (*bool*) – Wheter 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*', 'vR'` for *bra*, *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'  ->---M[i+1]-- ... --M[L-1]----.
|                 |               |          |
|                 |               |         RP[-1]
|                 |               |          |
|      'vL*' -<---N[i+1]*- ... --N[L-1]*---.
```

Parameters

- **i** (*int*) – The returned *RP* will contain the contraction *strictly* right of site *i*.
- **store** (*bool*) – Wheter to store the calculated *RP* in *self* (`True`) or discard them (`False`).

Returns **RP_i** – Contraction of everything left of site *i*, with labels `'vL*', 'vL'` for *bra*, *ket*.

Return type *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 storde part scrictly 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 examples 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 wich the expectation value should be taken, All operators should all have the same number of legs (namely *2 n*). If less than `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, `exp_vals[i] = <bra|ops[i]|ket>`, where `ops[i]` acts on site(s) `j, j+1, ..., j+{n-1}` with `j=sites[i]`.

Return type 1D ndarray

Examples

One site examples (n=1):

```
>>> env.expectation_value('Sz')
[Sz0, Sz1, ..., Sz{L-1}]
>>> env.expectation_value(['Sz', 'Sx'])
```

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```
[Sz0, Sx1, Sz2, Sx3, ... ]
>>> env.expectation_value('Sz', sites=[0, 3, 4])
[Sz0, Sz3, Sz4]
```

Two site example (n=2), assuming homogeneous sites:

```
>>> SzSx = npc.outer(psi.sites[0].Sz.replace_labels(['p', 'p*'], ['p0', 'p0*
↪']),
                     psi.sites[1].Sx.replace_labels(['p', 'p*'], ['p1', 'p1*
↪']))
>>> env.expectation_value(SzSx)
[Sz0Sx1, Sz1Sx2, Sz2Sx3, ... ]   # with len L-1 for finite bc, or L for␣
↪infinite
```

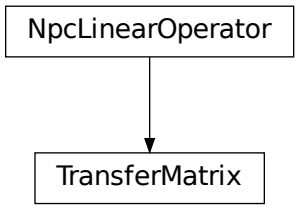
Example measuring <bra|SzSx|ket> on each second site, for inhomogeneous sites:

```
>>> SzSx_list = [npc.outer(psi.sites[i].Sz.replace_labels(['p', 'p*'], ['p0',
↪'p0*']),
...                         psi.sites[i+1].Sx.replace_labels(['p', 'p*'], ['p1
↪', 'p1*']))
...               for i in range(0, psi.L-1, 2)]
>>> env.expectation_value(SzSx_list, range(0, psi.L-1, 2))
[Sz0Sx1, Sz2Sx3, Sz4Sx5, ...]
```

TransferMatrix

- full name: tenpy.networks.mps.TransferMatrix
- parent module: *tenpy.networks.mps*
- type: class

Inheritance Diagram



Methods

`TransferMatrix.__init__`(bra, ket[, ...])	Initialize self.
`TransferMatrix.adjoint`()	Return the hermitian conjugate of *self*
`TransferMatrix.eigenvectors`([num_ev, ...])	Find (dominant) eigenvector(s) of self using `scipy.sparse`.
`TransferMatrix.initial_guess`([diag])	Return a diagonal matrix as initial guess for the eigenvector.
`TransferMatrix.matvec`(vec)	Given *vec* as an npc.Array, apply the transfer matrix.
`TransferMatrix.to_matrix`()	Contract *self* to a matrix.

Class Attributes and Properties

`TransferMatrix.acts_on`

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 mean 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 $(TM)^n RP$ (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:

```
|    ---M[i]---M[i+1]- ... --M[i+L]---
|       |       |              |
|    ---N[j]*--N[j+1]* ... --N[j+L]*--
```

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:

```
|  (vL.vL*) ->-TM->- (vR.vR*)   acting on  (vL.vL*) ->-RP
```

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*) – Wheter *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 to `'(vR.vR*)'` for `transpose=True`.

Type *`LegPipe`*

label_split

`['vL', 'vL*']` if `tranpose=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

_contract_legs

Number of physical legs per site + 1.

Type int

matvec(*vec*)

Given *vec* as an npc.Array, apply the transfer matrix.

Parameters **vec** (*Array*) – Vector to act on with the transfermatrix. If not *transposed*, *vec* is the right part *RP* of an environment, with legs `'(vL.vL*)'` in a pipe or splitted. If *transposed*, the left part *LP* of an environment with legs `'(vR*.vR)'`.

Returns **mat_vec** – The tranfer 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(*num_ev=1*, *max_num_ev=None*, *max_tol=1e-12*, *which='LM'*, *v0=None*, ***kwargs*)

Find (dominant) eigenvector(s) of self using `scipy.sparse`.

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()` somtimes 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.speigs*.
- ****kwargs** – Further keyword arguments given to *speigs()*.

Returns

- **eta** (*1D ndarray*) – The eigenvalues, sorted according to *which*.
- **w** (list of *Array*) – The eigenvectors corresponding to *eta*, as npc.Array with LegPipe.

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*, *mode='random'*, *seed=None*)

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:

```
|   -- B[0] -- B[1] -- B[2] -- ...
|       |       |       |
```

We use the following label convention for the *B* (where arrows indicate *qconj*):

```
|  vL ->- B ->- vR
|         |
|         ^
|         p
```

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 *bc_coupling* of *tenpy.models.model.CouplingModel*) are the following:

bc	description
'finite'	Finite MPS, `G0 s1 G1 ... s{L-1} G{l-1}`. This is acchieved by using a trivial left and right bond `s[0] = s[-1] = np.array([1.])`.
'segment'	Generalization of 'finite', describes an MPS embedded in left and right environments. The left environment is described by `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 `... s L s L [s0 G0 s1 G1 ... s{L-1} G{L-1} s{L}] R s R s R ...` (where we save the part in the brackets `[ ... ]`).
'infinite'	infinite MPS (iMPS): we save a 'MPS unit cell' `[s0 G0 s1 G1 ... 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.

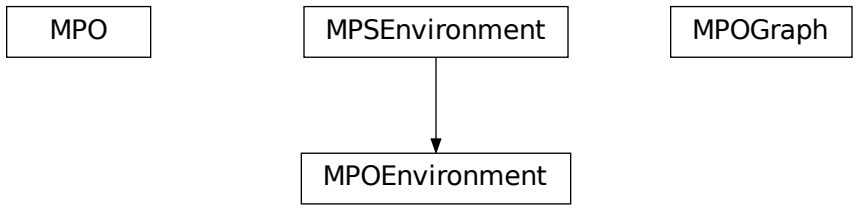
An MPS can be in different 'canonical forms' (see [Vidal2004], [Schollwoeck2011]). To take care of the different canonical forms, algorithms should use functions like *get_theta()*, *get_B()* and *set_B()* instead of accessing them directly, as they return the *B* in the desired form (which can be chosen 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 *MPS.form*.

form	tuple	description
`'B'`	(0, 1)	right canonical: `_B[i] = -- Gamma[i] -- s[i+1]--` The default form, which algorithms asssume.
`'C'`	(0.5, 0.5)	symmetric form: `_B[i] = -- s[i]**0.5 -- Gamma[i] -- s[i+1]**0.5--`
`'A'`	(1, 0)	left canonical: `_B[i] = -- s[i] -- Gamma[i] --`.
`'G'`	(0, 0)	Save only `_B[i] = -- Gamma[i] --`.
`'Th'`	(1, 1)	Form of a local wave function *theta* with singular value on both sides. `psi.get_B(i, 'Th') is equivalent to ``psi.get_theta(i, n=1)`.`
`None`	`None`	General non-canoncial form. Valid form for initialization, but you need to call `canonical_form()` (or similar) before using algorithms.

7.10.3 mpo

- full name: tenpy.networks.mpo
- parent module: `tenpy.networks`
- type: module

Classes



`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.
`MPOGraph`(sites[, bc, max_range])	Representation of an MPO by a graph, based on a 'finite state machine'.

MPO

- full name: tenpy.networks.mpo.MPO
- parent module: *tenpy.networks.mpo*
- type: class

Inheritance Diagram

Methods

MPO.__init__(sites, Ws[, bc, IdL, IdR, ...])	Initialize self.
MPO.dagger()	Return hermition conjugate copy of self.
MPO.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
MPO.expectation_value(psi[, tol, max_range])	Calculate <psi|self|psi>/<psi|psi>.
MPO.from_grids(sites, grids[, bc, IdL, IdR, ...])	Initialize an MPO from *grids*.
MPO.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
MPO.get_IdL(i)	Return index of *IdL* at bond to the *left* of site *i*.
MPO.get_IdR(i)	Return index of *IdR* at bond to the *right* of site *i*.
MPO.get_W(i[, copy])	Return *W* at site *i*.
MPO.get_full_hamiltonian([maxsize])	extract the full Hamiltonian as a d**L``x``d**L matrix.
MPO.get_grouped_mpo(blocklen)	group each *blocklen* subsequent tensors and return result as a new MPO.
MPO.group_sites([n, grouped_sites])	Modify *self* inplace to group sites.
MPO.is_equal(other[, eps, max_range])	Check if *self* and *other* represent the same MPO to precision *eps*.
MPO.is_hermitian([eps, max_range])	Check if *self* is a hermitian MPO.
MPO.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
MPO.set_W(i, W)	Set *W* at site *i*.
MPO.sort_legcharges()	Sort virtual legs by charges.
MPO.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.
MPO.variance(psi[, exp_val])	Calculate <psi|self^2|psi> - <psi|self|psi>^2.

Class Attributes and Properties

`MPO.L`	Number of physical sites; for an iMPO the len of the MPO unit cell.
`MPO.chi`	Dimensions of the virtual bonds.
`MPO.dim`	List of local physical dimensions.
`MPO.finite`	Distinguish MPO vs iMPO.

class `tenpy.networks.mpo.`**`MPO`**(*sites*, *Ws*, *bc='finite'*, *IdL=None*, *IdR=None*, *max_range=None*, *explicit_plus_hc=False*)

Bases: `object`

Matrix product operator, finite (MPO) or infinite (iMPO).

Parameters

- **sites** (list of `Site`) – Defines the local Hilbert space for each site.
- **Ws** (list of `Array`) – The matrices of the MPO. Should have labels `wL, wR, p, p*`.
- **bc** (*`{'finite' | 'segment' | 'infinite'}`*) – Boundary conditions as described in `mps`. `'finite'` requires `Ws[0].get_leg('wL').ind_len = 1`.
- **IdL** (*`(iterable of) {int | None}`*) – Indices on the bonds, which correpond to 'only identities to the left'. A single entry holds for all bonds.
- **IdR** (*`(iterable of) {int | None}`*) – Indices on the bonds, which correpond to 'only identities to the right'.
- **max_range** (*`int | np.inf | None`*) – Maximum range of hopping/interactions (in unit of sites) of the MPO. `None` for unknown.
- **explicit_plus_hc** (*`bool`*) – If True, this flag indicates that the hermitian conjugate of the MPO should be computed and added at runtime, i.e., *self* is not (necessarily) hermitian.

chinfo

The nature of the charge.

Type `ChargeInfo`

sites

Defines the local Hilbert space for each site.

Type list of `Site`

dtype

The data type of the *_W*.

Type type

bc

Boundary conditions as described in `mps`. `'finite'` requires `Ws[0].get_leg('wL').ind_len = 1`.

Type {'finite' | 'segment' | 'infinite'}

IdL

Indices on the bonds (length *L`+1), which correpond to 'only identities to the left'. ``None`* for bonds where it is not set. In standard form, this is *0* (except for unset bonds in finite case)

Type list of {int | None}

IdR
Indices on the bonds (length *L`+1), which correpond to 'only identities to the right'. ``None`* for bonds where it is not set. In standard form, this is the last index on the bond (except for unset bonds in finite case).

Type list of {int | None}

max_range
Maximum range of hopping/interactions (in unit of sites) of the MPO. `None` for unknown.

Type int | np.inf | None

grouped
Number of sites grouped together, see `group_sites()`.

Type int

explicit_plus_hc
If True, this flag indicates that the hermitian conjugate of the MPO should be computed and added at runtime, i.e., *self* is not (necessarily) hermitian.

Type bool

_W
The matrices of the MPO. Labels are `'wL', 'wR', 'p', 'p*'`.

Type list of `Array`

_valid_bc
Class attribute. Valid boundary conditions; the same as for an MPS.

Type tuple of str

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 `sites`, `chinfo`, `max_range` (under these names), `_W` as `"tensors"`, `IdL` as `"index_identity_left"`, `IdR` as `"index_identity_right"`, and `bc` as `"boundary_condition"`. Moreover, it saves `L`, `explicit_plus_hc` and `grouped` as HDF5 attributes, as well as the maximum of `chi` under the name `max_bond_dimension`.

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_grids(*sites*, *grids*, *bc='finite'*, *IdL=None*, *IdR=None*, *Ws_qtotal=None*, *leg0=None*, *max_range=None*, *explicit_plus_hc=False*)

Initialize an MPO from *grids*.

Parameters

- **sites** (list of `Site`) – Defines the local Hilbert space for each site.
- **grids** (*`list of list of list of entries`*) – For each site (outer-most list) a matrix-grid (corresponding to `wL, wR`) with entries being or representing (see *`grid_insert_ops()`*) onsite-operators.
- **bc** (*`{'finite' | 'segment' | 'infinite'}`*) – Boundary conditions as described in *`mps`*.
- **IdL** (*`(iterable of) {int | None}`*) – Indices on the bonds, which correpond to 'only identities to the left'. A single entry holds for all bonds.
- **IdR** (*`(iterable of) {int | None}`*) – Indices on the bonds, which correpond to 'only identities to the right'.
- **Ws_qtotal** (*`(list of) total charge`*) – The *qtotal* to be used for each grid. Defaults to zero charges.
- **leg0** (`LegCharge`) – LegCharge for 'wL' of the left-most *W*. By default, construct it.
- **max_range** (*`int | np.inf | None`*) – Maximum range of hopping/interactions (in unit of sites) of the MPO. `None` for unknown.
- **explicit_plus_hc** (*`bool`*) – If True, the Hermitian conjugate of the MPO is computed at runtime, rather than saved in the MPO.

See also:

grid_insert_ops() used to plug in *entries* of the grid.

tenpy.linalg.np_conserved.grid_outer() used for final conversion.

test_sanity()

Sanity check, raises ValueErrors, if something is wrong.

property L

Number of physical sites; for an iMPO the len of the MPO unit cell.

property dim

List of local physical dimensions.

property finite

Distinguish MPO vs iMPO.

True for an MPO (`bc='finite', 'segment'`), False for an iMPO (`bc='infinite'`).

property chi

Dimensions of the virtual bonds.

get_W(*i*, *copy=False*)

Return *W* at site *i*.

set_W(*i*, *W*)

Set *W* at site *i*.

get_IdL(*i*)

Return index of *IdL* at bond to the *left* of site *i*.

May be `None`.

get_IdR(*i*)
Return index of *IdR* at bond to the *right* of site *i*.

May be `None`.

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 unit cell will be increased from *L* to `factor*L`.

group_sites(*n=2*, *grouped_sites=None*)
Modify *self* inplace 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).

Parameters

- **n** (*int*) – Number of sites to be grouped together.
- **grouped_sites** (None | list of *GroupedSite*) – The sites grouped together.

sort_legcharges()
Sort virtual legs by charges. In place.

The MPO seen as matrix of the `wL, wR` legs is usually very sparse. This sparsity is captured by the LegCharges for these bonds not being sorted and bunched. This requires a tensordot to do more block-multiplications with smaller blocks. This is in general faster for large blocks, but might lead to a larger overhead for small blocks. Therefore, this function allows to sort the virtual legs by charges.

expectation_value(*psi*, *tol=1e-10*, *max_range=100*)
Calculate `<psi|self|psi>/<psi|psi>`.

For a finite MPS, simply contract the network `<psi|self|psi>`. For an infinite MPS, it assumes that *self* is the a of terms, with *IdL* and *IdR* defined on each site. Under this assumption, it calculates the expectation value of terms with the left-most non-trivial operator inside the MPO unit cell and returns the average value per site.

Parameters

- **psi** (*MPS*) – State for which the expectation value should be taken.
- **tol** (*float*) – Ignored for finite *psi*. For infinite MPO containing exponentially decaying long-range terms, stop evaluating further terms if the terms in *LP* have norm < *tol*.
- **max_range** (*int*) – Ignored for finite *psi*. Contract at most `self.L * max_range` sites, even if *tol* is not reached. In that case, issue a warning.

Returns **exp_val** – The expectation value of *self* with respect to the state *psi*. For an infinite MPS: the density per site.

Return type float/complex

variance(*psi*, *exp_val=None*)
Calculate `<psi|self^2|psi> - <psi|self|psi>^2`.

Works only for finite systems. Ignores the *norm* of *psi*.

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?

Parameters

- **psi** (*MPS*) – State for which the variance should be taken.
- **exp_val** (*float/complex | None*) – The result of `<psi|self|psi> = self.expectation_value(psi)` if known; otherwise obtained from *expectation_value()*. (Set this to 0 to obtain only the part `<psi|self^2|psi>`.)

dagger()
Return hermition conjugate copy of self.

is_hermitian(*eps=1e-10*, *max_range=None*)
Check if *self* is a hermitian MPO.

Shorthand for `self.is_equal(self.dagger(), eps, max_range)`.

is_equal(*other*, *eps=1e-10*, *max_range=None*)
Check if *self* and *other* represent the same MPO to precision *eps*.

To compare them efficiently we view *self* and *other* as MPS and compare the overlaps `abs(<self|self> + <other|other> - 2 Re(<self|other>)) < eps*(<self|self>+<other|other>)`

Parameters

- **other** (*MPO*) – The MPO to compare to.
- **eps** (*float*) – Precision threshold what counts as zero.
- **max_range** (*None | int*) – Ignored for finite MPS; for finite MPS we consider only the terms contained in the sites with indices `range(self.L + max_range)`. None defaults to *max_range* (or *L* in case this is infinite or None).

Returns **equal** – Whether *self* equals *other* to the desired precision.

Return type bool

get_grouped_mpo(*blocklen*)
group each *blocklen* subsequent tensors and return result as a new MPO.

Deprecated since version 0.5.0: Make a copy and use *group_sites()* instead.

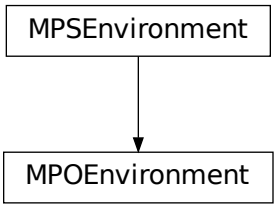
get_full_hamiltonian(*maxsize=1000000.0*)
extract the full Hamiltonian as a `d**L``x``d**L` matrix.

Deprecated since version 0.5.0: Use *tenpy.algorithms.exact_diag.ExactDiag.from_H_mpo()* instead.

MPOEnvironment

- full name: tenpy.networks.mpo.MPOEnvironment
- parent module: *tenpy.networks.mpo*
- type: class

Inheritance Diagram



Methods

`MPOEnvironment.__init__`(bra, H, ket[, ...])	Initialize self.
`MPOEnvironment.del_LP`(i)	Delete stored part strictly to the left of site *i*.
`MPOEnvironment.del_RP`(i)	Delete storde part scrictly to the right of site *i*.
`MPOEnvironment.expectation_value`(ops[, ...])	Expectation value `<bra|ops|ket>` of (n-site) operator(s).
`MPOEnvironment.full_contraction`(i0)	Calculate the energy by a full contraction of the network.
`MPOEnvironment.get_LP`(i[, store])	Calculate LP at given site from nearest available one (including *i*).
`MPOEnvironment.get_LP_age`(i)	Return number of physical sites in the contractions of get_LP(i).
`MPOEnvironment.get_RP`(i[, store])	Calculate RP at given site from nearest available one (including *i*).
`MPOEnvironment.get_RP_age`(i)	Return number of physical sites in the contractions of get_RP(i).
`MPOEnvironment.get_initialization_data`()	Return data for (re-)initialization.
`MPOEnvironment.init_LP`(i)	Build initial left part `LP`.
`MPOEnvironment.init_RP`(i)	Build initial right part `RP` for an MPS/MPOEnvironment.
`MPOEnvironment.set_LP`(i, LP, age)	Store part to the left of site *i*.
`MPOEnvironment.set_RP`(i, RP, age)	Store part to the right of site *i*.
`MPOEnvironment.test_sanity`()	Sanity check, raises ValueErrors, if something is wrong.

class `tenpy.networks.mpo.`**`MPOEnvironment`**(*bra*, *H*, *ket*, *init_LP=None*, *init_RP=None*, *age_LP=0*, *age_RP=0*)

Bases: *`tenpy.networks.mps.MPSEnvironment`*

Stores partial contractions of $< bra|H|ket >$ for an MPO H.

The network for a contraction $< bra|H|ket >$ of an MPO H bewteen two MPS looks like:

```
|      .------>-M[0]-->-M[1]-->-M[2]-->- ...  ->--.
|      |         |        |        |                |
|      |         ^        ^        ^                |
```

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```
|      |         |        |        |                   |
|      LP[0] ->-W[0]-->-W[1]-->-W[2]-->- ...  ->- RP[-1]
|      |         |        |        |                   |
|      |         ^        ^        ^                   |
|      |         |        |        |                   |
|      .------<-N[0]*-<-N[1]*-<-N[2]*-<- ...  -<--.
```

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 *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*.

Parameters

- **bra** (*MPS*) – The MPS to project on. Should be given in usual 'ket' form; we call *conj()* on the matrices directly.
- **H** (*MPO*) – The MPO sandwiched between *bra* and *ket*. Should have 'IdL' and 'IdR' set on the first and last bond.
- **ket** (`MPS`) – The MPS on which *H* acts. May be identical with *bra*.
- **init_LP** (`None` | *Array*) – Initial very left part `LP`. If `None`, build trivial one with :meth`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*.

H

The MPO sandwiched between *bra* and *ket*.

Type *MPO*

test_sanity()

Sanity check, raises ValueErrors, if something is wrong.

init_LP(*i*)

Build initial left part `LP`.

Parameters **i** (*int*) – Build `LP` left of site *i*.

Returns **init_LP** – Identity contractible with the *vL* leg of `.ket.get_B(i)`, multiplied with a unit vector nonzero in `H.IdL[i]`, with labels `'vR*', 'wR', 'vR'`.

Return type *Array*

init_RP(*i*)

Build initial right part `RP` for an MPS/MPOEnvironment.

Parameters **i** (*int*) – Build `RP` right of site *i*.

Returns **init_RP** – Identity contractible with the *vR* leg of `self.get_B(i)`, multiplied with a unit vector nonzero in `H.IdR[i]`, with labels `'vL*', 'wL', 'vL'`.

Return type *Array*

get_LP(*i*, *store=True*)

Calculate LP at given site from nearest available one (including *i*).

The returned `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*) – Wheter 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'  ->---M[i+1]-- ... --M[L-1]----.
|                 |               |          |
|      'wL'  ->---W[i+1]-- ... --W[L-1]----RP[-1]
|                 |               |          |
|      'vL*' -<---N[i+1]*- ... --N[L-1]*---.
```

Parameters

- **i** (*int*) – The returned *RP* will contain the contraction *strictly* rigth of site *i*.
- **store** (*bool*) – Wheter 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.

del_LP(*i*)
Delete stored part strictly to the left of site *i*.

del_RP(*i*)
Delete storde part scrictly to the right of site *i*.

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 examples 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 wich the expectation value should be taken, All operators should all have the same number of legs (namely *2 n*). If less than `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, `exp_vals[i] = <bra|ops[i]|ket>`, where `ops[i]` acts on site(s) `j, j+1, ..., j+{n-1}` with `j=sites[i]`.

Return type 1D ndarray

Examples

One site examples (n=1):

```
>>> env.expectation_value('Sz')
[Sz0, Sz1, ..., Sz{L-1}]
>>> env.expectation_value(['Sz', 'Sx'])
[Sz0, Sx1, Sz2, Sx3, ... ]
>>> env.expectation_value('Sz', sites=[0, 3, 4])
[Sz0, Sz3, Sz4]
```

Two site example (n=2), assuming homogeneous sites:

```
>>> SzSx = npc.outer(psi.sites[0].Sz.replace_labels(['p', 'p*'], ['p0', 'p0*
↪']),
                     psi.sites[1].Sx.replace_labels(['p', 'p*'], ['p1', 'p1*
↪']))
>>> env.expectation_value(SzSx)
[Sz0Sx1, Sz1Sx2, Sz2Sx3, ... ]   # with len L-1 for finite bc, or L for␣
↪infinite
```

Example measuring <bra|SzSx|ket> on each second site, for inhomogeneous sites:

```
>>> SzSx_list = [npc.outer(psi.sites[i].Sz.replace_labels(['p', 'p*'], ['p0',
↪'p0*']),
...                         psi.sites[i+1].Sx.replace_labels(['p', 'p*'], ['p1
↪', 'p1*']))
...               for i in range(0, psi.L-1, 2)]
>>> env.expectation_value(SzSx_list, range(0, psi.L-1, 2))
[Sz0Sx1, Sz2Sx3, Sz4Sx5, ...]
```

---

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*.

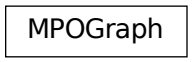
set_RP(*i*, *RP*, *age*)

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

MPOGraph.__init__(sites[, bc, max_range])	Initialize self.
MPOGraph.add(i, keyL, keyR, opname, strength)	Insert an edge into the graph.
MPOGraph.add_missing_IdL_IdR()	Add missing identity ('Id') edges connecting 'IdL'->'IdL' and ``'IdR'->'IdR'.
MPOGraph.add_string(i, j, key[, opname, ...])	Insert a bunch of edges for an 'operator string' into the graph.
MPOGraph.build_MPO([Ws_qtotal, leg0])	Build the MPO represented by the graph (*self*).
MPOGraph.from_term_list(term_list, sites, bc)	Initialize form a list of operator terms and prefactors.
MPOGraph.from_terms(onsite_terms, ...)	Initialize an *MPOGraph* from OnsiteTerms and CouplingTerms.
MPOGraph.has_edge(i, keyL, keyR)	True if there is an edge from *keyL* on bond (i-1, i) to *keyR* on bond (i, i+1).
MPOGraph.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.

Class Attributes and Properties

MPOGraph.L	Number of physical sites; for infinite boundaries the length of the unit cell.

class tenpy.networks.mpo.**MPOGraph**(*sites*, *bc='finite'*, *max_range=None*)

Bases: object

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 virtul 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 'idenity 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.

Type list of set of keys

graph

For each site *i* a dictionary `{keyL: {keyR: [(opname, strength)]}}` with `keyL in vertices[i]` and `keyR in vertices[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(*onsite_terms*, *coupling_terms*, *sites*, *bc*)

Initialize an *`MPOGraph`* from OnsiteTerms and CouplingTerms.

Parameters

- **onsite_terms** (*`OnsiteTerms`*) – Onsite terms to be added to the new *`MPOGraph`*.
- **coupling_terms** (*`CouplingTerms`* | *`MultiCouplingTerms`*) – Coupling terms to be added to the new *`MPOGraph`*.

- **sites** (list of *Site*) – Local sites of the Hilbert space.
- **bc** (`'finite' | 'infinite'`) – MPO boundary conditions.

Returns **graph** – Initialized with the given terms.

Return type *MPOGraph*

See also:

from_term_list() equivalent for other representation terms.

classmethod from_term_list(*term_list*, *sites*, *bc*)

Initialize form 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.

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*, *keyL*, *keyR*, *opname*, *strength*, *check_op=True*, *skip_existing=False*)

Insert an edge into the graph.

Parameters

- **i** (*int*) – Site index at which the edge of the graph is to be inserted.
- **keyL** (*hashable*) – The state at bond (i-1, i) to connect from.
- **keyR** (*hashable*) – The state at bond (i, i+1) to connect to.
- **opname** (*str*) – Name of the operator.
- **strength** (*str*) – Prefactor of the operator to be inserted.
- **check_op** (*bool*) – Whether to check that 'opname' exists on the given *site*.
- **skip_existing** (*bool*) – If `True`, skip adding the graph node if it exists (with same keys and *opname*).

add_string(*i*, *j*, *key*, *opname='Id'*, *check_op=True*, *skip_existing=True*)

Insert a bunch of edges for an 'operator string' into the graph.

Terms like $S_i^z S_j^z$ actually stand for $S_i^z \otimes \prod_{i<k<j} \mathbb{1}_k \otimes S_j^z$. This function adds the $\mathbb{1}$ terms to the graph.

Parameters

- **j** (*i,*) – 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.

- **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, key, key)`.
- **opname** (*str*) – Name of the operator to be used for the string. Useful for the Jordan-Wigner transformation to fermions.
- **skip_existing** (*bool*) – Whether existing graph nodes should be skipped.

Returns **label_j** – The *key* on the left of site j to connect to. Usually the same as the parameter *key*, except if `j - i > self.L`, in which case we use the additional labels `(key, 1)`, `(key, 2)`, ... to generate couplings over multiple unit cells.

Return type hashable

add_missing_IdL_IdR()

Add missing identity ('Id') edges connecting `'IdL'->'IdL' and ``'IdR'->'IdR'`.

For `bc='infinite'`, insert missing identities at *all* bonds. For `bc='finite' | 'segment'` only insert `'IdL'->'IdL'` to the left of the rightmost existing 'IdL' and `'IdR'->'IdR'` to the right of the leftmost existing 'IdR'.

This function should be called *after* all other operators have been inserted.

has_edge(*i*, *keyL*, *keyR*)

True if there is an edge from *keyL* on bond (i-1, i) to *keyR* on bond (i, i+1).

build_MPO(*Ws_qtotal=None*, *leg0=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.
- **leg0** (None | `npc.LegCharge`) – The charges to be used for the very first leg (which is a gauge freedom). If `None` (default), use zeros.

Returns **mpo** – the MPO which self represents.

Return type *MPO*

Functions

grid_insert_ops(site, grid)	Replaces entries representing operators in a grid of `W[i]` with npc.Arrays.

grid_insert_ops

- full name: tenpy.networks.mpo.grid_insert_ops
- parent module: *tenpy.networks.mpo*
- type: function

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`*}

Module description

Matrix product operator (MPO).

An MPO is the generalization of an *`MPS`* to operators. Graphically:

```
|       ^         ^         ^
|       |         |         |
|  ->- W[0] ->- W[1] ->- W[2] ->- ...
|       |         |         |
|       ^         ^         ^
```

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 canoncial 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
```

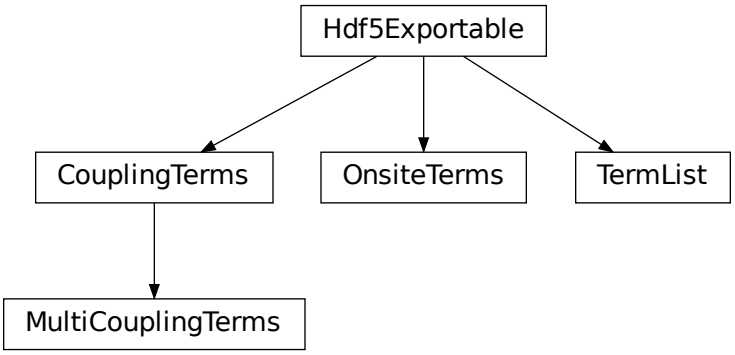
If an MPO describes a sum of local terms (e.g. most Hamiltonians), some bond indices correspond to 'only identities to the left/right'. We store these indices in *IdL* and *IdR* (if there are such indices).

Similar as for the MPS, a bond index `i` is *left* of site *i*, i.e. between sites `i-1` and `i`.

7.10.4 terms

- full name: tenpy.networks.terms
- parent module: *`tenpy.networks`*
- type: module

Classes

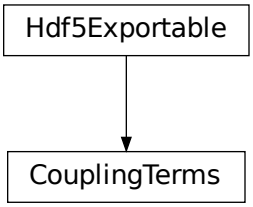


`CouplingTerms`(L)	Operator names, site indices and strengths representing two-site coupling terms.
`MultiCouplingTerms`(L)	Operator names, site indices and strengths representing general M-site coupling terms.
`OnsiteTerms`(L)	Operator names, site indices and strengths representing onsite terms.
`TermList`(terms, strength)	A list of terms (=operator names and sites they act on) and associated strengths.

CouplingTerms

- full name: tenpy.networks.terms.CouplingTerms
- parent module: `tenpy.networks.terms`
- type: class

Inheritance Diagram



Methods

`CouplingTerms.__init__`(L)	Initialize self.
`CouplingTerms.add_coupling_term`(strength, i, ...)	Add a two-site coupling term on given MPS sites.
`CouplingTerms.add_to_graph`(graph)	Add terms from `coupling_terms` to an MPOGraph.
`CouplingTerms.coupling_term_handle_JW`(..., ...])	Helping function to call before `add_multi_coupling_term()`.
`CouplingTerms.from_hdf5`(hdf5_loader, h5gr, ...)	Load instance from a HDF5 file.
`CouplingTerms.max_range`()	Determine the maximal range in `coupling_terms`.
`CouplingTerms.plot_coupling_terms`(ax, lat[, ...])	"Plot coupling terms into a given lattice.
`CouplingTerms.remove_zeros`([tol_zero])	Remove entries close to 0 from `coupling_terms`.
`CouplingTerms.save_hdf5`(hdf5_saver, h5gr, ...)	Export *self* into a HDF5 file.
`CouplingTerms.to_TermList`()	Convert `onsite_terms` into a *`TermList`*.
`CouplingTerms.to_nn_bond_Arrays`(sites)	Convert the `coupling_terms` into Arrays on nearest neighbor bonds.

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* occuring 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.
- **`j`** (*`i,`*) – 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.

- **op2** (*op1,*) – 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.

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

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'`.

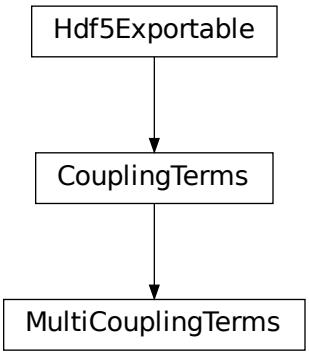
Parameters

- **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.

MultiCouplingTerms

- full name: tenpy.networks.terms.MultiCouplingTerms
- parent module: *tenpy.networks.terms*
- type: class

Inheritance Diagram



Methods

`MultiCouplingTerms.__init__`(L)	Initialize self.
MultiCouplingTerms.add_coupling_term(...[, ...])	Add a two-site coupling term on given MPS sites.
MultiCouplingTerms.add_multi_coupling_term(...)	Add a multi-site coupling term.
MultiCouplingTerms.add_to_graph(graph[, _i, ...])	Add terms from `coupling_terms` to an MPOGraph.
MultiCouplingTerms.coupling_term_handle_JW(...)	Helping function to call before `add_multi_coupling_term()`.
MultiCouplingTerms.from_hdf5(hdf5_loader, ...)	Load instance from a HDF5 file.
MultiCouplingTerms.max_range()	Determine the maximal range in `coupling_terms`.
MultiCouplingTerms.multi_coupling_term_handle_JW(...)	Helping function to call before `add_multi_coupling_term()`.
MultiCouplingTerms.plot_coupling_terms(ax, lat)	"Plot coupling terms into a given lattice.
MultiCouplingTerms.remove_zeros([tol_zero, _d0])	Remove entries close to 0 from `coupling_terms`.
MultiCouplingTerms.save_hdf5(hdf5_saver, ...)	Export *self* into a HDF5 file.

continues on next page

Table 161 – continued from previous page

MultiCouplingTerms.to_TermList()	Convert `onsite_terms` into a *TermList*.
MultiCouplingTerms.to_nn_bond_Arrays(sites)	Convert the `coupling_terms` into Arrays on nearest neighbor bonds.

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.

L

Number of sites.

Type int

coupling_terms

Nested dictionaries of the following form:

```
{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*M` dictionaries. Note that always `i < j < k < ... < l`, but entries with `j,k,l >= 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*, *ijkl*, *ops_ijkl*, *op_string='Id'*)

Add a multi-site coupling term.

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, ... = ijkl*, 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_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*. A single name holds for all in-between segments.

multi_coupling_term_handle_JW(*strength*, *term*, *sites*, *op_string=None*)

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.

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* occuring in a term of `coupling_terms`.

Return type int

add_to_graph(*graph*, *_i=None*, *_d1=None*, *_label_left=None*)

Add terms from `coupling_terms` to an MPOGraph.

Parameters

- **graph** (*MPOGraph*) – The graph into which the terms from `coupling_terms` should be added.
- **_d1, _label_left** (*_i,*) – Should not be given; only needed for recursion.

remove_zeros(*tol_zero=1e-15*, *_d0=None*)

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.
- **_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.
- **j** (*i,*) – 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.

- **op2** (*op1,*) – 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.

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

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.

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.

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*.

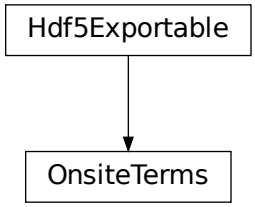
Returns **H_bond** – The *coupling_terms* rewritten as `sum_i H_bond[i]` for MPS indices `i`. `H_bond[i]` acts on sites `(i-1, i)`, `None` represents 0. Legs of each `H_bond[i]` are `['p0', 'p0*', 'p1', 'p1*']`.

Return type list of {*Array* | None}

OnsiteTerms

- full name: tenpy.networks.terms.OnsiteTerms
- parent module: *tenpy.networks.terms*
- type: class

Inheritance Diagram



Methods

`OnsiteTerms.__init__`(L)	Initialize self.
`OnsiteTerms.add_onsite_term`(strength, i, op)	Add a onsite term on a given MPS site.
`OnsiteTerms.add_to_graph`(graph)	Add terms from `onsite_terms` to an MPOGraph.
`OnsiteTerms.add_to_nn_bond_Arrays`(H_bond, ...)	Add `self.onsite_terms` into nearest-neighbor bond arrays.
`OnsiteTerms.from_hdf5`(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
`OnsiteTerms.remove_zeros`([tol_zero])	Remove entries close to 0 from `onsite_terms`.
`OnsiteTerms.save_hdf5`(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
`OnsiteTerms.to_Arrays`(sites)	Convert the `onsite_terms` into a list of np_conserved Arrays.
`OnsiteTerms.to_TermList`()	Convert `onsite_terms` into a *`TermList`*.

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 meth:*add_onsite_term*. For each index *i* a dictionary `{'opname': strength}` defining the onsite terms.

Type list of dict

`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'`.

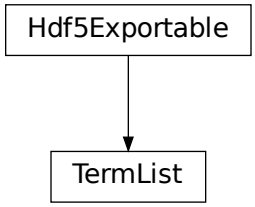
Parameters

- **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



Methods

`TermList.__init__`(terms, strength)	Initialize self.
TermList.from_hdf5(hdf5_loader, h5gr, subpath)	Load instance from a HDF5 file.
TermList.order_combine(sites)	Order and combine operators in each term.
TermList.save_hdf5(hdf5_saver, h5gr, subpath)	Export *self* into a HDF5 file.
TermList.to_OnsiteTerms_CouplingTerms(sites)	Convert to *OnsiteTerms* and *CouplingTerms*

class tenpy.networks.terms.**TermList**(*terms*, *strength*)

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.

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 pref-

actor or strength (e.g. expectation value).

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 (e.g. expectation value).

Type 1D ndarray

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.

Parameters **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

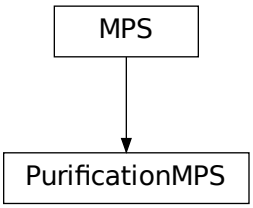
Classes to store a collection of operator names and sites they act on, together with prefactors.

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.

7.10.5 purification_mps

- full name: tenpy.networks.purification_mps
- parent module: *tenpy.networks*
- type: module

Classes

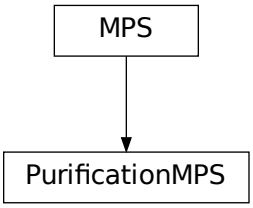


PurificationMPS(sites, Bs, SVs[, bc, form, norm])	An MPS representing a finite-temperature ensemble using purification.

PurificationMPS

- full name: tenpy.networks.purification_mps.PurificationMPS
- parent module: *tenpy.networks.purification_mps*
- type: class

Inheritance Diagram



Methods

PurificationMPS.__init__(sites, Bs, SVs[, ...])	Initialize self.
PurificationMPS.add(other, alpha, beta[, cutoff])	Return an MPS which represents alpha|self> + beta |others>.
PurificationMPS.apply_local_op(i, op[, ...])	Apply a local (one or multi-site) operator to *self*.
PurificationMPS.average_charge([bond])	Return the average charge for the block on the left of a given bond.
PurificationMPS.canonical_form([renormalize])	Bring self into canonical 'B' form, (re-)calculate singular values.
PurificationMPS.canonical_form_finite([...])	Bring a finite (or segment) MPS into canonical form (in place).
PurificationMPS.canonical_form_infinite([...])	Bring an infinite MPS into canonical form (in place).
PurificationMPS.charge_variance([bond])	Return the charge variance on the left of a given bond.
PurificationMPS.compute_K(perm[, swap_op, ...])	Compute the momentum quantum numbers of the entanglement spectrum for 2D states.
PurificationMPS.convert_form([new_form])	Tranform self into different canonical form (by scaling the legs with singular values).
PurificationMPS.copy()	Returns a copy of *self*.
PurificationMPS.correlation_function(ops1, ops2)	Correlation function <psi|op1_i op2_j|psi>/<psi|psi> of single site operators.
PurificationMPS.correlation_length([target, ...])	Calculate the correlation length by diagonalizing the transfer matrix.
PurificationMPS.enlarge_mps_unit_cell([factor])	Repeat the unit cell for infinite MPS boundary conditions; in place.
PurificationMPS.entanglement_entropy([n, ...])	Calculate the (half-chain) entanglement entropy for all nontrivial bonds.
PurificationMPS.entanglement_entropy_segment([...])	Calculate entanglement entropy for general geometry of the bipartition.
PurificationMPS.entanglement_spectrum([...])	return entanglement energy spectrum.
PurificationMPS.expectation_value(ops[, ...])	Expectation value <psi|ops|psi>/<psi|psi> of (n-site) operator(s).
PurificationMPS.expectation_value_multi_sites(...)	Expectation value <psi|op0_{i0}op1_{i0+1}...opN_{i0+N}|psi>/<psi|psi>.
PurificationMPS.expectation_value_term(term)	Expectation value <psi|op_{i0}op_{i1}...op_{iN}|psi>/<psi|psi>.
PurificationMPS.expectation_value_terms_sum(...)	Calculate expectation values for a bunch of terms and sum them up.
PurificationMPS.from_Bflat(sites, Bflat[, ...])	Construct a matrix product state from a set of numpy arrays *Bflat* and singular vals.
PurificationMPS.from_full(sites, psi[, ...])	Construct an MPS from a single tensor *psi* with one leg per physical site.
PurificationMPS.from_hdf5(hdf5_loader, h5gr, ...)	Load instance from a HDF5 file.
PurificationMPS.from_infiniteT(sites[, bc, form])	Initial state corresponding to infinite-Temperature ensemble.

continues on next page

Table 166 – continued from previous page

PurificationMPS.from_lat_product_state(lat, ...)	Construct an MPS from a product state given in lattice coordinates.
PurificationMPS.from_product_state(sites, ...)	Construct a matrix product state from a given product state.
PurificationMPS.from_singlets(site, L, pairs)	Create an MPS of entangled singlets.
PurificationMPS.gauge_total_charge([qtotal, ...])	Gauge the legcharges of the virtual bonds such that the MPS has a total *qtotal*.
PurificationMPS.get_B(i[, form, copy, ...])	Return (view of) *B* at site *i* in canonical form.
PurificationMPS.get_SL(i)	Return singular values on the left of site *i*
PurificationMPS.get_SR(i)	Return singular values on the right of site *i*
PurificationMPS.get_grouped_mps(blocklen)	contract blocklen subsequent tensors into a single one and return result as a new MPS.
PurificationMPS.get_op(op_list, i)	Given a list of operators, select the one corresponding to site *i*.
PurificationMPS.get_rho_segment(segment)	Return reduced density matrix for a segment.
PurificationMPS.get_theta(i[, n, cutoff, ...])	Calculates the *n*-site wavefunction on `sites[i:i+n]`.
PurificationMPS.get_total_charge([...])	Calculate and return the *qtotal* of the whole MPS (when contracted).
PurificationMPS.group_sites([n, grouped_sites])	Modify *self* inplace to group sites.
PurificationMPS.group_split([trunc_par])	Modify *self* inplace to split previously grouped sites.
PurificationMPS.increase_L([new_L])	Modify *self* inplace to enlarge the MPS unit cell; in place.
PurificationMPS.mutinf_two_site([max_range, ...])	Calculate the two-site mutual information $I(i:j)$.
PurificationMPS.norm_test()	Check that self is in canonical form.
PurificationMPS.overlap(other[, ...])	Compute overlap `<self|other>`.
PurificationMPS.permute_sites(perm[, ...])	Applies the permutation perm to the state (inplace).
PurificationMPS.probability_per_charge([bond])	Return probabilites of charge value on the left of a given bond.
PurificationMPS.roll_mps_unit_cell([shift])	Shift the section we define as unit cellof an infinite MPS; in place.
PurificationMPS.save_hdf5(hdf5_saver, h5gr, ...)	Export *self* into a HDF5 file.
PurificationMPS.set_B(i, B[, form])	Set *B* at site *i*.
PurificationMPS.set_SL(i, S)	Set singular values on the left of site *i*
PurificationMPS.set_SR(i, S)	Set singular values on the right of site *i*
PurificationMPS.swap_sites(i[, swapOP, ...])	Swap the two neighboring sites *i* and *i+1* (inplace).
PurificationMPS.test_sanity()	Sanity check, raises ValueErrors, if something is wrong.

Class Attributes and Properties

`PurificationMPS.L`	Number of physical sites; for an iMPS the len of the MPS unit cell.
`PurificationMPS.chi`	Dimensions of the (nontrivial) virtual bonds.
`PurificationMPS.dim`	List of local physical dimensions.
`PurificationMPS.finite`	Distinguish MPS vs iMPS.
`PurificationMPS.nontrivial_bonds`	Slice of the non-trivial bond indices, depending on `self.bc`.

class tenpy.networks.purification_mps.**PurificationMPS**(*sites*, *Bs*, *SVs*, *bc='finite'*, *form='B'*, *norm=1.0*)

Bases: `tenpy.networks.mps.MPS`

An MPS representing a finite-temperature ensemble using purification.

Similar as an MPS, but each B has now the four legs `'vL', 'vR', 'p', 'q'`. From the point of algorithms, it is to be considered as a ususal MPS by combining the legs p and q, but all physical operators act only on the p part. For example, the right-canonical form is defined as if the legs 'p' and 'q' would be combined, e.g. a right-canonical B full-fills:

```
npc.tensordot(B, B.conj(),axes=[['vR', 'p', 'q'], ['vR*', 'p*', 'q*']]) == \
    npc.eye_like(B, axes='vL')  # up to round-off errors
```

For expectation values / correlation functions, all operators are to understood to act on p only, i.e. they act trivial on q, so we just trace over `'q', 'q*'`.

See also the docstring of the module for details.

test_sanity()

Sanity check, raises ValueErrors, if something is wrong.

classmethod from_infiniteT(*sites*, *bc='finite'*, *form='B'*)

Initial state corresponding to infinite-Temperature ensemble.

Parameters

- **sites** (list of `Site`) – The sites defining the local Hilbert space.
- **bc** (`{'finite', 'segment', 'infinite'}`) – MPS boundary conditions as described in `MPS`.
- **form** ((list of) `{'B' | 'A' | 'C' | 'G' | None` | tuple(float, float)}) – The canonical form of the stored 'matrices', see table in `mps`. A single choice holds for all of the entries.

Returns **infiniteT_MPS** – Describes the infinite-temperature (grand canonical) ensemble, i.e. expectation values give a trace over all basis states.

Return type `PurificationMPS`

entanglement_entropy_segment(*segment=[0]*, *first_site=None*, *n=1*, *legs='p'*)

Calculate entanglement entropy for general geometry of the bipartition.

This function is similar as `entanglement_entropy()`, but for more general geometry of the region A to be a segment of a *few* sites.

This is acchieved by explicitly calculating the reduced density matrix of A and thus works only for small segments.

Parameters

- **segment** (*list of int*) – Given a first site *i*, the region `A_i` is defined to be `[i+j for j in segment]`.
- **first_site** (`None` | (iterable of) int) – Calculate the entropy for segments starting at these sites. `None` defaults to `range(L-segment[-1])` for finite or *range(L)* for infinite boundary conditions.
- **n** (*int | float*) – Selects which entropy to calculate; *n=1* (default) is the ususal von-Neumann entanglement entropy, otherwise the *n*-th Renyi entropy.
- **leg** (*'p', 'q', 'pq'*) – Whether we look at the entanglement entropy in both (*pq*) or only one of auxiliar (*q*) and physical (*p*) space.

Returns entropies – `entropies[i]` contains the entropy for the the region `A_i` defined above.

Return type 1D ndarray

mutinf_two_site (*max_range=None*, *n=1*, *legs='p'*)

Calculate the two-site mutual information $I(i:j)$.

Calculates $I(i:j) = S(i) + S(j) - S(i,j)$, where $S(i)$ is the single site entropy on site i and $S(i,j)$ the two-site entropy on sites i, j.

Parameters

- **max_range** (*int*) – Maximal distance `|i-j|` for which the mutual information should be calculated. `None` defaults to *L-1*.
- **n** (*float*) – Selects the entropy to use, see *entropy()*.
- **leg** (*'p', 'q', 'pq'*) – Whether we look at the entanglement entropy in both (*pq*) or only one of auxiliar (*q*) and physical (*p*) space.

Returns

- **coords** (*2D array*) – Coordinates for the mutinf array.
- **mutinf** (*1D array*) – `mutinf[k]` is the mutual information $I(i:j)$ between the sites `i, j = coords[k]`.

swap_sites (*i*, *swapOP='auto'*, *trunc_par={}*)

Swap the two neighboring sites *i* and *i+1* (inplace).

Exchange two neighboring sites: form theta, 'swap' the physical legs and split with an svd. While the 'swap' is just a transposition/relabeling for bosons, one needs to be careful about the sign for fermions.

Parameters

- **i** (*int*) – Swap the two sites at positions *i* and *i+1*.
- **swap_op** (`None` | `'auto'` | *Array*) – The operator used to swap the phyiscal legs of the two-site wave function *theta*. For `None`, just transpose/relabel the legs, for `'auto'` also take care of fermionic signs. Alternative give an npc *Array* which represents the full operator used for the swap. Should have legs `['p0', 'p1', 'p0*', 'p1*']` whith `'p0', 'p1*'` contractible.
- **trunc_par** (*dict*) – Parameters for truncation, see `truncate()`. *chi_max* defaults to `max(self.chi)`.

Returns trunc_err – The error of the represented state introduced by the truncation after the swap.

Return type *TruncationError*

property L
Number of physical sites; for an iMPS the len of the MPS unit cell.

add(*other*, *alpha*, *beta*, *cutoff=1e-15*)
Return an MPS which represents `alpha|self> + beta |others>`.

Works only for 'finite', 'segment' boundary conditions. For 'segment' boundary conditions, the virtual legs on the very left/right are assumed to correspond to each other (i.e. self and other have the same state outside of the considered segment). Takes into account `norm`.

Parameters

- **other** (`MPS`) – Another MPS of the same length to be added with self.
- **beta** (*alpha,*) – Prefactors for self and other. We calculate `alpha * |self> + beta * |other>`
- **cutoff** (*float | None*) – Cutoff of singular values used in the SVDs.

Returns

- **sum** (`MPS`) – An MPS representing `alpha|self> + beta |other>`. Has same total charge as *self*.
- **U_L, V_R** (*Array*) – Only returned for `'segment'` boundary conditions. The unitaries defining the new left and right Schmidt states in terms of the old ones, with legs `'vL', 'vR'`.

apply_local_op(*i*, *op*, *unitary=None*, *renormalize=False*, *cutoff=1e-13*)
Apply a local (one or multi-site) operator to *self*.

Note that this destroys the canonical form if the local operator is non-unitary. Therefore, this function calls *canonical_form()* if necessary.

Parameters

- **i** (*int*) – (Left-most) index of the site(s) on which the operator should act.
- **op** (*str | npc.Array*) – A physical operator acting on site *i*, with legs `'p', 'p*'` for a single-site operator or with legs `['p0', 'p1', ...], ['p0*', 'p1*', ...]` for an operator acting on *n*>=2 sites. Strings (like `'Id', 'Sz'`) are translated into single-site operators defined by `sites`.
- **unitary** (*None | bool*) – Whether *op* is unitary, i.e., whether the canonical form is preserved (`True`) or whether we should call *canonical_form()* (`False`). `None` checks whether `norm(op dagger(op) - identity)` is smaller than *cutoff*.
- **renormalize** (*bool*) – Whether the final state should keep track of the norm (False, default) or be renormalized to have norm 1 (True).
- **cutoff** (*float*) – Cutoff for singular values if *op* acts on more than one site (see *from_full()*). (And used as cutoff for a unspecified *unitary*.)

average_charge(*bond=0*)
Return the average charge for the block on the left of a given bond.

For example for particle number conservation, define $N_b = sum_{i<b} n_i$ for a given bond b. Then this function returns $< \psi | N_b | \psi >$.

Parameters **bond** (*int*) – The bond to be considered. The returned charges are summed over the sites left of *bond*.

Returns **average_charge** – For each type of charge in `chinfo` the average value when summing the charge values over sites left of the given bond.

Return type 1D array

canonical_form(*renormalize=True*)

Bring self into canonical 'B' form, (re-)calculate singular values.

Simply calls `canonical_form_finite()` or `canonical_form_infinite()`.

canonical_form_finite(*renormalize=True*, *cutoff=0.0*)

Bring a finite (or segment) MPS into canonical form (in place).

If any site is in `form` `None`, it does *not* use any of the singular values *S* (for 'finite' boundary conditions, or only the very left *S* for 'segment' b.c.). If all sites have a *form*, it respects the *form* to ensure that one *S* is included per bond. The final state is always in right-canonical 'B' form.

Performs one sweep left to right doing QR decompositions, and one sweep right to left doing SVDs calculating the singular values.

Parameters

- **renormalize** (*bool*) – Whether a change in the norm should be discarded or used to update `norm`.
- **cutoff** (*float | None*) – Cutoff of singular values used in the SVDs.

Returns **U_L, V_R** – Only returned for `'segment'` boundary conditions. The unitaries defining the new left and right Schmidt states in terms of the old ones, with legs `'vL', 'vR'`.

Return type *Array*

canonical_form_infinite(*renormalize=True*, *tol_xi=1000000.0*)

Bring an infinite MPS into canonical form (in place).

If any site is in `form` `None`, it does *not* use any of the singular values *S*. If all sites have a *form*, it respects the *form* to ensure that one *S* is included per bond. The final state is always in right-canonical 'B' form.

Proceeds in three steps, namely 1) diagonalize right and left transfermatrix on a given bond to bring that bond into canonical form, and then 2) sweep right to left, and 3) left to right to bringing other bonds into canonical form.

Parameters

- **renormalize** (*bool*) – Whether a change in the norm should be discarded or used to update `norm`.
- **tol_xi** (*float*) – Raise an error if the correlation length is larger than that (which indicates a degenerate "cat" state, e.g., for spontaneous symmetry breaking).

charge_variance(*bond=0*)

Return the charge variance on the left of a given bond.

For example for particle number conservation, define $N_b = sum_{i<b} n_i$ for a given bond b. Then this function returns $< \psi | N_b^2 | \psi > - (< \psi | N_b | \psi >)^2$.

Parameters **bond** (*int*) – The bond to be considered. The returned charges are summed over the sites left of *bond*.

Returns **average_charge** – For each type of charge in `chinfo` the variance of of the charge values left of the given bond.

Return type 1D array

property chi

Dimensions of the (nontrivial) virtual bonds.

compute_K(*perm*, *swap_op='auto'*, *trunc_par=None*, *canonicalize=1e-06*, *verbose=0*)

Compute the momentum quantum numbers of the entanglement spectrum for 2D states.

Works for an infinite MPS living on a cylinder, infinitely long in *x* direction and with periodic boundary conditions in *y* directions. If the state is invariant under 'rotations' around the cylinder axis, one can find the momentum quantum numbers of it. (The rotation is nothing more than a translation in *y*.) This function permutes some sites (on a copy of *self*) to enact the rotation, and then finds the dominant eigenvector of the mixed transfer matrix to get the quantum numbers, along the lines of [PollmannTurner2012], see also (the appendix and Fig. 11 in the arXiv version of) [CincioVidal2013].

Parameters

- **perm** (1D ndarray | `Lattice`) – Permuation to be applied to the physical indices, see `permute_sites()`. If a lattice is given, we use it to read out the lattice structure and shift each site by one lattice-vector in y-direction (assuming periodic boundary conditions). (If you have a `CouplingModel`, give its *lat* attribute for this argument)
- **swap_op** (`None` | `'auto'` | `Array`) – The operator used to swap the phyiscal legs of a two-site wave function *theta*, see `swap_sites()`.
- **trunc_par** (`dict`) – Parameters for truncation, see `truncate()`. If not set, *chi_max* defaults to `max(self.chi)`.
- **canonicalize** (`float`) – Check that *self* is in canonical form; call `canonical_form()` if `norm_test()` yields `np.linalg.norm(self.norm_test()) > canonicalize`.
- **verbose** (`float`) – Level of verbosity, print status messages if verbose > 0.

Returns

- **U** (`Array`) – Unitary representation of the applied permutation on left Schmidt states.
- **W** (*ndarray*) – 1D array of the form `S**2 exp(i K)`, where *S* are the Schmidt values on the left bond. You can use `np.abs()` and `np.angle()` to extract the Schmidt values *S* and momenta *K* from *W*.
- **q** (`LegCharge`) – LegCharge corresponding to *W*.
- **ov** (*complex*) – The eigenvalue of the mixed transfer matrix <*psi*|*T*|*psi*> per `L` sites. An absolute value different smaller than 1 indicates that the state is not invariant under the permutation or that the truncation error *trunc_err* was too large!
- **trunc_err** (`TruncationError`) – The error of the represented state introduced by the truncation after swaps when performing the truncation.

convert_form(*new_form='B'*)

Tranform self into different canonical form (by scaling the legs with singular values).

Parameters **new_form** ((list of) {`'B' | 'A' | 'C' | 'G' | 'Th' | None` | tuple(float, float)}) – The form the stored 'matrices'. The table in module doc-string. A single choice holds for all of the entries.

:raises ValueError : if trying to convert from a `None` form. Use `canonical_form()` instead!:

copy()

Returns a copy of *self*.

The copy still shares the sites, chinfo, and LegCharges of the B tensors, but the values of B and S are deeply copied.

correlation_function(*ops1*, *ops2*, *sites1=None*, *sites2=None*, *opstr=None*, *str_on_first=True*, *hermitian=False*, *autoJW=True*)

Correlation function `<psi|op1_i op2_j|psi>/<psi|psi>` of single site operators.

Given the MPS in canonical form, it calculates 2-site correlation functions. For examples the contraction for a two-site operator on site *i* would look like:

```
|           .--S--B[i]--B[i+1]--...--B[j]---.
|           |     |     |             |      |
|           |     |     |             op2    |
|           |     op1   |             |      |
|           |     |     |             |      |
|           .--S--B*[i]-B*[i+1]-...--B*[j]--.
```

Onsite terms are taken in the order `<psi | op1 op2 | psi>`.

If *opstr* is given and `str_on_first=True`, it calculates:

```
|           for i < j                                for i > j
|
|           .--S--B[i]---B[i+1]--...- B[j]---.     .--S--B[j]---B[j+1]--...-␣
↪B[i]---.
|           |     |      |             |      |     |     |      |             |␣
↪     |
|           |     opstr  opstr        op2    |     |     op2    |             |␣
↪     |
|           |     |      |             |      |     |     |      |             |␣
↪     |
|           |     op1    |             |      |     |     opstr  opstr       ␣
↪op1    |
|           |     |      |             |      |     |     |      |             |␣
↪     |
|           .--S--B*[i]--B*[i+1]-...- B*[j]--.     .--S--B*[j]--B*[j+1]-...-␣
↪B*[i]--.
```

For `i==j`, no *opstr* is included. For `str_on_first=False`, the *opstr* on site `min(i, j)` is always left out.

Strings (like `'Id', 'Sz'`) in the arguments are translated into single-site operators defined by the *Site* on which they act. Each operator should have the two legs `'p', 'p*'`.

Parameters

- **ops1** ((list of) { *Array* | str }) – First operator of the correlation function (acting after ops2). If a list is given, `ops1[i]` acts on site *i* of the MPS.
- **ops2** ((list of) { *Array* | str }) – Second operator of the correlation function (acting before ops1). If a list is given, `ops2[j]` acts on site *j* of the MPS.
- **sites1** (*None | int | list of int*) – List of site indices *i*; a single *int* is translated to `range(0, sites1)`. `None` defaults to all sites `range(0, L)`. Is sorted before use, i.e. the order is ignored.
- **sites2** (*None | int | list of int*) – List of site indices; a single *int* is translated to `range(0, sites2)`. `None` defaults to all sites `range(0, L)`. Is sorted before use, i.e. the order is ignored.
- **opstr** (None | (list of) { *Array* | str }) – Ignored by default (`None`). Operator(s) to be inserted between `ops1` and `ops2`. If less than *L* operators are given, we repeat them periodically. If given as a list, `opstr[r]` is inserted at site *r* (independent of *sites1* and *sites2*).
- **str_on_first** (*bool*) – Whether the *opstr* is included on the site `min(i, j)`. Note the order, which is chosen that way to handle fermionic Jordan-Wigner strings correctly. (In other words: choose `str_on_first=True` for fermions!)

- **hermitian** (*bool*) – Optimization flag: if `sites1 == sites2` and `Ops1[i]^\dagger == Ops2[i]` (which is not checked explicitly!), the resulting `C[x, y]` will be hermitian. We can use that to avoid calculations, so `hermitian=True` will run faster.
- **autoJW** (*bool*) – *Ignored* if *opstr* is given. If *True*, auto-determine if a Jordan-Wigner string is needed. Works only if exclusively strings were used for *op1* and *op2*.

Returns

C – The correlation function `C[x, y] = <psi|ops1[i] ops2[j]|psi>`, where `ops1[i]` acts on site `i=sites1[x]` and `ops2[j]` on site `j=sites2[y]`. If *opstr* is given, it gives (for `str_on_first=True`):

- For `i < j: C[x, y] = <psi|ops1[i] prod_{i <= r < j} opstr[r] ops2[j]|psi>`.
- For `i > j: C[x, y] = <psi|prod_{j <= r < i} opstr[r] ops1[i] ops2[j]|psi>`.
- For `i = j`: `C[x, y] = <psi|ops1[i] ops2[j]|psi>`.

The condition `<= r` is replaced by a strict `< r`, if `str_on_first=False`.

Return type 2D ndarray

Examples

For a spin chain:

```
>>> psi.correlation_function("A", "B")
[[A0B0,     A0B1, ..., A0B{L-1}],
 [A1B0,     A1B1, ..., A1B{L-1}],
 ...,
 [A{L-1}B0, ALB1, ..., A{L-1}B{L-1}],
]
```

To evaluate the correlation function for a single *i*, you can use `sites1=[i]`:

```
>>> psi.correlation_function("A", "B", [3])
[[A3B0,     A3B1, ..., A3B{L-1}]]
```

For fermions, it auto-determines that/whether a Jordan Wigner string is needed:

```
>>> CdC = psi.correlation_function("Cd", "C")  # optionally: use␣
↪`hermitian=True`
>>> psi.correlation_function("C", "Cd")[1, 2] == -CdC[1, 2]
True
>>> np.all(np.diag(CdC) == psi.expectation_value("Cd C"))  # "Cd C" is␣
↪equivalent to "N"
True
```

See also:

expectation_value_term() best for a single combination of *i* and *j*.

correlation_length(*target=1*, *tol_ev0=1e-08*, *charge_sector=0*)

Calculate the correlation length by diagonalizing the transfer matrix.

Assumes that *self* is in canonical form.

Works only for infinite MPS, where the transfer matrix is a useful concept. Assuming a single-site unit cell, any correlation function splits into $C(A_i, B_j) = A_i' T^{j-i-1} B_j'$ with some parts left and right and the $j-i-1$-th power of the transfer matrix in between. The largest eigenvalue is 1 (if self is properly normalized) and gives the dominant contribution of $A_i' E_1 * 1^{j-i-1} * E_1^T B_j' =< A >< B >$, and the second largest one gives a contribution $\propto \lambda_2^{j-i-1}$. Thus $\lambda_2 = \exp(-\frac{1}{\xi})$.

More general for a *L*-site unit cell we get $\lambda_2 = \exp(-\frac{L}{\xi})$, where the *xi* is given in units of 1 lattice spacing in the MPS.

Warning: For a higher-dimensional lattice (which the MPS class doesn't know about), the correct unit is the lattice spacing in x-direction, and the correct formula is $\lambda_2 = \exp(-\frac{L_x}{\xi})$, where *L_x* is the number of lattice spacings in the infinite direction within the MPS unit cell, e.g. the number of "rings" of a cylinder in the MPS unit cell. To get to these units, divide the returned *xi* by the number of sites within a "ring", for a lattice given in `N_sites_per_ring`.

Parameters

- **target** (*int*) – We look for the *target* + 1 largest eigenvalues.
- **tol_ev0** (*float*) – Print warning if largest eigenvalue deviates from 1 by more than *tol_ev0*.
- **charge_sector** (None | charges | `0`) – Selects the charge sector in which the dominant eigenvector of the TransferMatrix is. `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.

Returns **xi** – If *target`=1, return just the correlation length, otherwise an array of the `target* largest correlation lengths. It is measured in units of a single lattice spacing in the MPS language, see the warning above.

Return type float | 1D array

property dim

List of local physical dimensions.

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 unit cell will be increased from *L* to `factor*L`.

entanglement_entropy(*n=1*, *bonds=None*, *for_matrix_S=False*)

Calculate the (half-chain) entanglement entropy for all nontrivial bonds.

Consider a bipartition of the sytem into $A = \{j : j <= i_b\}$ and $B = \{j : j > i_b\}$ and the reduced density matrix $\rho_A = tr_B(\rho)$. The von-Neumann entanglement entropy is defined as $S(A, n = 1) = -tr(\rho_A \log(\rho_A)) = S(B, n = 1)$. The generalization for `n != 1, n>0` are the Renyi entropies: $S(A, n) = \frac{1}{1-n} \log(tr(\rho_A^2)) = S(B, n = 1)$

This function calculates the entropy for a cut at different bonds *i*, for which the the eigenvalues of the reduced density matrix ρ_A and ρ_B is given by the squared schmidt values *S* of the bond.

Parameters

- **n** (*int/float*) – Selects which entropy to calculate; *n=1* (default) is the ususal von-Neumann entanglement entropy.

- **bonds** (None | (iterable of) int) – Selects the bonds at which the entropy should be calculated. None defaults to range(0, L+1)[self.nontrivial_bonds].
- **for_matrix_S** (*bool*) – Switch calculate the entanglement entropy even if the *_S* are matrices. Since $O(\chi^3)$ is expensive compared to the ususal $O(\chi)$, we raise an error by default.

Returns **entropies** – Entanglement entropies for half-cuts. *entropies[j]* contains the entropy for a cut at bond bonds[j] (i.e. left to site bonds[j]).

Return type 1D ndarray

entanglement_spectrum(*by_charge=False*)

return entanglement energy spectrum.

Parameters **by_charge** (*bool*) – Wheter we should sort the spectrum on each bond by the possible charges.

Returns **ent_spectrum** – For each (non-trivial) bond the entanglement spectrum. If *by_charge* is False, return (for each bond) a sorted 1D ndarray with the convention $S_i^2 = e^{-\xi_i}$, where S_i labels a Schmidt value and ξ_i labels the entanglement 'energy' in the returned spectrum. If *by_charge* is True, return a a list of tuples (charge, sub_spectrum) for each possible charge on that bond.

Return type list

expectation_value(*ops*, *sites=None*, *axes=None*)

Expectation value <psi|ops|psi>/<psi|psi> of (n-site) operator(s).

Given the MPS in canonical form, it calculates n-site expectation values. For example the contraction for a two-site (n = 2) operator on site i would look like:

```
|           .--S--B[i]--B[i+1]--.
|           |     |     |       |
|           |     |-----|       |
|           |     | op  |       |
|           |     |-----|       |
|           |     |     |       |
|           .--S--B*[i]-B*[i+1]-.
```

Parameters

- **ops** ((list of) { *Array* | str }) – The operators, for wich the expectation value should be taken, All operators should all have the same number of legs (namely *2 n*). If less than *self.L* operators are given, we repeat them periodically. Strings (like 'Id', 'Sz') are translated into single-site operators defined by sites.
- **sites** (*None | list of int*) – 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 operators (n = 1), or (['p0', 'p1', ... 'p{n-1}'], ['p0*', 'p1*', ... 'p{n-1}*']) for $n > 1$.

Returns **exp_vals** – Expectation values, exp_vals[i] = <psi|ops[i]|psi>, where ops[i] acts on site(s) j, j+1, ..., j+{n-1} with j=sites[i].

Return type 1D ndarray

Examples

One site examples (n=1):

```
>>> psi.expectation_value('Sz')
[Sz0, Sz1, ..., Sz{L-1}]
>>> psi.expectation_value(['Sz', 'Sx'])
[Sz0, Sx1, Sz2, Sx3, ... ]
>>> psi.expectation_value('Sz', sites=[0, 3, 4])
[Sz0, Sz3, Sz4]
```

Two site example (n=2), assuming homogeneous sites:

```
>>> SzSx = npc.outer(psi.sites[0].Sz.replace_labels(['p', 'p*'], ['p0', 'p0*
↪']),
                     psi.sites[1].Sx.replace_labels(['p', 'p*'], ['p1', 'p1*
↪']))
>>> psi.expectation_value(SzSx)
[Sz0Sx1, Sz1Sx2, Sz2Sx3, ... ]   # with len L-1 for finite bc, or L for␣
↪infinite
```

Example measuring <psi|SzSx|psi2> on each second site, for inhomogeneous sites:

```
>>> SzSx_list = [npc.outer(psi.sites[i].Sz.replace_labels(['p', 'p*'], ['p0',
↪'p0*']),
                           psi.sites[i+1].Sx.replace_labels(['p', 'p*'], ['p1
↪', 'p1*']))
                 for i in range(0, psi.L-1, 2)]
>>> psi.expectation_value(SzSx_list, range(0, psi.L-1, 2))
[Sz0Sx1, Sz2Sx3, Sz4Sx5, ...]
```

expectation_value_multi_sites (*operators*, *i0*)

Expectation value `<psi|op0_{i0}op1_{i0+1}...opN_{i0+N}|psi>/<psi|psi>`.

Calculates the expectation value of a tensor product of single-site operators acting on different sites next to each other. In other words, evaluate the expectation value of a term `op0_i0 op1_{i0+1} op2_{i0+2} ....`

> **Warning:** This function does *not* automatically add Jordan-Wigner strings! For correct handling of fermions, use *`expectation_value_term()`* instead.

Parameters

- **operators** (List of { *`Array`* | str }) – List of one-site operators. This method calculates the expectation value of the n-sites operator given by their tensor product.
- **i0** (*`int`*) – The left most index on which an operator acts, i.e., `operators[i]` acts on site `i + i0`.

Returns exp_val – The expectation value of the tensorproduct of the given onsite operators, `<psi|operators[0]_{i0} operators[1]_{i0+1} ... |psi>/<psi|psi>`, where `|psi>` is the represented MPS.

Return type float/complex

expectation_value_term(*term*, *autoJW=True*)

Expectation value `<psi|op_{i0}op_{i1}...op_{iN}|psi>/<psi|psi>`.

Calculates the expectation value of a tensor product of single-site operators acting on different sites *i0*, *i1*, ... (not necessarily next to each other). In other words, evaluate the expectation value of a term `op0_i0 op1_i1 op2_i2 ....`

For example the contraction of three one-site operators on sites *i0*, *i1=i0+1*, *i2=i0+3* would look like:

```
|          .--S--B[i0]---B[i0+1]--B[i0+2]--B[i0+3]--.
|          |     |       |        |        |        |
|          |    op1     op2       |       op3       |
|          |     |       |        |        |        |
|          .--S--B*[i0]--B*[i0+1]-B*[i0+2]-B*[i0+3]-.
```

Parameters

- **term** (*list of (str, int)*) – List of tuples `op, i` where *i* is the MPS index of the site the operator named *op* acts on. The order inside *term* determines the order in which they act (in the mathematical convention: the last operator in *term* is right-most, so it acts first on a Ket).
- **autoJW** (*bool*) – If True (default), automatically insert Jordan Wigner strings for Fermions as needed.

Returns **exp_val** – The expectation value of the tensorproduct of the given onsite operators, `<psi|op_i0 op_i1 ... op_iN |psi>/<psi|psi>`, where `|psi>` is the represented MPS.

Return type float/complex

See also:

correlation_function() efficient way to evaluate many correlation functions.

Examples

```
>>> a = psi.expectation_value_term([('Sx', 2), ('Sz', 4)])
>>> b = psi.expectation_value_term([('Sz', 4), ('Sx', 2)])
>>> c = psi.expectation_value_multi_sites(['Sz', 'Id', 'Sz'], i0=2)
>>> assert a == b == c
```

expectation_value_terms_sum(*term_list*, *prefactors=None*)

Calculate expectation values for a bunch of terms and sum them up.

This is equivalent to the following expression:

```
sum([self.expectation_value_term(term)*strength for term, strength in term_
↪list])
```

However, for effiency, the term_list is converted to an MPO and the expectation value of the MPO is evaluated.

Note: Due to the way MPO expectation values are evaluated for infinite systems, it works only if all terms in the *term_list* start within the MPS unit cell.

Deprecated since version 0.4.0: *prefactor* will be removed in version 1.0.0. Instead, directly give just `TermList(term_list, prefactors)` as argument.

Parameters

- **term_list** (*TermList*) – The terms and prefactors (*strength*) to be summed up.
- **prefactors** – Instead of specifying a *TermList*, one can also specify the term_list and strength separately. This is deprecated.

Returns

- **terms_sum** (*list of (complex) float*) – Equivalent to the expression `sum([self.expectation_value_term(term)*strength for term, strength in term_list])`.
- *_mpo* – Intermediate results: the generated MPO. For a finite MPS, `terms_sum = _mpo.expectation_value(self)`, for an infinite MPS `terms_sum = _mpo.expectation_value(self) * self.L`

See also:

expectation_value_term() evaluates a single *term*.

tenpy.networks.mpo.MPO.expectation_value() expectation value density of an MPO.

property finite

Distinguish MPS vs iMPS.

True for an MPS (`bc='finite', 'segment'`), False for an iMPS (`bc='infinite'`).

classmethod from_Bflat(*sites*, *Bflat*, *SVs=None*, *bc='finite'*, *dtype=None*, *permute=True*, *form='B'*, *legL=None*)

Construct a matrix product state from a set of numpy arrays *Bflat* and singular vals.

Parameters

- **sites** (list of *Site*) – The sites defining the local Hilbert space.
- **Bflat** (*iterable of numpy ndarrays*) – The matrix defining the MPS on each site, with legs `'p', 'vL', 'vR'` (physical, virtual left/right).
- **SVs** (list of 1D array | `None`) – The singular values on *each* bond. Should always have length *L+1*. By default (`None`), set all singular values to the same value. Entries out of *nontrivial_bonds* are ignored.
- **bc** (*{'infinite', 'finite', 'segmemt'}*) – MPS boundary conditions. See docstring of `MPS`.
- **dtype** (*type or string*) – The data type of the array entries. Defaults to the common dtype of *Bflat*.
- **permute** (*bool*) – The `Site` might permute the local basis states if charge conservation gets enabled. If *permute* is True (default), we permute the given *Bflat* locally according to each site's `perm`. The *p_state* argument should then always be given as if *conserve=None* in the Site.
- **form** ((list of) {`'B' | 'A' | 'C' | 'G' | None` | tuple(float, float)}) – Defines the canonical form of *Bflat*. See module doc-string. A single choice holds for all of the entries.
- **leg_L** (LegCharge | `None`) – Leg charges at bond 0, which are purely conventional. If `None`, use trivial charges.

Returns **mps** – An MPS with the matrices *Bflat* converted to npc arrays.

Return type `MPS`

classmethod from_full(*sites*, *psi*, *form=None*, *cutoff=1e-16*, *normalize=True*, *bc='finite'*, *outer_S=None*)

Construct an MPS from a single tensor *psi* with one leg per physical site.

Performs a sequence of SVDs of psi to split off the *B* matrices and obtain the singular values, the result will be in canonical form. Obviously, this is only well-defined for *finite* or *segment* boundary conditions.

Parameters

- **sites** (list of `Site`) – The sites defining the local Hilbert space.
- **psi** (`Array`) – The full wave function to be represented as an MPS. Should have labels `'p0', 'p1', ..., 'p{L-1}'`. Additionally, it may have (or must have for 'segment' *bc*) the legs `'vL', 'vR'`, which are trivial for 'finite' *bc*.
- **form** (`'B' | 'A' | 'C' | 'G' | None`) – The canonical form of the resulting MPS, see module doc-string. `None` defaults to 'A' form on the first site and 'B' form on all following sites.
- **cutoff** (`float`) – Cutoff of singular values used in the SVDs.
- **normalize** (`bool`) – Whether the resulting MPS should have 'norm' 1.
- **bc** (`'finite' | 'segment'`) – Boundary conditions.
- **outer_S** (`None | (array, array)`) – For 'semgent' *bc* the singular values on the left and right of the considered segment, *None* for 'finite' boundary conditions.

Returns **psi_mps** – MPS representation of *psi*, in canonical form and possibly normalized.

Return type `MPS`

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_lat_product_state(*lat*, *p_state*, ***kwargs*)

Construct an MPS from a product state given in lattice coordinates.

This is a wrapper around `from_product_state()`. The purpuse is to make the *p_state* argument independent of the *order* of the *Lattice*, and specify it in terms of lattice indices instead.

Parameters

- **lat** (`Lattice`) – The underlying lattice defining the geometry and Hilbert Space.
- **p_state** (`array_like of {int | str | 1D array}`) – Defines the product state to be represented. Should be of dimension *lat.dim`+1, entries are indexed by lattice indices. Entries of the array as for the `p_state* argument of `from_product_state()`. It gets tiled to the shape `lat.shape`, if it is smaller.

- ****kwargs** – Other keyword arguments as definied in *from_product_state()*. *bc* is set by default from `lat.bc_MPS`.

Returns **product_mps** – An MPS representing the specified product state.

Return type `MPS`

Examples

Let's first consider a *Ladder* composed of a *SpinHalfSite* and a *FermionSite*.

```
>>> spin_half = tenpy.networks.site.SpinHalfSite()
>>> fermion = tenpy.networks.site.FermionSite()
>>> ladder_i = tenpy.models.lattice.Ladder(2, [spin_half, fermion], bc_MPS=
↪"infinite")
```

To initialize a state of up-spins on the spin sites and half-filled ferions, you can use:

```
>>> p_state = [["up", "empty"], ["up", "full"]]
>>> psi = tenpy.networks.MPS.from_lat_product_state(ladder_i, p_state)
```

Note that the same *p_state* works for a finite lattice of even length, say `L=10`, as well. We then just "tile" in x-direction, i.e., repeat the specified state 5 times:

```
>>> ladder_f = tenpy.models.lattice.Ladder(10, [spin_half, fermion], bc_MPS=
↪"finite")
>>> psi = tenpy.networks.MPS.from_lat_product_state(ladder_f, p_state)
```

You can also easily half-fill a *Honeycomb*, for example with only the *A* sites occupied, or as stripe parallel to the x-direction (*stripe_x*, alternating along *y* axis), or as stripes parallel to the y-direction (*stripe_y*, alternating along *x* axis).

```
>>> honeycomb = tenpy.models.lattice.Honeycomb([4, 4], [fermion, fermion], bc_
↪MPS="finite")
>>> p_state_only_A = [[["empty", "full"]]]
>>> psi_only_A = tenpy.networks.MPS.from_lat_product_state(honeycomb, p_state_
↪only_A)
>>> p_state_stripe_x = [[["empty", "empty"],
...                      ["full", "full"]]]
>>> psi_stripe_x = tenpy.networks.MPS.from_lat_product_state(honeycomb, p_
↪state_stripe_x)
>>> p_state_stripe_y = [[["empty", "empty"]],
...                      [["full", "full"]]]
>>> psi_stripe_y = tenpy.networks.MPS.from_lat_product_state(honeycomb, p_
↪state_stripe_y)
```

---

classmethod from_product_state(*sites*, *p_state*, *bc='finite'*, *dtype=<class 'numpy.float64'>*, *permute=True*, *form='B'*, *chargeL=None*)

Construct a matrix product state from a given product state.

Parameters

- **sites** (list of *Site*) – The sites defining the local Hilbert space.
- **p_state** (*list of {int | str | 1D array}*) – Defines the product state to be represented; one entry for each *site* of the MPS. An entry of *str* type is translated to an *int* with the help of *state_labels()*. An entry of *int* type represents the physical index

of the state to be used. An entry which is a 1D array defines the complete wavefunction on that site; this allows to make a (local) superposition.

- **bc** (*{'infinite', 'finite', 'segmemt'}*) – MPS boundary conditions. See docstring of `MPS`.
- **dtype** (*type or string*) – The data type of the array entries.
- **permute** (*bool*) – The `Site` might permute the local basis states if charge conservation gets enabled. If *permute* is True (default), we permute the given *p_state* locally according to each site's `perm`. The *p_state* entries should then always be given as if *conserve=None* in the Site.
- **form** ((list of) {`'B' | 'A' | 'C' | 'G' | None` | tuple(float, float)}) – Defines the canonical form. See module doc-string. A single choice holds for all of the entries.
- **chargeL** (*charges*) – Leg charges at bond 0, which are purely conventional.

Returns **product_mps** – An MPS representing the specified product state.

Return type `MPS`

Examples

Example to get a Neel state for a `TIChain`:

```
>>> M = TFIChain({'L': 10})
>>> p_state = ["up", "down"] * (L//2)  # repeats entries L/2 times
>>> psi = MPS.from_product_state(M.lat.mps_sites(), p_state, bc=M.lat.bc_MPS)
```

The meaning of the labels `"up","down"` is defined by the `Site`, in this example a *SpinHalfSite*.

Extending the example, we can replace the spin in the center with one with arbitrary angles `theta, phi` in the bloch sphere:

```
>>> M = TFIChain({'L': 8, 'conserve': None})
>>> p_state = ["up", "down"] * (L//2)  # repeats entries L/2 times
>>> bloch_sphere_state = np.array([np.cos(theta/2), np.exp(1.j*phi)*np.
↪sin(theta/2)])
>>> p_state[L//2] = bloch_sphere_state   # replace one spin in center
>>> psi = MPS.from_product_state(M.lat.mps_sites(), p_state, bc=M.lat.bc_MPS,␣
↪dtype=np.complex)
```

Note that for the more general *SpinChain*, the order of the two entries for the `bloch_sphere_state` would be *exactly the opposite* (when we keep the the north-pole of the bloch sphere being the up-state). The reason is that the *SpinChain* uses the general *SpinSite*, where the states are orderd ascending from `'down'` to `'up'`. The *SpinHalfSite* on the other hand uses the order `'up', 'down'` where that the Pauli matrices look as usual.

Moreover, note that you can not write this bloch state (for `theta != 0, pi`) when conserving symmetries, as the two physical basis states correspond to different symmetry sectors.

---

classmethod from_singlets(*site*, *L*, *pairs*, *up='up'*, *down='down'*, *lonely=[]*, *lonely_state='up'*, *bc='finite'*)

Create an MPS of entangled singlets.

Parameters

- **site** (*Site*) – The *site* defining the local Hilbert space, taken uniformly for all sites.
- **L** (*int*) – The number of sites.

- **pairs** (*list of (int, int)*) – Pairs of sites to be entangled; the returned MPS will have a singlet for each pair in *pairs*.
- **down** (*up,*) – A singlet is defined as `(|up down> - |down up>)/2**0.5`, `up` and `down` give state indices or labels defined on the corresponding site.
- **lonely** (*list of int*) – Sites which are not included into a singlet pair.
- **lonely_state** (*int | str*) – The state for the lonely sites.
- **bc** (*{'infinite', 'finite', 'segmemt'}*) – MPS boundary conditions. See docstring of `MPS`.

Returns **singlet_mps** – An MPS representing singlets on the specified pairs of sites.

Return type `MPS`

gauge_total_charge (*qtotal=None*, *vL_leg=None*, *vR_leg=None*)

Gauge the legcharges of the virtual bonds such that the MPS has a total *qtotal*.

Parameters

- **qtotal** (*(list of) charges*) – If a single set of charges is given, it is the desired total charge of the MPS (which *get_total_charge()* will return afterwards). By default (`None`), use 0 charges, unless vL_leg and vR_leg are specified, in which case we adjust the total charge to match these legs.
- **vL_leg** (*None | LegCharge*) – Desired new virtual leg on the very left. Needs to have the same block strucuture as current leg, but can have shifted charge entries.
- **vR_leg** (*None | LegCharge*) – Desired new virtual leg on the very right. Needs to have the same block strucuture as current leg, but can have shifted charge entries. Should be *vL_leg.conj()* for infinite MPS, if *qtotal* is not given.

get_B (*i*, *form='B'*, *copy=False*, *cutoff=1e-16*, *label_p=None*)

Return (view of) *B* at site *i* in canonical form.

Parameters

- **i** (*int*) – Index choosing the site.
- **form** (`'B' | 'A' | 'C' | 'G' | 'Th' | None` | tuple(float, float)) – The (canonical) form of the returned B. For `None`, return the matrix in whatever form it is. If any of the tuple entry is None, also don't scale on the corresponding axis.
- **copy** (*bool*) – Whether to return a copy even if *form* matches the current form.
- **cutoff** (*float*) – During DMRG with a mixer, *S* may be a matrix for which we need the inverse. This is calculated as the Penrose pseudo-inverse, which uses a cutoff for the singular values.
- **label_p** (*None | str*) – Ignored by default (`None`). Otherwise replace the physical label `'p'` with `'p'+label_p'`. (For derived classes with more than one "physical" leg, replace all the physical leg labels accordingly.)

Returns **B** – The MPS 'matrix' *B* at site *i* with leg labels `'vL', 'p', 'vR'`. May be a view of the matrix (if `copy=False`), or a copy (if the form changed or `copy=True`).

Return type *Array*

:raises ValueError : if self is not in canoncial form and *form* is not None.:

get_SL (*i*)

Return singular values on the left of site *i*

get_SR(*i*)
Return singular values on the right of site *i*

get_grouped_mps(*blocklen*)
contract blocklen subsequent tensors into a single one and return result as a new MPS.

blocklen = number of subsequent sites to be combined.

Returns

Return type new MPS object with bunched sites.

get_op(*op_list*, *i*)
Given a list of operators, select the one corresponding to site *i*.

Parameters

- **op_list** (*(list of) {str | npc.array}*) – List of operators from which we choose. We assume that `op_list[j]` acts on site `j`. If the length is shorter than *L*, we repeat it periodically. Strings are translated using *get_op()* of site *i*.
- **i** (*int*) – Index of the site on which the operator acts.

Returns **op** – One of the entries in *op_list*, not copied.

Return type npc.array

get_rho_segment(*segment*)
Return reduced density matrix for a segment.

Note that the dimension of rho_A scales exponentially in the length of the segment.

Parameters **segment** (*iterable of int*) – Sites for which the reduced density matrix is to be calculated. Assumed to be sorted.

Returns **rho** – Reduced density matrix of the segment sites. Labels `'p0', 'p1', ..., 'pk', 'p0*', 'p1*', ..., 'pk*'` with `k=len(segment)`.

Return type *Array*

get_theta(*i*, *n=2*, *cutoff=1e-16*, *formL=1.0*, *formR=1.0*)
Calculates the *n*-site wavefunction on `sites[i:i+n]`.

Parameters

- **i** (*int*) – Site index.
- **n** (*int*) – Number of sites. The result lives on `sites[i:i+n]`.
- **cutoff** (*float*) – During DMRG with a mixer, *S* may be a matrix for which we need the inverse. This is calculated as the Penrose pseudo-inverse, which uses a cutoff for the singular values.
- **formL** (*float*) – Exponent for the singular values to the left.
- **formR** (*float*) – Exponent for the singular values to the right.

Returns **theta** – The n-site wave function with leg labels `vL, p0, p1, .... p{n-1}, vR`. In Vidal's notation (with s=lambda, G=Gamma): `theta = s**form_L G_i s G_{i+1} s ... G_{i+n-1} s**form_R`.

Return type *Array*

get_total_charge(*only_physical_legs=False*)
Calculate and return the *qtotal* of the whole MPS (when contracted).

Parameters **only_physical_legs** (*bool*) – For `'finite'` boundary conditions, the total charge can be gauged away by changing the LegCharge of the trivial legs on the left and right of the MPS. This option allows to project out the trivial legs to get the actual "physical" total charge.

Returns **qtotal** – The sum of the *qtotal* of the individual *B* tensors.

Return type charges

group_sites(*n=2*, *grouped_sites=None*)

Modify *self* inplace 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).

Parameters

- **n** (*int*) – Number of sites to be grouped together.
- **grouped_sites** (None | list of `GroupedSite`) – The sites grouped together.

See also:

group_split() Reverts the grouping.

group_split(*trunc_par=None*)

Modify *self* inplace to split previously grouped sites.

Parameters **trunc_par** (*dict*) – Parameters for truncation, see `truncate()`. Defaults to `{'chi_max': max(self.chi)}`.

Returns **trunc_err** – The error introduced by the truncation for the splitting.

Return type `TruncationError`

See also:

group_sites() Should have been used before to combine sites.

increase_L(*new_L=None*)

Modify *self* inplace to enlarge the MPS unit cell; in place.

Deprecated since version 0.5.1: This method will be removed in version 1.0.0. Use the equivalent `psi.enlarge_mps_unit_cell(new_L//psi.L)` instead of `psi.increase_L(new_L)`.

Parameters **new_L** (*int*) – New number of sites. Needs to be an integer multiple of `L`. Defaults to `2*self.L`.

property nontrivial_bonds

Slice of the non-trivial bond indices, depending on `self.bc`.

norm_test()

Check that self is in canonical form.

Returns

norm_error – For each site the norm error to the left and right. The error `norm_error[i, 0]` is defined as the norm-difference between the following networks:

```
|   --theta[i]---.       --s[i]--.
|       |        |    vs         |
|   --theta*[i]--.       --s[i]--.
```

Similarly, `norm_errror[i, 1]` is the norm-difference of:

```
|   .--theta[i]---          .--s[i+1]--
|   |    |           vs     |
|   .--theta*[i]--          .--s[i+1]--
```

Return type array, shape (L, 2)

overlap(*other*, *charge_sector=None*, *ignore_form=False*, ***kwargs*)

Compute overlap `<self|other>`.

Parameters

- **other** (`MPS`) – An MPS with the same physical sites.
- **charge_sector** (None | charges | `0`) – Selects the charge sector in which the dominant eigenvector of the TransferMatrix is. `None` stands for *all* sectors, `0` stands for the sector of zero charges. If a sector is given, it *assumes* the dominant eigenvector is in that charge sector.
- **ignore_form** (*bool*) – If `False` (default), take into account the canonical form `form` at each site. If `True`, we ignore the canonical form (i.e., whether the MPS is in left, right, mixed or no canonical form) and just contract all the `_B` as they are. (This can give different results!)
- ****kwargs** – Further keyword arguments given to `TransferMatrix.eigenvectors()`; only used for infinite boundary conditions.

Returns overlap – The contraction `<self|other> * self.norm * other.norm` (i.e., taking into account the `norm` of both MPS). For an infinite MPS, `<self|other>` is the overlap per unit cell, i.e., the largest eigenvalue of the TransferMatrix.

Return type dtype.type

permute_sites(*perm*, *swap_op='auto'*, *trunc_par={}*, *verbose=0*)

Applies the permutation perm to the state (inplace).

Parameters

- **perm** (*ndarray[ndim=1, int]*) – The applied permutation, such that `psi.permute_sites(perm)[i] = psi[perm[i]]` (where `[i]` indicates the *i*-th site).
- **swap_op** (`None` | `'auto'` | *Array*) – The operator used to swap the phyiscal legs of a two-site wave function *theta*, see *swap_sites()*.
- **trunc_par** (*dict*) – Parameters for truncation, see `truncate()`. *chi_max* defaults to `max(self.chi)`.
- **verbose** (*float*) – Level of verbosity, print status messages if verbose > 0.

Returns trunc_err – The error of the represented state introduced by the truncation after the swaps.

Return type *TruncationError*

probability_per_charge(*bond=0*)

Return probabilites of charge value on the left of a given bond.

For example for particle number conservation, define $N_b = sum_{i<b} n_i$ for a given bond b. This function returns the possible values of *N_b* as rows of *charge_values*, and for each row the probabilty that this combination occurs in the given state.

Parameters **bond** (*int*) – The bond to be considered. The returned charges are summed on the left of this bond.

Returns

- **charge_values** (*2D array*) – Columns correspond to the different charges in *self.chinfo*. Rows are the different charge fluctuations at this bond
- **probabilities** (*1D array*) – For each row of *charge_values* the probablity for these values of charge fluctuations.

roll_mps_unit_cell(*shift=1*)

Shift the section we define as unit cellof an infinite MPS; in place.

Suppose we have a unit cell with tensors `[A, B, C, D]` (repeated on both sites). With `shift = 1`, the new unit cell will be `[D, A, B, C]`, whereas `shift = -1` will give `[B, C, D, A]`.

Parameters **shift** (*int*) – By how many sites to move the tensors to the right.

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 `sites`, `chinfo` (under these names), `_B` as `"tensors"`, `_S` as `"singular_values"`, `bc` as `"boundary_condition"`, and `form` converted to a single array of shape (L, 2) as `"canonical_form"`, Moreover, it saves `norm`, *L*, `grouped` and `_transfermatrix_keep` (as "transfermatrix_keep") as HDF5 attributes, as well as the maximum of *chi* under the name "max_bond_dimension".

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.

set_B(*i*, *B*, *form='B'*)

Set *B* at site *i*.

Parameters

- **i** (*int*) – Index choosing the site.
- **B** (*Array*) – The 'matrix' at site *i*. No copy is made! Should have leg labels `'vL', 'p', 'vR'` (not necessarily in that order).
- **form** (`'B' | 'A' | 'C' | 'G' | 'Th' | None` | tuple(float, float)) – The (canonical) form of the *B* to set. `None` stands for non-canonical form.

set_SL(*i*, *S*)

Set singular values on the left of site *i*

set_SR(*i*, *S*)

Set singular values on the right of site *i*

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 accieved 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 phyisical and auxiliar system.

For $T = \infty$, the density matrix ρ_∞ 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:

```
|          :   :   :   :   :   :
|          |   |   |   |   |   |
|          |-------------------|
|          |         O         |
|          |-------------------|
|          |   |   |   |   |   |
|          :   :   :   :   :   :
```

Clearly, we get the same result, if we insert an identity operator, written as MPO, on the top and bottom:

```
|          :   :   :   :   :   :
|          |   |   |   |   |   |
|          B---B---B---B---B---B
|          |   |   |   |   |   |
|          |-------------------|
|          |         O         |
|          |-------------------|
|          |   |   |   |   |   |
|          B*--B*--B*--B*--B*--B*
|          |   |   |   |   |   |
|          :   :   :   :   :   :
```

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 expecation 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 expecation 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:

$$< A(t)B(0) > \propto < \phi| \exp(-\beta H/2) \exp(+iHt) A \exp(-iHt) B \exp(-\beta H/2) |\phi >$$

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 $\exp(-\beta H/2)\ldots$) 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 `purification_tebd`), 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 Barthel (2016), arXiv:1607.01696 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*.

7.11 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 libary. Common to all tools is that they are not just useful for a single algorithm but fairly general.

Submodules

hdf5_io	Tools to save and load data (from TeNPy) to disk.
params	Tools to handle config options/paramters for algorithms.
misc	Miscellaneous tools, somewhat random mix yet often helpful.
math	Different math functions needed at some point in the library.
fit	tools to fit to an algebraic decay.
string	Tools for handling strings.
process	Tools to read out total memory usage and get/set the number of threads.
optimization	Optimization options for this library.

7.11.1 hdf5_io

- full name: tenpy.tools.hdf5_io
- parent module: *tenpy.tools*
- type: module

Classes

Hdf5Exportable	Interface specification for a class to be exportable to our HDF5 format.
Hdf5Ignored([name])	Placeholder for a dataset/group to be ignored during both loading and saving.
Hdf5Loader(h5group[, ignore_unknown])	Class to load and import object from a HDF5 file.
Hdf5Saver(h5group[, format_selection])	Engine to save simple enough objects into a HDF5 file.

Hdf5Exportable

- full name: tenpy.tools.hdf5_io.Hdf5Exportable
- parent module: *tenpy.tools.hdf5_io*
- type: class

Inheritance Diagram

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

- **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.

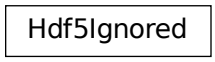
Returns **obj** – Newly generated class instance containing the required data.

Return type cls

Hdf5Ignored

- full name: tenpy.tools.hdf5_io.Hdf5Ignored
- parent module: `tenpy.tools.hdf5_io`
- type: class

Inheritance Diagram



Methods

`Hdf5Ignored.__init__`([name])	Initialize self.

class tenpy.tools.hdf5_io.**Hdf5Ignored**(*name='unknown'*)

Bases: `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 *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

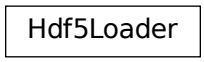
See above.

Type str

Hdf5Loader

- full name: tenpy.tools.hdf5_io.Hdf5Loader
- parent module: *tenpy.tools.hdf5_io*
- type: class

Inheritance Diagram



Methods

Hdf5Loader.__init__(h5group[, ignore_unknown])	Initialize self.
Hdf5Loader.find_class(module, classname)	Get the class of the qualified *classname* in a given python *module*.
Hdf5Loader.get_attr(h5gr, attr_name)	Return attribute h5gr.attrs[attr_name], if existent.
Hdf5Loader.load([path])	Load a Python object from the dataset.
Hdf5Loader.load_dataset(h5gr, type_info, subpath)	Load a h5py Dataset and convert it into the desired type.
Hdf5Loader.load_dict(h5gr, type_info, subpath)	Load a dictionary in the format according to *type_info*.
Hdf5Loader.load_dtype(h5gr, type_info, subpath)	Load a numpy.dtype.
Hdf5Loader.load_general_dict(h5gr, ...)	Load a dictionary with general keys.
Hdf5Loader.load_hdf5exportable(h5gr, ...)	Load an instance of a userdefined class.
Hdf5Loader.load_ignored(h5gr, type_info, subpath)	Ignore the group to be loaded.
Hdf5Loader.load_list(h5gr, type_info, subpath)	Load a list.
Hdf5Loader.load_none(h5gr, type_info, subpath)	Load the None object from a dataset.
Hdf5Loader.load_range(h5gr, type_info, subpath)	Load a range.
Hdf5Loader.load_set(h5gr, type_info, subpath)	Load a set.
Hdf5Loader.load_simple_dict(h5gr, type_info, ...)	Load a dictionary with simple keys.
Hdf5Loader.load_tuple(h5gr, type_info, subpath)	Load a tuple.
Hdf5Loader.memorize_load(h5gr, obj)	Store objects already loaded in the memo_load.

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_class(*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_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.

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_ignored(obj, path, type_repr)	Don't save the Hdf5Ignored object; just return None.
Hdf5Saver.save_iterable(obj, path, type_repr)	Save an iterable *obj* like a list, tuple or set; in dispatch table.
Hdf5Saver.save_iterable_content(obj, h5gr, ...)	Save contents of an iterable *obj* in the existing *h5gr*.
Hdf5Saver.save_none(obj, path, type_repr)	Save the None object as a string (dataset); in dispatch table.
Hdf5Saver.save_range(obj, path, type_repr)	Save a range object; in dispatch table.

Class Attributes and Properties

Hdf5Saver.dispatch_save

class tenpy.tools.hdf5_io.**Hdf5Saver**(*h5group*, *format_selection=None*)

Bases: object

Engine 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_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.

Exceptions

Hdf5ExportError	This exception is raised when something went wrong during export to hdf5.
Hdf5FormatError	Common base class for errors regarding our HDF5 format.
Hdf5ImportError	This exception is raised when something went wrong during import from hdf5.

Hdf5ExportError

- full name: tenpy.tools.hdf5_io.Hdf5ExportError
- parent module: *tenpy.tools.hdf5_io*
- type: exception

exception 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

exception 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

exception tenpy.tools.hdf5_io.**Hdf5ImportError**
This exception is raised when something went wrong during import from hdf5.

Functions

load(filename)	Load data from file with given *filename*.
load_from_hdf5(h5group[, path, ignore_unknown])	Load an object from hdf5 file or group.
save(data, filename[, mode])	Save *data* to file with given *filename*.
save_to_hdf5(h5group, obj[, path])	Save an object *obj* into a hdf5 file or group.
valid_hdf5_path_component(name)	Determine if *name* is a valid HDF5 path component.

load

- full name: tenpy.tools.hdf5_io.load
- parent module: *tenpy.tools.hdf5_io*
- type: function

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.

Returns **data** – The object loaded from the file.

Return type obj

load_from_hdf5

- full name: tenpy.tools.hdf5_io.load_from_hdf5
- parent module: *tenpy.tools.hdf5_io*
- type: function

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

`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:

ending	description
.pkl	Pickle without compression
.pklz	Pickle with gzip compression.
.hdf5	Hdf5 file (using *h5py*).

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 exisiting 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

`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

`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

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

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).

Global module constants used for our HDF5 format

Names of HDF5 attributes:

`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

`tenpy.tools.hdf5_io.`**`ATTR_MODULE = 'module'`**

Attribute name for the module where ATTR_CLASS can be retrieved

`tenpy.tools.hdf5_io.`**`ATTR_LEN = 'len'`**

Attribute name for the length of iterables, e.g, list, tuple

`tenpy.tools.hdf5_io.`**`ATTR_FORMAT = 'format'`**

indicates the *ATTR_TYPE* format used by *Hdf5Exportable*

Names for the `ATTR_TYPE` attribute:

`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

`tenpy.tools.hdf5_io.REPR_INT = 'int'`
saved object represents a (python) int

`tenpy.tools.hdf5_io.REPR_FLOAT = 'float'`
saved object represents a (python) float

`tenpy.tools.hdf5_io.REPR_STR = 'str'`
saved object represents a (python unicode) string

`tenpy.tools.hdf5_io.REPR_COMPLEX = 'complex'`
saved object represents a complex number

`tenpy.tools.hdf5_io.REPR_INT64 = 'np.int64'`
saved object represents a np.int64

`tenpy.tools.hdf5_io.REPR_FLOAT64 = 'np.float64'`
saved object represents a np.float64

`tenpy.tools.hdf5_io.REPR_INT32 = 'np.int32'`
saved object represents a np.int32

`tenpy.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

`tenpy.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

`tenpy.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

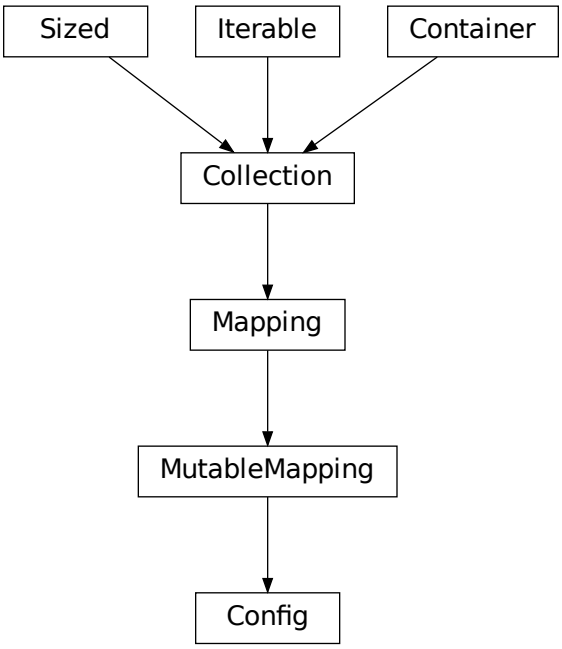
`tenpy.tools.hdf5_io.TYPES_FOR_HDF5_DATASETS = ((<class 'numpy.ndarray'>, 'array'), (<class`
tuple of (type, type_repr) which h5py can save as datasets; one entry for each type.

Todo: For memory caching with big MPO environments, we need a Hdf5Cacher clearing the memo's every now and then (triggered by what?).

7.11.2 params

- full name: tenpy.tools.params
- parent module: *tenpy.tools*
- type: module

Classes



`Config`(config, name)	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 higer *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 dicionary 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.
- **descr** (*str*) – A short description for verbose output, like 'TEBD', 'XXZ_model', 'truncation'.
- **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:

```
>>> def model_calc_U(U_param):
>>>     dt = get_parameter(U_param, 'dt', 0.01, 'TEBD')
>>>     # ... calculate exp(-i * dt* H) ....
```

Then, when you call *time_evolution* without any parameters, it just uses the default value:

```
>>> tenpy.algorithms.tebd.time_evolution(..., dict())  # uses dt=0.01
```

If you provide the special keyword `'verbose'` you can triger this function to print the used parameter values:

```
>>> tenpy.algorithms.tebd.time_evolution(..., dict(verbose=1))
parameter 'dt'=0.01 (default) for TEBD
```

Of course you can also provide the parameter to use a non-default value:

```
>>> tenpy.algorithms.tebd.time_evolution(..., dict(dt=0.1, verbose=1))
parameter 'dt'=0.1 for TEBD
```

---

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}".

Returns **unused_keys** – The set of keys of the params which was not used

Return type set

Module description

Tools to handle config options/paramters for algorithms.

See the doc-string of `Config` for details.

7.11.3 misc

- full name: tenpy.tools.misc
- parent module: *tenpy.tools*
- type: module

Functions

add_with_None_0(a, b)	Return `a + b`, treating *None* as zero.
any_nonzero(params, keys[, verbose_msg])	Check for any non-zero or non-equal entries in some parameters.
anynan(a)	check whether any entry of a ndarray *a* is 'NaN'.
argsort(a[, sort])	wrapper around np.argsort to allow sorting ascending/descending and by magnitude.
atleast_2d_pad(a[, pad_item])	Transform *a* into a 2D array, filling missing places with *pad_item*.
build_initial_state(size, states, filling[, ...])	
chi_list(chi_max[, dchi, nsweeps, verbose])	
inverse_permutation(perm)	reverse sorting indices.
lexsort(a[, axis])	wrapper around `np.lexsort`: allow for trivial case `a.shape[0] = 0` without sorting
list_to_dict_list(l)	Given a list *l* of objects, construct a lookup table.
pad(a[, w_l, v_l, w_r, v_r, axis])	Pad an array along a given *axis*.
setup_executable(mod, run_defaults[, ...])	Read command line arguments and turn into useable dicts.
to_array(a[, shape])	Convert *a* to an numpy array and tile to matching dimension/shape.
to_iterable(a)	If *a* is a not iterable or a string, return `[a]`, else return `a`.
to_iterable_of_len(a, L)	If a is a non-string iterable of length *L*, return *a*, otherwise return [a]*L.
transpose_list_list(D[, pad])	Returns a list of lists T, such that `T[i][j] = D[j][i]`.
zero_if_close(a[, tol])	set real and/or imaginary part to 0 if their absolute value is smaller than *tol*.

add_with_None_0

- full name: tenpy.tools.misc.add_with_None_0
- parent module: *tenpy.tools.misc*
- type: function

`tenpy.tools.misc.`**`add_with_None_0`**(*a*, *b*)

Return `a + b`, treating *None* as zero.

Parameters **b** (*a,*) – 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

`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.
- **sort** (`'m>', 'm<', '>', '<', None`) – Specify how the arguments should be sorted.

sort	order
`'m>', 'LM'`	Largest magnitude first
`'m<', 'SM'`	Smallest magnitude first
`'>', 'LR', 'LA'`	Largest real part first
`'<', 'SR', 'SA'`	Smallest real part first
`'LI'`	Largest imaginary part first
`'Si'`	Smallest imaginary part first
`None`	numpy default: same as '<'

- ****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

```
>>> 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

`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

`tenpy.tools.misc.`**`chi_list`**(*chi_max*, *dchi=20*, *nsweeps=20*, *verbose=0*)

inverse_permutation

- full name: tenpy.tools.misc.inverse_permutation
- parent module: *tenpy.tools.misc*
- type: function

`tenpy.tools.misc.`**`inverse_permutation`**(*perm*)

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, `inverse_permutation(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

`tenpy.tools.misc.`**`lexsort`**(*a*, *axis=-1*)

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 iterabele 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** (*ieterable, 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 numpys 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

`tenpy.tools.misc.`**`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

`tenpy.tools.misc.`**`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

`tenpy.tools.misc.`**`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 threashold which values to consider as '0'.

Module description

Miscellaneous tools, somewhat random mix yet often helpful.

7.11.4 math

- full name: tenpy.tools.math
- parent module: *tenpy.tools*
- type: module

Functions

entropy(p[, n])	Calculate the entropy of a distribution.
gcd(a, b)	Computes the greatest common divisor (GCD) of two numbers.
gcd_array(a)	Return the greatest common divisor of all of entries in *a*
lcm(a, b)	Returns the least common multiple (LCM) of two positive numbers.
matvec_to_array(H)	transform an linear operator with a *matvec* method into a dense numpy array.
perm_sign(p)	Given a permutation *p* of numbers, returns its sign.
qr_li(A[, cutoff])	QR decomposition with cutoff to discard nearly linear dependent columns in *Q*.
rq_li(A[, cutoff])	RQ decomposition with cutoff to discard nearly linear dependent columns in *Q*.
speigs(A, k, *args, **kwargs)	Wrapper around `scipy.sparse.linalg.eigs()`, lifting the restriction `k < rank(A)-1`.
speigsh(A, k, *args, **kwargs)	Wrapper around `scipy.sparse.linalg.eigsh()`, lifting the restriction `k < rank(A)-1`.

entropy

- full name: tenpy.tools.math.entropy
- parent module: *tenpy.tools.math*
- type: function

`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

`tenpy.tools.math.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

`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

```
>>> for p in itertools.permutations(range(3))]):
...     print('{p!s}: {sign!s}'.format(p=p, sign=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

`tenpy.tools.math.`**`qr_li`**(*A*, *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] < cuttoff`, reverse the permututation 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 = 1* and upper right *R* with diagonal entries larger than *cutoff*.

Return type `numpy.ndarray`

rq_li

- full name: tenpy.tools.math.rq_li
- parent module: *tenpy.tools.math*
- type: function

`tenpy.tools.math.`**`rq_li`**(*A*, *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 <= 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 < 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 < 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 `kwargs['return_eigenvectors'] == True`.

Module description

Different math functions needed at some point in the library.

`tenpy.tools.math.`**`LeviCivita3 = array([[[ 0, 0, 0], [ 0, 0, 1], [ 0, -1, 0]], [[ 0, 0, -1],`**
Levi-Civita Symbol of int type

7.11.5 fit

- full name: tenpy.tools.fit
- parent module: *tenpy.tools*
- type: module

Functions

alg_decay(x, a, b, c)	define the algebraic decay.
alg_decay_fit(x, y[, npts, power_range, . . .])	Fit y to the form `a*x**(-b) + c`.
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(x, ys[, npts, power_range, . . .])	Fit arrays of y's to the form a * x**(-b) + c.
lin_fit_res(x, y)	Returns the least-square residue of a linear fit y vs x.
linear_fit(x, y)	Perform a linear fit of y to ax + b.
plot_alg_decay_fit(plot_module, x, y, fit_par)	Given x, y, and fit_par (output from alg_decay_fit), produces a plot of the algebraic decay fit.

alg_decay

- full name: tenpy.tools.fit.alg_decay
- parent module: *tenpy.tools.fit*
- type: function

`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*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 * x**(-b) + c.

Returns arrays of [a, b, c].

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, whoses key/items are passed to the plot function. plot_fit_args is a dictionary that controls how the fit is shown.

Module description

tools to fit to an algebraic decay.

7.11.6 string

- full name: tenpy.tools.string
- parent module: *tenpy.tools*
- type: module

Functions

is_non_string_iterable(x)	Check if x is a non-string iterable, (e.g., list, tuple, dictionary, np.ndarray)
to_mathematica_lists(a)	convert nested *a* to string readable by mathematica using curly brackets '{...}'.
vert_join(strlist[, valign, halign, delim])	Join strings with multilines vertically such that they appear next to each other.

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='t'*, *halign='l'*, *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

```
>>> print vert_join(['a\nsample\nmultiline\nstring', 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.

7.11.7 process

- full name: tenpy.tools.process
- parent module: *tenpy.tools*
- type: module

Functions

load_omp_library([libs, verbose])	Tries to load openMP library.
memory_usage()	Return memory usage of the running python process.
mkl_get_nthreads()	wrapper around MKL `get_max_threads`.
mkl_set_nthreads(n)	wrapper around MKL `set_num_threads`.
omp_get_nthreads()	wrapper around OpenMP `get_max_threads`.
omp_set_nthreads(n)	wrapper around OpenMP `set_nthreads`.

load_omp_library

- full name: tenpy.tools.process.load_omp_library
- parent module: *tenpy.tools.process*
- type: function

`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*) – wheter to print the name of the loaded library.

Returns **omp** – OpenMP shared libary if found, otherwise None. Once it was sucessfully 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

`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

`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

`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

`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

`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.

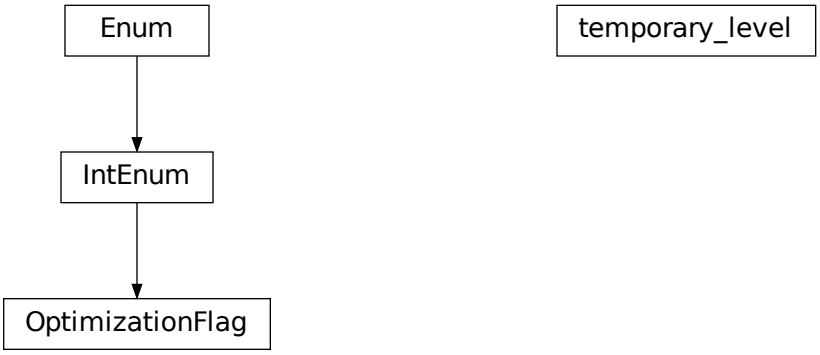
If your python is compiled against MKL (e.g. if you use *anaconda* as recommended in INSTALL), it will by default use as many threads as CPU cores are available. If you run a job on a cluster, you should limit this to the number of cores you reserved – otherwise your colleagues might get angry... A simple way to achieve this is to set a suitable enviornment 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 failsave 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()`.

7.11.8 optimization

- full name: tenpy.tools.optimization
- parent module: `tenpy.tools`
- type: module

Classes

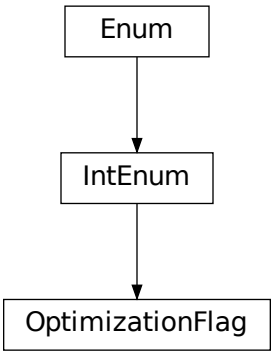


`OptimizationFlag`	Options for the global 'optimization level' used for dynamical optimizations.
`temporary_level`(temporary_level)	Context manager to temporarily set the optimization level to a different value.

OptimizationFlag

- full name: tenpy.tools.optimization.OptimizationFlag
- parent module: *tenpy.tools.optimization*
- type: class

Inheritance Diagram



Class Attributes and Properties

`OptimizationFlag.default`
`OptimizationFlag.none`
`OptimizationFlag.safe`
`OptimizationFlag.skip_arg_checks`

class `tenpy.tools.optimization.`**`OptimizationFlag`**

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.

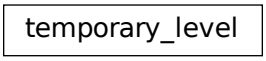
Level	Flag	Description
0	none	Don't do any optimizations, i.e., run many sanity checks. Used for testing.
1	default	Skip really unnecessary sanity checks, but also don't try any optional optimizations if they might give an overhead.
2	safe	Activate safe optimizations in algorithms, even if they might give a small overhead. Example: Try to compress the MPO representing the hamiltonian.
3	skip_arg_checks	Unsafe! Skip (some) class sanity tests and (function) argument checks.

> **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 parmeters and disabled optimiztions! 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



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

get_level()	Return the global optimization level.
optimize([level_compare])	Called by algorithms to check whether it should (try to) do some optimizations.
set_level([level])	Set the global optimization level.
to_OptimizationFlag(level)	Convert strings and int to a valid OptimizationFlag.
use_cython([func, replacement, check_doc])	Decorator to replace a function with a Cython-equivalent from _npc_helper.pyx.

get_level

- full name: tenpy.tools.optimization.get_level
- parent module: *tenpy.tools.optimization*
- type: function

tenpy.tools.optimization.**get_level**()
Return the global optimization level.

optimize

- full name: tenpy.tools.optimization.optimize
- parent module: *tenpy.tools.optimization*
- type: function

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

`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), 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:

```
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 optimiztion, 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 parmeters! 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!

`tenpy.tools.optimization.`**`bottleneck = None`**

`tenpy.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()`.

7.12 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.

`tenpy.version.`**`version = '0.6.0'`**

current release version as a string

`tenpy.version.`**`released = True`**

whether this is a released version or modified

`tenpy.version.`**`short_version = 'v0.6.0'`**

same as version, but with 'v' in front

`tenpy.version.`**`git_revision = '288f9c5e2217ea1688113f3429c7d38f16294458'`**

the hash of the last git commit (if available)

`tenpy.version.`**`full_version = '0.6.0'`**

if not released additional info with part of git revision

tenpy.version.**version_summary = 'tenpy 0.6.0 (not compiled),\ngit revision 288f9c5e2217ea1**

summary of the tenpy, python, numpy and scipy versions used

CHAPTER

EIGHT

INDICES AND TABLES

- genindex
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- search

BIBLIOGRAPHY

[TeNPyNotes] "Efficient numerical simulations with Tensor Networks: Tensor Network Python (TeNPy)" J. Hauschild, F. Pollmann, SciPost Phys. Lect. Notes 5 (2018), arXiv:1805.00055, doi:10.21468/SciPostPhysLectNotes.5

[TeNPySource] https://github.com/tenpy/tenpy

[TeNPyDoc] Online documentation, https://tenpy.readthedocs.io/

[TeNPyForum] Community forum for discussions, FAQ and announcements, https://tenpy.johannes-hauschild.de

[Cirac2009] "Renormalization and tensor product states in spin chains and lattices" J. I. Cirac and F. Verstraete, Journal of Physics A: Mathematical and Theoretical, 42, 50 (2009) arXiv:0910.1130 doi:10.1088/1751-8113/42/50/504004

[Verstraete2009] "Matrix Product States, Projected Entangled Pair States, and variational renormalization group methods for quantum spin systems" F. Verstraete and V. Murg and J.I. Cirac, Advances in Physics 57 2, 143-224 (2009) arXiv:0907.2796 doi:10.1080/14789940801912366

[Schollwoeck2011] "The density-matrix renormalization group in the age of matrix product states" U. Schollwoeck, Annals of Physics 326, 96 (2011), arXiv:1008.3477 doi:10.1016/j.aop.2010.09.012

[Stoudenmire2011] "Studying Two Dimensional Systems With the Density Matrix Renormalization Group" E.M. Stoudenmire, Steven R. White, Ann. Rev. of Cond. Mat. Physics, 3: 111-128 (2012), arXiv:1105.1374 doi:10.1146/annurev-conmatphys-020911-125018

[Eisert2013] "Entanglement and tensor network states" J. Eisert, Modeling and Simulation 3, 520 (2013) arXiv:1308.3318

[Orus2014] "A Practical Introduction to Tensor Networks: Matrix Product States and Projected Entangled Pair States" R. Orus, Annals of Physics 349, 117-158 (2014) arXiv:1306.2164 doi:10.1016/j.aop.2014.06.013

[Hubig2019] "Time-evolution methods for matrix-product states" S. Paeckel, T. Köhler, A. Swoboda, S. R. Manmana, U. Schollwöck, C. Hubig, arXiv:1901.05824

[White1992] "Density matrix formulation for quantum renormalization groups" S. White, Phys. Rev. Lett. 69, 2863 (1992) doi:10.1103/PhysRevLett.69.2863, S. White, Phys. Rev. B 84, 10345 (1992) doi:10.1103/PhysRevB.48.10345

[Vidal2004] "Efficient Simulation of One-Dimensional Quantum Many-Body Systems" G. Vidal, Phys. Rev. Lett. 93, 040502 (2004), arXiv:quant-ph/0310089 doi:10.1103/PhysRevLett.93.040502

[White2005] "Density matrix renormalization group algorithms with a single center site" S. White, Phys. Rev. B 72, 180403(R) (2005), arXiv:cond-mat/0508709 doi:10.1103/PhysRevB.72.180403

[Vidal2007] "Entanglement Renormalization" G. Vidal, Phys. Rev. Lett. 99, 220405 (2007), arXiv:cond-mat/0512165, doi:10.1103/PhysRevLett.99.220405

[McCulloch2008] "Infinite size density matrix renormalization group, revisited" I. P. McCulloch, arXiv:0804.2509

[Singh2009] "Tensor network decompositions in the presence of a global symmetry" S. Singh, R. Pfeifer, G. Vidal, Phys. Rev. A 82, 050301(R), arXiv:0907.2994 doi:10.1103/PhysRevA.82.050301

[Singh2010] "Tensor network states and algorithms in the presence of a global U(1) symmetry" S. Singh, R. Pfeifer, G. Vidal, Phys. Rev. B 83, 115125, arXiv:1008.4774 doi:10.1103/PhysRevB.83.115125

[Haegeman2011] "Time-Dependent Variational Principle for Quantum Lattices" J. Haegeman, J. I. Cirac, T. J. Osborne, I. Pizorn, H. Verschelde, F. Verstraete, Phys. Rev. Lett. 107, 070601 (2011), arXiv:1103.0936 doi:10.1103/PhysRevLett.107.070601

[Karrasch2013] "Reducing the numerical effort of finite-temperature density matrix renormalization group calculations" C. Karrasch, J. H. Bardarson, J. E. Moore, New J. Phys. 15, 083031 (2013), arXiv:1303.3942 doi:10.1088/1367-2630/15/8/083031

[Hubig2015] "Strictly single-site DMRG algorithm with subspace expansion" C. Hubig, I. P. McCulloch, U. Schollwoeck, F. A. Wolf, Phys. Rev. B 91, 155115 (2015), arXiv:1501.05504 doi:10.1103/PhysRevB.91.155115

[Haegeman2016] "Unifying time evolution and optimization with matrix product states" J. Haegeman, C. Lubich, I. Oseledets, B. Vandereycken, F. Verstraete, Phys. Rev. B 94, 165116 (2016), arXiv:1408.5056 doi:10.1103/PhysRevB.94.165116

[Hauschild2018] "Finding purifications with minimal entanglement" J. Hauschild, E. Leviatan, J. H. Bardarson, E. Altman, M. P. Zaletel, F. Pollmann, Phys. Rev. B 98, 235163 (2018), arXiv:1711.01288 doi:10.1103/PhysRevB.98.235163

[Resta1997] "Quantum-Mechanical Position Operator in Extended Systems" R. Resta, Phys. Rev. Lett. 80, 1800 (1997) doi:10.1103/PhysRevLett.80.1800

[Neupert2011] "Fractional quantum Hall states at zero magnetic field" Titus Neupert, Luiz Santos, Claudio Chamon, and Christopher Mudry, Phys. Rev. Lett. 106, 236804 (2011), arXiv:1012.4723 doi:10.1103/PhysRevLett.106.236804

[Yang2012] "Topological flat band models with arbitrary Chern numbers" Shuo Yang, Zheng-Cheng Gu, Kai Sun, and S. Das Sarma, Phys. Rev. B 86, 241112(R) (2012), arXiv:1205.5792, doi:10.1103/PhysRevB.86.241112

[CincioVidal2013] "Characterizing Topological Order by Studying the Ground States on an Infinite Cylinder" L. Cincio, G. Vidal, Phys. Rev. Lett. 110, 067208 (2013), arXiv:1208.2623 doi:10.1103/PhysRevLett.110.067208

[Schuch2013] "Condensed Matter Applications of Entanglement Theory" N. Schuch, Quantum Information Processing. Lecture Notes of the 44th IFF Spring School (2013) arXiv:1306.5551

[PollmannTurner2012] "Detection of symmetry-protected topological phases in one dimension" F. Pollmann, A. Turner, Phys. Rev. B 86, 125441 (2012), arXiv:1204.0704 doi:10.1103/PhysRevB.86.125441

[Grushin2015] "Characterization and stability of a fermionic =1/3 fractional Chern insulator" Adolfo G. Grushin, Johannes Motruk, Michael P. Zaletel, and Frank Pollmann, Phys. Rev. B 91, 035136 (2015), arXiv:1407.6985 doi:10.1103/PhysRevB.91.035136

[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.

[pip] "pip - the Python Package installer", https://pip.pypa.io/en/stable/ Traditional way to handle installed python packages with `pip install ...` and `pip uninstall ...` on the command line.

[matplotlib] "Matplotlib", https://matplotlib.org/ A Python 2D plotting library. Some TeNPy functions expect `matplotlib.axes.Axes` as arguments to plot into.

[HDF5] "Hierarchical Data Format 5 (R)", https://portal.hdfgroup.org/display/HDF5/HDF5 A file format and library for saving data (including metadata). We use it through the python interface of the *h5py <https://docs.h5py.org/en/stable/>*, see *Saving to disk: input/output*.

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