

# **QuTiP: Quantum Toolbox in Python**

*Release 5.0.0*

**P.D. Nation, J.R. Johansson, A.J.G. Pitchford, C. Granade, A.L. C**

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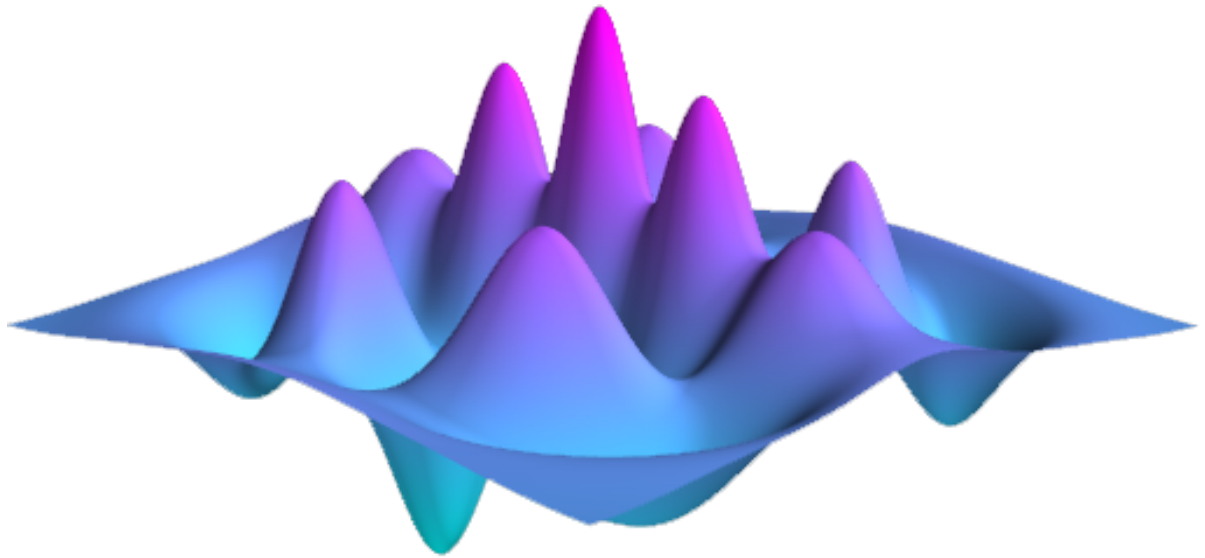


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# Chapter 1

## Frontmatter

### 1.1 About This Documentation

This document contains a user guide and automatically generated API documentation for QuTiP. A PDF version of this text is available at the [documentation page](#).

For more information see the [QuTiP project web page](#).

**Author**

J.R. Johansson

**Author**

P.D. Nation

**Author**

Alexander Pitchford

**Author**

Arne Grimsmo

**Author**

Chris Grenade

**Author**

Nathan Shammah

**Author**

Shahnawaz Ahmed

**Author**

Neill Lambert

**Author**

Eric Giguere

**Author**

Boxi Li

**Author**

Jake Lishman

**Author**

Simon Cross

**release**

5.0.0

**copyright**

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## 1.2 Citing This Project

If you find this project useful, then please cite:

J. R. Johansson, P.D. Nation, and F. Nori, “QuTiP 2: A Python framework for the dynamics of open quantum systems”, *Comp. Phys. Comm.* **184**, 1234 (2013).

or

J. R. Johansson, P.D. Nation, and F. Nori, “QuTiP: An open-source Python framework for the dynamics of open quantum systems”, *Comp. Phys. Comm.* **183**, 1760 (2012).

which may also be downloaded from <https://arxiv.org/abs/1211.6518> or <https://arxiv.org/abs/1110.0573>, respectively.

## 1.3 Funding

QuTiP is developed under the auspice of the non-profit organizations:



QuTiP was partially supported by







## 1.4 About QuTiP

Every quantum system encountered in the real world is an open quantum system. For although much care is taken experimentally to eliminate the unwanted influence of external interactions, there remains, if ever so slight, a coupling between the system of interest and the external world. In addition, any measurement performed on the system necessarily involves coupling to the measuring device, therefore introducing an additional source of external influence. Consequently, developing the necessary tools, both theoretical and numerical, to account for the interactions between a system and its environment is an essential step in understanding the dynamics of practical quantum systems.

In general, for all but the most basic of Hamiltonians, an analytical description of the system dynamics is not possible, and one must resort to numerical simulations of the equations of motion. In absence of a quantum computer, these simulations must be carried out using classical computing techniques, where the exponentially increasing dimensionality of the underlying Hilbert space severely limits the size of system that can be efficiently simulated. However, in many fields such as quantum optics, trapped ions, superconducting circuit devices, and most recently nanomechanical systems, it is possible to design systems using a small number of effective oscillator and spin components, excited by a limited number of quanta, that are amenable to classical simulation in a truncated Hilbert space.

The Quantum Toolbox in Python, or QuTiP, is an open-source framework written in the Python programming language, designed for simulating the open quantum dynamics of systems such as those listed above. This framework distinguishes itself from other available software solutions in providing the following advantages:

- QuTiP relies entirely on open-source software. You are free to modify and use it as you wish with no licensing fees or limitations.
- QuTiP is based on the Python scripting language, providing easy to read, fast code generation without the need to compile after modification.
- The numerics underlying QuTiP are time-tested algorithms that run at C-code speeds, thanks to the [Numpy](#), [Scipy](#), and [Cython](#) libraries, and are based on many of the same algorithms used in propriety software.
- QuTiP allows for solving the dynamics of Hamiltonians with (almost) arbitrary time-dependence, including collapse operators.
- Time-dependent problems can be automatically compiled into C++-code at run-time for increased performance.
- Takes advantage of the multiple processing cores found in essentially all modern computers.
- QuTiP was designed from the start to require a minimal learning curve for those users who have experience using the popular quantum optics toolbox by Sze M. Tan.
- Includes the ability to create high-quality plots, and animations, using the excellent [Matplotlib](#) package.

For detailed information about new features of each release of QuTiP, see the [Change Log](#).

## 1.5 QuTiP Plugins

Several libraries depend on QuTiP heavily making QuTiP a super-library

### **Matsubara**

[Matsubara](#) is a plugin to study the ultrastrong coupling regime with structured baths

### **QNET**

[QNET](#) is a computer algebra package for quantum mechanics and photonic quantum networks

## 1.6 Libraries Using QuTiP

Several libraries rely on QuTiP for quantum physics or quantum information processing. Some of them are:

### **Krotov**

[Krotov](#) focuses on the python implementation of Krotov's method for quantum optimal control

### **pyEPR**

[pyEPR](#) interfaces classical distributed microwave analysis with that of quantum structures and hamiltonians by providing easy to use analysis function and automation for the design of quantum chips

### **scQubits**

[scQubits](#) is a Python library which provides a convenient way to simulate superconducting qubits by providing an interface to QuTiP

### **SimulaQron**

[SimulaQron](#) is a distributed simulation of the end nodes in a quantum internet with the specific goal to explore application development

### **QInfer**

[QInfer](#) is a library for working with sequential Monte Carlo methods for parameter estimation in quantum information

### **QPtomographer**

[QPtomographer](#) derive quantum error bars for quantum processes in terms of the diamond norm to a reference quantum channel

### **QuNetSim**

[QuNetSim](#) is a quantum networking simulation framework to develop and test protocols for quantum networks

### **qupulse**

[qupulse](#) is a toolkit to facilitate experiments involving pulse driven state manipulation of physical qubits

### **Pulser**

[Pulser](#) is a framework for composing, simulating and executing pulse sequences for neutral-atom quantum devices.

## 1.7 Contributing to QuTiP

We welcome anyone who is interested in helping us make QuTiP the best package for simulating quantum systems. There are *detailed instructions on how to contribute code and documentation* in the developers' section of this guide. You can also help out our users by answering questions in the [QuTiP discussion mailing list](#), or by raising issues in [the main GitHub repository](#) if you find any bugs. Anyone who contributes code will be duly recognized. Even small contributions are noted. See *Contributors* for a list of people who have helped in one way or another.



# Chapter 2

## Installation

### 2.1 Quick Start

From QuTiP version 4.6 onwards, you should be able to get a working version of QuTiP with the standard

```
pip install qutip
```

It is not recommended to install any packages directly into the system Python environment; consider using `pip` or `conda` virtual environments to keep your operating system space clean, and to have more control over Python and other package versions.

You do not need to worry about the details on the rest of this page unless this command did not work, but do also read the next section for the list of optional dependencies. The rest of this page covers *installation directly from conda*, *installation from source*, and *additional considerations when working on Windows*.

### 2.2 General Requirements

QuTiP depends on several open-source libraries for scientific computing in the Python programming language. The following packages are currently required:

Package	Version	Details
<b>Python</b>	3.6+	
<b>NumPy</b>	1.16+	
<b>SciPy</b>	1.0+	Lower versions may have missing features.

In addition, there are several optional packages that provide additional functionality:

Package	Version	Details
<code>matplotlib</code>	1.2.1+	Needed for all visualisation tasks.
<code>cython</code>	0.29.20+	Needed for compiling some time-dependent Hamiltonians.
<code>cvxpy</code>	1.0+	Needed to calculate diamond norms.
C++ Compiler	GCC 4.7+, MS VS 2015	Needed for compiling Cython files, made when using string-format time-dependence.
<code>pytest</code> , <code>pytest-rerunfailures</code>	5.3+	For running the test suite.
LaTeX	TeXLive 2009+	Needed if using LaTeX in matplotlib figures, or for nice circuit drawings in IPython.

In addition, there are several additional packages that are not dependencies, but may give you a better programming experience. [IPython](#) provides an improved text-based Python interpreter that is far more full-featured than the default interpreter, and runs in a terminal. If you prefer a more graphical set-up, [Jupyter](#) provides a notebook-style interface to mix code and mathematical notes together. Alternatively, [Spyder](#) is a free integrated development environment for Python, with several nice features for debugging code. QuTiP will detect if it is being used within one of these richer environments, and various outputs will have enhanced formatting.

## 2.3 Installing with conda

If you already have your conda environment set up, and have the `conda-forge` channel available, then you can install QuTiP using:

```
conda install qutip
```

This will install the minimum set of dependences, but none of the optional packages.

### 2.3.1 Adding the conda-forge channel

To install QuTiP from conda, you will need to add the conda-forge channel. The following command adds this channel with lowest priority, so conda will still try and install all other packages normally:

```
conda config --append channels conda-forge
```

If you want to change the order of your channels later, you can edit your `.condarc` (user home folder) file manually, but it is recommended to keep defaults as the highest priority.

### 2.3.2 New conda environments

The default Anaconda environment has all the Python packages needed for running QuTiP installed already, so you will only need to add the `conda-forge` channel and then install the package. If you have only installed Miniconda, or you want a completely clean virtual environment to install QuTiP in, the conda package manager provides a convenient way to do this.

To create a conda environment for QuTiP called `qutip-env`:

```
conda create -n qutip-env python qutip
```

This will automatically install all the necessary packages, and none of the optional packages. You activate the new environment by running

```
conda activate qutip-env
```

You can also install any more optional packages you want with `conda install`, for example `matplotlib`, `ipython` or `jupyter`.

## 2.4 Installation of the pre-release of version 5

QuTiP version 5 has been in development for some time and brings many new features, heavily reworks the core functionalities of QuTiP. It is available as a pre-release on PyPI. Anyone wanting to try the new features can install it with:

```
pip install --pre qutip
```

We expect the pre-release to fully work. If you find any bugs, confusing documentation or missing features, please tell create an issue on [github](#).

This version breaks compatibility with QuTiP 4.7 in many small ways. Please see the [Change Log](#) for a list of changes, new features and deprecations.

## 2.5 Installing from Source

Official releases of QuTiP are available from the download section on [the project's web pages](#), and the latest source code is available in [our GitHub repository](#). In general we recommend users to use the latest stable release of QuTiP, but if you are interested in helping us out with development or wish to submit bug fixes, then use the latest development version from the GitHub repository.

You can install from source by using the [Python-recommended PEP 517 procedure](#), or if you want more control or to have a development version, you can use the [low-level build procedure with setuptools](#).

### 2.5.1 PEP 517 Source Builds

The easiest way to build QuTiP from source is to use a PEP-517-compatible builder such as the `build` package available on `pip`. These will automatically install all build dependencies for you, and the `pip` installation step afterwards will install the minimum runtime dependencies. You can do this by doing (for example)

```
pip install build
python -m build <path to qutip>
pip install <path to qutip>/dist/qutip-<version>.whl
```

The first command installs the reference PEP-517 build tool, the second effects the build and the third uses `pip` to install the built package. You will need to replace `<path to qutip>` with the actual path to the QuTiP source code. The string `<version>` will depend on the version of QuTiP, the version of Python and your operating system. It will look something like `4.6.0-cp39-cp39-manylinux1_x86_64`, but there should only be one `.whl` file in the `dist/` directory, which will be the correct one.

### 2.5.2 Direct Setuptools Source Builds

This is the method to have the greatest amount of control over the installation, but it the most error-prone and not recommended unless you know what you are doing. You first need to have all the runtime dependencies installed. The most up-to-date requirements will be listed in `pyproject.toml` file, in the `build-system.requires` key. As of the 4.6.0 release, the build requirements can be installed with

```
pip install setuptools wheel packaging 'cython>=0.29.20' 'numpy>=1.16.6,<1.20' 'scipy>=1.0'
```

or similar with `conda` if you prefer. You will also need to have a functional C++ compiler installed on your system. This is likely already done for you if you are on Linux or macOS, but see the [section on Windows installations](#) if that is your operating system.

To install QuTiP from the source code run:

```
python setup.py install
```

To install OpenMP support, if available, run:

```
python setup.py install --with-openmp
```

This will attempt to load up OpenMP libraries during the compilation process, which depends on you having suitable C++ compiler and library support. If you are on Linux this is probably already done, but the compiler macOS ships with does not have OpenMP support. You will likely need to refer to external operating-system-specific guides for more detail here, as it may be very non-trivial to correctly configure.

If you wish to contribute to the QuTiP project, then you will want to create your own fork of [the QuTiP git repository](#), clone this to a local folder, and install it into your Python environment using:

```
python setup.py develop
```

When you do `import qutip` in this environment, you will then load the code from your local fork, enabling you to edit the Python files and have the changes immediately available when you restart your Python interpreter, without needing to rebuild the package. Note that if you change any Cython files, you will need to rerun the build command.

You should not need to use `sudo` (or other superuser privileges) to install into a personal virtual environment; if it feels like you need it, there is a good chance that you are installing into the system Python environment instead.

## 2.6 Installation on Windows

As with other operating systems, the easiest method is to use `pip install qutip`, or use the conda procedure described above. If you want to build from source or use runtime compilation with Cython, you will need to have a working C++ compiler.

You can [download the Visual Studio IDE from Microsoft](#), which has a free Community edition containing a sufficient C++ compiler. This is the recommended compiler toolchain on Windows. When installing, be sure to select the following components:

- Windows “X” SDK (where “X” stands for your version: 7/8/8.1/10)
- Visual Studio C++ build tools

You can then follow the [installation from source](#) section as normal.

---

**Important:** In order to prevent issues with the PATH environment variable not containing the compiler and associated libraries, it is recommended to use the developer command prompt in the Visual Studio installation folder instead of the built-in command prompt.

---

The Community edition of Visual Studio takes around 10GB of disk space. If this is prohibitive for you, it is also possible to install [only the build tools and necessary SDKs](#) instead, which should save about 2GB of space.

## 2.7 Verifying the Installation

QuTiP includes a collection of built-in test scripts to verify that an installation was successful. To run the suite of tests scripts you must also have the `pytest` testing library. After installing QuTiP, leave the installation directory, run Python (or IPython), and call:

```
import qutip.testing
qutip.testing.run()
```



This will take between 10 and 30 minutes, depending on your computer. At the end, the testing report should report a success; it is normal for some tests to be skipped, and for some to be marked “xfail” in yellow. Skips may be tests that do not run on your operating system, or tests of optional components that you have not installed the dependencies for. If any failures or errors occur, please check that you have installed all of the required modules. See the next section on how to check the installed versions of the QuTiP dependencies. If these tests still fail, then head on over to the [QuTiP Discussion Board](#) or the [GitHub issues page](#) and post a message detailing your particular issue.

## 2.8 Checking Version Information

QuTiP includes an “about” function for viewing information about QuTiP and the important dependencies installed on your system. To view this information:

```
import qutip
qutip.about()
```



# Chapter 3

## Users Guide

### 3.1 Guide Overview

The goal of this guide is to introduce you to the basic structures and functions that make up QuTiP. This guide is divided up into several sections, each highlighting a specific set of functionalities. In combination with the examples that can be found on the project web page <https://qutip.org/tutorials.html>, this guide should provide a more or less complete overview of QuTip. We also provide the API documentation in *API documentation*.

#### 3.1.1 Organization

QuTiP is designed to be a general framework for solving quantum mechanics problems such as systems composed of few-level quantum systems and harmonic oscillators. To this end, QuTiP is built from a large (and ever growing) library of functions and classes; from `qutip.states.basis` to *[qutip.wigner](#)*. The general organization of QuTiP, highlighting the important API available to the user, is shown in the figure below.

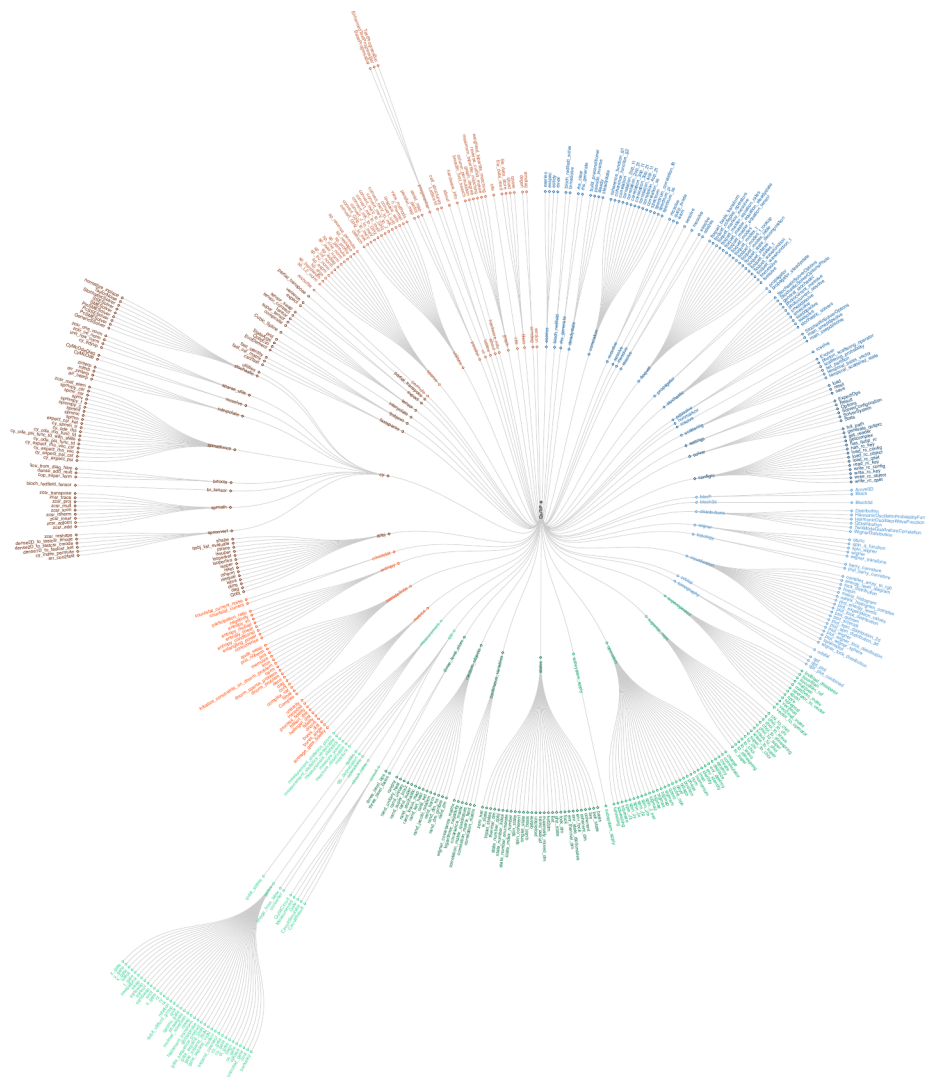


Fig. 1: Tree-diagram of the 468 user accessible functions and classes in QuTiP 4.6. A vector image of the code tree is in `qutip_tree.pdf`.

## 3.2 Basic Operations on Quantum Objects

### 3.2.1 First things first

**Warning:** Do not run QuTiP from the installation directory.

To load the qutip modules, first call the import statement:

```
from qutip import *
```

This will load all of the user available functions. Often, we also need to import the NumPy and Matplotlib libraries with:

```
import numpy as np
import matplotlib.pyplot as plt
```

In the rest of the documentation, functions are written using `qutip.module.function()` notation which links to the corresponding function in the QuTiP API: [Functions](#). However, in calling `import *`, we have already loaded all of the QuTiP modules. Therefore, we will only need the function name and not the complete path when calling the function from the interpreter prompt, Python script, or Jupyter notebook.

## 3.2.2 The quantum object class

### Introduction

The key difference between classical and quantum mechanics is the use of operators instead of numbers as variables. Moreover, we need to specify state vectors and their properties. Therefore, in computing the dynamics of quantum systems, we need a data structure that encapsulates the properties of a quantum operator and ket/bra vectors. The quantum object class, `qutip.Qobj`, accomplishes this using matrix representation.

To begin, let us create a blank `Qobj`:

```
print(Qobj())
```

**Output:**

```
Quantum object: dims = [[1], [1]], shape = (1, 1), type = bra
Qobj data =
[[0.]]
```

where we see the blank `Qobj` object with dimensions, shape, and data. Here the data corresponds to a 1x1-dimensional matrix consisting of a single zero entry.

---

**Hint:** By convention, the names of Python classes, such as `Qobj()`, are capitalized whereas the names of functions are not.

---

We can create a `Qobj` with a user defined data set by passing a list or array of data into the `Qobj`:

```
print(Qobj([[1],[2],[3],[4],[5]]))
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[1.]
 [2.]
 [3.]
 [4.]
 [5.]]
```

```
x = np.array([[1, 2, 3, 4, 5]])
print(Qobj(x))
```

**Output:**

```
Quantum object: dims = [[1], [5]], shape = (1, 5), type = bra
Qobj data =
[[1. 2. 3. 4. 5.]]
```

```
r = np.random.rand(4, 4)
print(Qobj(r))
```

### Output:

```
Quantum object: dims = [[4], [4]], shape = (4, 4), type = oper, isherm = False
Qobj data =
[[0.37454012 0.95071431 0.73199394 0.59865848]
 [0.15601864 0.15599452 0.05808361 0.86617615]
 [0.60111501 0.70807258 0.02058449 0.96990985]
 [0.83244264 0.21233911 0.18182497 0.18340451]]
```

Notice how both the dims and shape change according to the input data. Although dims and shape appear to be the same, dims keep track of the shapes for individual components of a multipartite system, while shape does not. We refer the reader to the section [tensor products and partial traces](#) for more information.

---

**Note:** If you are running QuTiP from a python script you must use the `print` function to view the Qobj attributes.

---

## States and operators

Manually specifying the data for each quantum object is inefficient. Even more so when most objects correspond to commonly used types such as the ladder operators of a harmonic oscillator, the Pauli spin operators for a two-level system, or state vectors such as Fock states. Therefore, QuTiP includes predefined objects for a variety of states and operators:

States	Command (# means optional)	Inputs
Fock state ket vector	<code>basis(N, #m) / fock(N, #m)</code>	N = number of levels in Hilbert space, m = level containing excitation (0 if no m given)
Empty ket vector	<code>zero_ket(N)</code>	N = number of levels in Hilbert space,
Fock density matrix (outer product of basis)	<code>fock_dm(N, #p)</code>	same as <code>basis(N,m) / fock(N,m)</code>
Coherent state	<code>coherent(N, alpha)</code>	alpha = complex number (eigenvalue) for requested coherent state
Coherent density matrix (outer product)	<code>coherent_dm(N, alpha)</code>	same as <code>coherent(N,alpha)</code>
Thermal density matrix (for n particles)	<code>thermal_dm(N, n)</code>	n = particle number expectation value
Maximally mixed density matrix	<code>maximally_mixed_d</code>	N = number of levels in Hilbert space

Operators	Command (# means optional)	Inputs
Charge operator	<code>charge(N,M=-N)</code>	Diagonal operator with entries from M..0..N.
Commutator	<code>commutator(A, B, kind)</code>	Kind = 'normal' or 'anti'.
Diagonals operator	<code>qdiags(N)</code>	Quantum object created from arrays of diagonals at given offsets.
Displacement operator (Single-mode)	<code>displace(N,alpha)</code>	N=number of levels in Hilbert space, alpha = complex displacement amplitude.
Higher spin operators	<code>jmat(j,#s)</code>	j = integer or half-integer representing spin, s = 'x', 'y', 'z', '+', or '-'
Identity	<code>qeye(N)</code>	N = number of levels in Hilbert space.
Identity-like	<code>qeye_like(qobj)</code>	qobj = Object to copy dimensions from.
Lowering (destruction) operator	<code>destroy(N)</code>	same as above
Momentum operator	<code>momentum(N)</code>	same as above
Number operator	<code>num(N)</code>	same as above
Phase operator (Single-mode)	<code>phase(N, phi0)</code>	Single-mode Pegg-Barnett phase operator with ref phase phi0.
Position operator	<code>position(N)</code>	same as above
Raising (creation) operator	<code>create(N)</code>	same as above
Squeezing operator (Single-mode)	<code>squeeze(N, sp)</code>	N=number of levels in Hilbert space, sp = squeezing parameter.
Squeezing operator (Generalized)	<code>squeezing(q1, q2, sp)</code>	q1,q2 = Quantum operators (Qobj) sp = squeezing parameter.
Sigma-X	<code>sigmax()</code>	
Sigma-Y	<code>sigmay()</code>	
Sigma-Z	<code>sigmaz()</code>	
Sigma plus	<code>sigmap()</code>	
Sigma minus	<code>sigmam()</code>	
Tunneling operator	<code>tunneling(N,m)</code>	Tunneling operator with elements of the form $ N \rangle \langle N+m  +  N+m \rangle \langle N $ .

As an example, we give the output for a few of these functions:

```
>>> basis(5,3)
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [0.]
 [0.]
 [1.]
 [0.]]

>>> coherent(5,0.5-0.5j)
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[ 0.7788017 +0.j          ]
 [ 0.38939142-0.38939142j]
 [ 0.          -0.27545895j]
 [-0.07898617-0.07898617j]
 [-0.04314271+0.j          ]]

>>> destroy(4)
Quantum object: dims = [[4], [4]], shape = (4, 4), type = oper, isherm = False
```

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```
Qobj data =
[[0.      1.      0.      0.      ]
 [0.      0.      1.41421356 0.      ]
 [0.      0.      0.      1.73205081]
 [0.      0.      0.      0.      ]]

>>> sigmaz()
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[ 1.  0.]
 [ 0. -1.]]

>>> jmat(5/2.0, '+')
Quantum object: dims = [[6], [6]], shape = (6, 6), type = oper, isherm = False
Qobj data =
[[0.      2.23606798 0.      0.      0.      0.      ]
 [0.      0.      2.82842712 0.      0.      0.      ]
 [0.      0.      0.      3.      0.      0.      ]
 [0.      0.      0.      0.      2.82842712 0.      ]
 [0.      0.      0.      0.      0.      2.23606798]
 [0.      0.      0.      0.      0.      0.      ]]
```

## Qobj attributes

We have seen that a quantum object has several internal attributes, such as `data`, `dims`, and `shape`. These can be accessed in the following way:

```
>>> q = destroy(4)

>>> q.dims
[[4], [4]]

>>> q.shape
(4, 4)
```

In general, the attributes (properties) of a `Qobj` object (or any Python object) can be retrieved using the *Q.attribute* notation. In addition to the those shown with the `print` function, an instance of the `Qobj` class also has the following attributes:

Property	Attribute	Description
Data	<code>Q.data</code>	Matrix representing state or operator
Dimensions	<code>Q.dims</code>	List keeping track of shapes for individual components of a multipartite system (for tensor products and partial traces).
Shape	<code>Q.shape</code>	Dimensions of underlying data matrix.
is Hermitian?	<code>Q.isherm</code>	Is the operator Hermitian or not?
Type	<code>Q.type</code>	Is object of type 'ket', 'bra', 'oper', or 'super'?



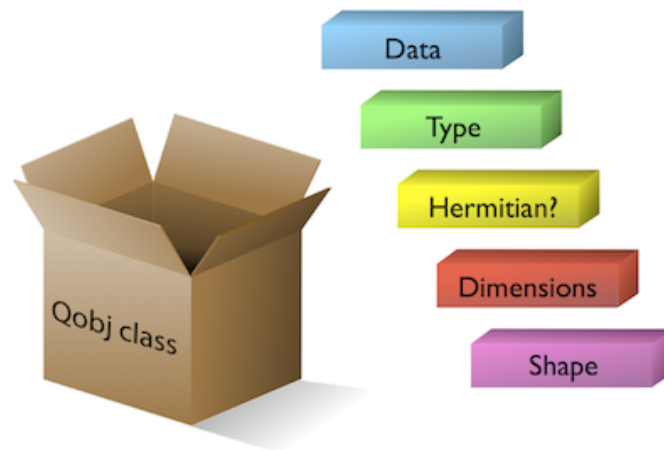


Fig. 2: The Qobj Class viewed as a container for the properties needed to characterize a quantum operator or state vector.

For the destruction operator above:

```
>>> q.type
'oper'

>>> q.isherm
False

>>> q.data
Dia(shape=(4, 4), num_diag=1)
```

The data attribute returns a Qutip diagonal matrix. Qobj instances store their data in Qutip matrix format. In the core qutip module, the Dense, CSR and Dia formats are available, but other packages can add other formats. For example, the qutip-jax module adds the Jax and JaxDia formats. One can always access the underlying matrix as a numpy array using [Qobj.full](#). It is also possible to access the underlying data in a common format using [Qobj.data\\_as](#).

```
>>> q.data_as("dia_matrix")
<4x4 sparse matrix of type '<class 'numpy.complex128'>'
  with 3 stored elements (1 diagonals) in DIAgonal format>
```

Conversion between storage type is done using the [Qobj.to](#) method.

```
>>> q.to("CSR").data
CSR(shape=(4, 4), nnz=3)

>>> q.to("CSR").data_as("CSR_matrix")
<4x4 sparse matrix of type '<class 'numpy.complex128'>'
  with 3 stored elements in Compressed Sparse Row format>
```

Note that [Qobj.data\\_as](#) does not do the conversion.

QuTiP will do conversion when needed to keep everything working in any format. However these conversions could slow down computation and it is recommended to keep to one format family where possible. For example, core QuTiP Dense and CSR work well together and binary operations between these formats is efficient. However binary operations between Dense and Jax should be avoided since it is not always clear whether the operation will be executed by Jax (possibly on a GPU if present) or numpy.

## Qobj Math

The rules for mathematical operations on Qobj instances are similar to standard matrix arithmetic:

```
>>> q = destroy(4)

>>> x = sigmax()

>>> q + 5
Quantum object: dims = [[4], [4]], shape = (4, 4), type = oper, isherm = False
Qobj data =
[[5.         1.         0.         0.         ]
 [0.         5.         1.41421356 0.         ]
 [0.         0.         5.         1.73205081]
 [0.         0.         0.         5.         ]]

>>> x * x
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[1. 0.]
 [0. 1.]]

>>> q ** 3
Quantum object: dims = [[4], [4]], shape = (4, 4), type = oper, isherm = False
Qobj data =
[[0.         0.         0.         2.44948974]
 [0.         0.         0.         0.         ]
 [0.         0.         0.         0.         ]
 [0.         0.         0.         0.         ]]

>>> x / np.sqrt(2)
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0.         0.70710678]
 [0.70710678 0.         ]]
```

Of course, like matrices, multiplying two objects of incompatible shape throws an error:

```
>>> print(q * x)
-----
TypeError                                Traceback (most recent call last)
<ipython-input-33-0b599f41213e> in <module>
----> 1 print(q * x)

~/Documents/qutip_dev/qutip/qutip/qobj.py in __mul__(self, other)
    553
    554         else:
--> 555             raise TypeError("Incompatible Qobj shapes")
    556
    557         elif isinstance(other, np.ndarray):

TypeError: Incompatible Qobj shapes
```

In addition, the logic operators “is equal” `==` and “is not equal” `!=` are also supported.

### 3.2.3 Functions operating on Qobj class

Like attributes, the quantum object class has defined functions (methods) that operate on Qobj class instances. For a general quantum object Q:

Function	Command	Description
Check Her-micity	<code>Q.check_herm()</code>	Check if quantum object is Hermitian
Conjugate	<code>Q.conj()</code>	Conjugate of quantum object.
Cosine	<code>Q.cosm()</code>	Cosine of quantum object.
Dagger (ad-joint)	<code>Q.dag()</code>	Returns adjoint (dagger) of object.
Diagonal	<code>Q.diag()</code>	Returns the diagonal elements.
Diamond Norm	<code>Q.dnorm()</code>	Returns the diamond norm.
Eigenenergies	<code>Q.eigenenergies()</code>	Eigenenergies (values) of operator.
Eigenstates	<code>Q.eigenstates()</code>	Returns eigenvalues and eigenvectors.
Exponential	<code>Q.expm()</code>	Matrix exponential of operator.
Full	<code>Q.full()</code>	Returns full (not sparse) array of Q's data.
Groundstate	<code>Q.groundstate()</code>	Eigenval & eigket of Qobj groundstate.
Matrix inverse	<code>Q.inv()</code>	Matrix inverse of the Qobj.
Matrix Ele-ment	<code>Q.matrix_element(bra, ket)</code>	Matrix element $\langle \text{bra}   Q   \text{ket} \rangle$
Norm	<code>Q.norm()</code>	Returns L2 norm for states, trace norm for operators.
Overlap	<code>Q.overlap(state)</code>	Overlap between current Qobj and a given state.
Partial Trace	<code>Q.ptrace(sel)</code>	Partial trace returning components selected using 'sel' parameter.
Permute	<code>Q.permute(order)</code>	Permutes the tensor structure of a composite object in the given order.
Projector	<code>Q.proj()</code>	Form projector operator from given ket or bra vector.
Sine	<code>Q.sinm()</code>	Sine of quantum operator.
Sqrt	<code>Q.sqrm()</code>	Matrix sqrt of operator.
Tidyup	<code>Q.tidyup()</code>	Removes small elements from Qobj.
Trace	<code>Q.tr()</code>	Returns trace of quantum object.
Conversion	<code>Q.to(dtype)</code>	Convert the matrix format CSR / Dense.
Transform	<code>Q.transform(inpt)</code>	A basis transformation defined by matrix or list of kets 'inpt'
Transpose	<code>Q.trans()</code>	Transpose of quantum object.
Truncate Neg	<code>Q.trunc_neg()</code>	Truncates negative eigenvalues
Unit	<code>Q.unit()</code>	Returns normalized (unit) vector $Q/Q.\text{norm}()$ .

```
>>> basis(5, 3)
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [0.]
 [0.]
 [1.]
 [0.]]

>>> basis(5, 3).dag()
Quantum object: dims = [[1], [5]], shape = (1, 5), type = bra
Qobj data =
[[0. 0. 0. 1. 0.]]

>>> coherent_dm(5, 1)
```

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```

Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[0.36791117 0.36774407 0.26105441 0.14620658 0.08826704]
 [0.36774407 0.36757705 0.26093584 0.14614018 0.08822695]
 [0.26105441 0.26093584 0.18523331 0.10374209 0.06263061]
 [0.14620658 0.14614018 0.10374209 0.05810197 0.035077 ]
 [0.08826704 0.08822695 0.06263061 0.035077 0.0211765 ]]

>>> coherent_dm(5, 1).diag()
array([0.36791117, 0.36757705, 0.18523331, 0.05810197, 0.0211765 ])

>>> coherent_dm(5, 1).full()
array([[0.36791117+0.j, 0.36774407+0.j, 0.26105441+0.j, 0.14620658+0.j,
        0.08826704+0.j],
       [0.36774407+0.j, 0.36757705+0.j, 0.26093584+0.j, 0.14614018+0.j,
        0.08822695+0.j],
       [0.26105441+0.j, 0.26093584+0.j, 0.18523331+0.j, 0.10374209+0.j,
        0.06263061+0.j],
       [0.14620658+0.j, 0.14614018+0.j, 0.10374209+0.j, 0.05810197+0.j,
        0.035077 +0.j],
       [0.08826704+0.j, 0.08822695+0.j, 0.06263061+0.j, 0.035077 +0.j,
        0.0211765 +0.j]])

>>> coherent_dm(5, 1).norm()
1.00000000175063126

>>> coherent_dm(5, 1).sqrtm()
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = False
Qobj data =
[[0.36791117+3.66778589e-09j 0.36774407-2.13388761e-09j
 0.26105441-1.51480558e-09j 0.14620658-8.48384618e-10j
 0.08826704-5.12182118e-10j]
 [0.36774407-2.13388761e-09j 0.36757705+2.41479965e-09j
 0.26093584-1.11446422e-09j 0.14614018+8.98971115e-10j
 0.08822695+6.40705133e-10j]
 [0.26105441-1.51480558e-09j 0.26093584-1.11446422e-09j
 0.18523331+4.02032413e-09j 0.10374209-3.39161017e-10j
 0.06263061-3.71421368e-10j]
 [0.14620658-8.48384618e-10j 0.14614018+8.98971115e-10j
 0.10374209-3.39161017e-10j 0.05810197+3.36300708e-10j
 0.035077 +2.36883273e-10j]
 [0.08826704-5.12182118e-10j 0.08822695+6.40705133e-10j
 0.06263061-3.71421368e-10j 0.035077 +2.36883273e-10j
 0.0211765 +1.71630348e-10j]]

>>> coherent_dm(5, 1).tr()
1.0

>>> (basis(4, 2) + basis(4, 1)).unit()
Quantum object: dims = [[4], [1]], shape = (4, 1), type = ket
Qobj data =
[[0.
 [0.70710678]
 [0.70710678]
 [0.
 ]]]

```

## 3.3 Manipulating States and Operators

### 3.3.1 Introduction

In the previous guide section *Basic Operations on Quantum Objects*, we saw how to create states and operators, using the functions built into QuTiP. In this portion of the guide, we will look at performing basic operations with states and operators. For more detailed demonstrations on how to use and manipulate these objects, see the examples on the [tutorials](#) web page.

### 3.3.2 State Vectors (kets or bras)

Here we begin by creating a Fock *basis* vacuum state vector  $|0\rangle$  with in a Hilbert space with 5 number states, from 0 to 4:

```
vac = basis(5, 0)

print(vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[1.]
 [0.]
 [0.]
 [0.]
 [0.]]
```

and then create a lowering operator ( $\hat{a}$ ) corresponding to 5 number states using the *destroy* function:

```
a = destroy(5)

print(a)
```

**Output:**

```
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = False
Qobj data =
[[0.      1.      0.      0.      0.      ]
 [0.      0.      1.41421356 0.      0.      ]
 [0.      0.      0.      1.73205081 0.      ]
 [0.      0.      0.      0.      2.      ]
 [0.      0.      0.      0.      0.      ]]
```

Now lets apply the destruction operator to our vacuum state *vac*,

```
print(a * vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [0.]
 [0.]
 [0.]
 [0.]]
```

We see that, as expected, the vacuum is transformed to the zero vector. A more interesting example comes from using the adjoint of the lowering operator, the raising operator  $\hat{a}^\dagger$ :

```
print(a.dag() * vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [1.]
 [0.]
 [0.]
 [0.]]
```

The raising operator has in indeed raised the state *vac* from the vacuum to the  $|1\rangle$  state. Instead of using the dagger `Qobj.dag()` method to raise the state, we could have also used the built in `create` function to make a raising operator:

```
c = create(5)
print(c * vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [1.]
 [0.]
 [0.]
 [0.]]
```

which does the same thing. We can raise the vacuum state more than once by successively apply the raising operator:

```
print(c * c * vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.      ]
 [0.      ]
 [1.41421356]
 [0.      ]
 [0.      ]]
```

or just taking the square of the raising operator  $(\hat{a}^\dagger)^2$ :

```
print(c ** 2 * vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.      ]
 [0.      ]]
```

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```
[1.41421356]
[0.         ]
[0.         ]]
```

Applying the raising operator twice gives the expected  $\sqrt{n+1}$  dependence. We can use the product of  $c * a$  to also apply the number operator to the state vector `vac`:

```
print(c * a * vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [0.]
 [0.]
 [0.]
 [0.] ]]
```

or on the  $|1\rangle$  state:

```
print(c * a * (c * vac))
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [1.]
 [0.]
 [0.]
 [0.] ]]
```

or the  $|2\rangle$  state:

```
print(c * a * (c**2 * vac))
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.         ]
 [0.         ]
 [2.82842712]
 [0.         ]
 [0.         ]]
```

Notice how in this last example, application of the number operator does not give the expected value  $n = 2$ , but rather  $2\sqrt{2}$ . This is because this last state is not normalized to unity as  $c|n\rangle = \sqrt{n+1}|n+1\rangle$ . Therefore, we should normalize our vector first:

```
print(c * a * (c**2 * vac).unit())
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
```

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```
[[0.]
 [0.]
 [2.]
 [0.]
 [0.]]
```

Since we are giving a demonstration of using states and operators, we have done a lot more work than we should have. For example, we do not need to operate on the vacuum state to generate a higher number Fock state. Instead we can use the *basis* (or *fock*) function to directly obtain the required state:

```
ket = basis(5, 2)

print(ket)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [0.]
 [1.]
 [0.]
 [0.]]
```

Notice how it is automatically normalized. We can also use the built in *num* operator:

```
n = num(5)

print(n)
```

**Output:**

```
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[0. 0. 0. 0. 0.]
 [0. 1. 0. 0. 0.]
 [0. 0. 2. 0. 0.]
 [0. 0. 0. 3. 0.]
 [0. 0. 0. 0. 4.]]
```

Therefore, instead of `c * a * (c ** 2 * vac).unit()` we have:

```
print(n * ket)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.]
 [0.]
 [2.]
 [0.]
 [0.]]
```

We can also create superpositions of states:



```
ket = (basis(5, 0) + basis(5, 1)).unit()

print(ket)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.70710678]
 [0.70710678]
 [0.         ]
 [0.         ]
 [0.         ]]
```

where we have used the `Qobj.unit` method to again normalize the state. Operating with the number function again:

```
print(n * ket)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[0.         ]
 [0.70710678]
 [0.         ]
 [0.         ]
 [0.         ]]
```

We can also create coherent states and squeezed states by applying the `displace` and `squeeze` functions to the vacuum state:

```
vac = basis(5, 0)

d = displace(5, 1j)

s = squeeze(5, np.complex(0.25, 0.25))

print(d * vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[ 0.60655682+0.j          ]
 [ 0.          +0.60628133j]
 [-0.4303874 +0.j          ]
 [ 0.          -0.24104351j]
 [ 0.14552147+0.j          ]]
```

```
print(d * s * vac)
```

**Output:**

```
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[ 0.65893786+0.08139381j]
```

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```
[ 0.10779462+0.51579735j]
[-0.37567217-0.01326853j]
[-0.02688063-0.23828775j]
[ 0.26352814+0.11512178j]]
```

Of course, displacing the vacuum gives a coherent state, which can also be generated using the built in [coherent](#) function.

### 3.3.3 Density matrices

One of the main purpose of QuTiP is to explore the dynamics of **open** quantum systems, where the most general state of a system is no longer a state vector, but rather a density matrix. Since operations on density matrices operate identically to those of vectors, we will just briefly highlight creating and using these structures.

The simplest density matrix is created by forming the outer-product  $|\psi\rangle\langle\psi|$  of a ket vector:

```
ket = basis(5, 2)

print(ket * ket.dag())
```

**Output:**

```
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[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.]
```

A similar task can also be accomplished via the [fock\\_dm](#) or [ket2dm](#) functions:

```
print(fock_dm(5, 2))
```

**Output:**

```
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[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.]
```

```
print(ket2dm(ket))
```

**Output:**

```
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[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.]
```

If we want to create a density matrix with equal classical probability of being found in the  $|2\rangle$  or  $|4\rangle$  number states we can do the following:

```
print(0.5 * ket2dm(basis(5, 4)) + 0.5 * ket2dm(basis(5, 2)))
```

Output:

```
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[0.  0.  0.  0.  0. ]
 [0.  0.  0.  0.  0. ]
 [0.  0.  0.5 0.  0. ]
 [0.  0.  0.  0.  0. ]
 [0.  0.  0.  0.  0.5]]
```

or use `0.5 * fock_dm(5, 2) + 0.5 * fock_dm(5, 4)`. There are also several other built-in functions for creating predefined density matrices, for example `coherent_dm` and `thermal_dm` which create coherent state and thermal state density matrices, respectively.

```
print(coherent_dm(5, 1.25))
```

Output:

```
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[0.20980701 0.26141096 0.23509686 0.15572585 0.13390765]
 [0.26141096 0.32570738 0.29292109 0.19402805 0.16684347]
 [0.23509686 0.29292109 0.26343512 0.17449684 0.1500487 ]
 [0.15572585 0.19402805 0.17449684 0.11558499 0.09939079]
 [0.13390765 0.16684347 0.1500487  0.09939079 0.0854655 ]]
```

```
print(thermal_dm(5, 1.25))
```

Output:

```
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[0.46927974 0.          0.          0.          0.          ]
 [0.          0.26071096 0.          0.          0.          ]
 [0.          0.          0.14483942 0.          0.          ]
 [0.          0.          0.          0.08046635 0.          ]
 [0.          0.          0.          0.          0.04470353]]
```

QuTiP also provides a set of distance metrics for determining how close two density matrix distributions are to each other. Included are the trace distance `tracedist`, fidelity `fidelity`, Hilbert-Schmidt distance `hilbert_dist`, Bures distance `bures_dist`, Bures angle `bures_angle`, and quantum Hellinger distance `hellinger_dist`.

```
x = coherent_dm(5, 1.25)

y = coherent_dm(5, np.complex(0, 1.25)) # <-- note the 'j'

z = thermal_dm(5, 0.125)

np.testing.assert_almost_equal(fidelity(x, x), 1)

np.testing.assert_almost_equal(hellinger_dist(x, y), 1.3819080728932833)
```

We also know that for two pure states, the trace distance (T) and the fidelity (F) are related by  $T = \sqrt{1 - F^2}$ , while

the quantum Hellinger distance (QHE) between two pure states  $|\psi\rangle$  and  $|\phi\rangle$  is given by  $QHE = \sqrt{2 - 2|\langle\psi|\phi\rangle|^2}$ .

```
np.testing.assert_almost_equal(tracedist(y, x), np.sqrt(1 - fidelity(y, x) ** 2))
```

For a pure state and a mixed state,  $1 - F^2 \leq T$  which can also be verified:

```
assert 1 - fidelity(x, z) ** 2 < tracedist(x, z)
```

### 3.3.4 Qubit (two-level) systems

Having spent a fair amount of time on basis states that represent harmonic oscillator states, we now move on to qubit, or two-level quantum systems (for example a spin-1/2). To create a state vector corresponding to a qubit system, we use the same *basis*, or *fock*, function with only two levels:

```
spin = basis(2, 0)
```

Now at this point one may ask how this state is different than that of a harmonic oscillator in the vacuum state truncated to two energy levels?

```
vac = basis(2, 0)
```

At this stage, there is no difference. This should not be surprising as we called the exact same function twice. The difference between the two comes from the action of the spin operators *sigmax*, *sigmay*, *sigmaz*, *sigmap*, and *sigmam* on these two-level states. For example, if *vac* corresponds to the vacuum state of a harmonic oscillator, then, as we have already seen, we can use the raising operator to get the  $|1\rangle$  state:

```
print(vac)
```

**Output:**

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[1.]
 [0.]]
```

```
c = create(2)
```

```
print(c * vac)
```

**Output:**

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[0.]
 [1.]]
```

For a spin system, the operator analogous to the raising operator is the sigma-plus operator *sigmap*. Operating on the *spin* state gives:

```
print(spin)
```

**Output:**

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[1.]
 [0.]]
```

```
print(sigmap() * spin)
```

**Output:**

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[0.]
 [0.]]
```

Now we see the difference! The `sigmap` operator acting on the `spin` state returns the zero vector. Why is this? To see what happened, let us use the `sigmaz` operator:

```
print(sigmaz())
```

**Output:**

```
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[ 1.  0.]
 [ 0. -1.]]
```

```
print(sigmaz() * spin)
```

**Output:**

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[1.]
 [0.]]
```

```
spin2 = basis(2, 1)
```

```
print(spin2)
```

**Output:**

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[0.]
 [1.]]
```

```
print(sigmaz() * spin2)
```

**Output:**

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[ 0.]
 [-1.]]
```

The answer is now apparent. Since the QuTiP `sigmaz` function uses the standard z-basis representation of the sigma-z spin operator, the `spin` state corresponds to the  $|\uparrow\rangle$  state of a two-level spin system while `spin2` gives the  $|\downarrow\rangle$  state. Therefore, in our previous example `sigmap() * spin`, we raised the qubit state out of the truncated two-level Hilbert space resulting in the zero state.

While at first glance this convention might seem somewhat odd, it is in fact quite handy. For one, the spin operators remain in the conventional form. Second, when the spin system is in the  $|\uparrow\rangle$  state:

```
print(sigmaz() * spin)
```

**Output:**

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[1.]
 [0.]]
```

the non-zero component is the zeroth-element of the underlying matrix (remember that python uses c-indexing, and matrices start with the zeroth element). The  $|\downarrow\rangle$  state therefore has a non-zero entry in the first index position. This corresponds nicely with the quantum information definitions of qubit states, where the excited  $|\uparrow\rangle$  state is label as  $|0\rangle$ , and the  $|\downarrow\rangle$  state by  $|1\rangle$ .

If one wants to create spin operators for higher spin systems, then the `jmat` function comes in handy.

### 3.3.5 Expectation values

Some of the most important information about quantum systems comes from calculating the expectation value of operators, both Hermitian and non-Hermitian, as the state or density matrix of the system varies in time. Therefore, in this section we demonstrate the use of the `expect` function. To begin:

```
vac = basis(5, 0)

one = basis(5, 1)

c = create(5)

N = num(5)

np.testing.assert_almost_equal(expect(N, vac), 0)

np.testing.assert_almost_equal(expect(N, one), 1)

coh = coherent_dm(5, 1.0j)

np.testing.assert_almost_equal(expect(N, coh), 0.9970555745806597)

cat = (basis(5, 4) + 1.0j * basis(5, 3)).unit()

np.testing.assert_almost_equal(expect(c, cat), 0.9999999999999998j)
```

The `expect` function also accepts lists or arrays of state vectors or density matrices for the second input:

```
states = [(c**k * vac).unit() for k in range(5)] # must normalize

print(expect(N, states))
```

**Output:**

```
[0. 1. 2. 3. 4.]
```

```
cat_list = [(basis(5, 4) + x * basis(5, 3)).unit() for x in [0, 1.0j, -1.0, -1.0j]]

print(expect(c, cat_list))
```

**Output:**

```
[ 0.+0.j  0.+1.j -1.+0.j  0.-1.j]
```

Notice how in this last example, all of the return values are complex numbers. This is because the `expect` function looks to see whether the operator is Hermitian or not. If the operator is Hermitian, then the output will always be real. In the case of non-Hermitian operators, the return values may be complex. Therefore, the `expect` function will return an array of complex values for non-Hermitian operators when the input is a list/array of states or density matrices.

Of course, the `expect` function works for spin states and operators:

```
up = basis(2, 0)
down = basis(2, 1)
np.testing.assert_almost_equal(expect(sigmaz(), up), 1)
np.testing.assert_almost_equal(expect(sigmaz(), down), -1)
```

as well as the composite objects discussed in the next section *Using Tensor Products and Partial Traces*:

```
spin1 = basis(2, 0)
spin2 = basis(2, 1)
two_spins = tensor(spin1, spin2)
sz1 = tensor(sigmaz(), qeye(2))
sz2 = tensor(qeye(2), sigmaz())
np.testing.assert_almost_equal(expect(sz1, two_spins), 1)
np.testing.assert_almost_equal(expect(sz2, two_spins), -1)
```

### 3.3.6 Superoperators and Vectorized Operators

In addition to state vectors and density operators, QuTiP allows for representing maps that act linearly on density operators using the Kraus, Liouville supermatrix and Choi matrix formalisms. This support is based on the correspondence between linear operators acting on a Hilbert space, and vectors in two copies of that Hilbert space,  $\text{vec} : \mathcal{L}(\mathcal{H}) \rightarrow \mathcal{H} \otimes \mathcal{H}$  [Hav03], [Wat13].

This isomorphism is implemented in QuTiP by the `operator_to_vector` and `vector_to_operator` functions:

```
psi = basis(2, 0)
rho = ket2dm(psi)
print(rho)
```

**Output:**

```
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[1.  0.]
 [0.  0.]]
```

```
vec_rho = operator_to_vector(rho)

print(vec_rho)
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [1]], shape = (4, 1), type = operator-ket
Qobj data =
[[1.]
 [0.]
 [0.]
 [0.]]
```

```
rho2 = vector_to_operator(vec_rho)

np.testing.assert_almost_equal((rho - rho2).norm(), 0)
```

The `Qobj.type` attribute indicates whether a quantum object is a vector corresponding to an operator (`operator-ket`), or its Hermitian conjugate (`operator-bra`).

Note that QuTiP uses the *column-stacking* convention for the isomorphism between  $\mathcal{L}(\mathcal{H})$  and  $\mathcal{H} \otimes \mathcal{H}$ :

```
A = Qobj(np.arange(4).reshape((2, 2)))

print(A)
```

**Output:**

```
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = False
Qobj data =
[[0. 1.]
 [2. 3.]]
```

```
print(operator_to_vector(A))
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [1]], shape = (4, 1), type = operator-ket
Qobj data =
[[0.]
 [2.]
 [1.]
 [3.]]
```

Since  $\mathcal{H} \otimes \mathcal{H}$  is a vector space, linear maps on this space can be represented as matrices, often called *superoperators*. Using the `Qobj`, the `spre` and `spost` functions, supermatrices corresponding to left- and right-multiplication respectively can be quickly constructed.

```
X = sigmax()

S = spre(X) * spost(X.dag()) # Represents conjugation by X.
```

Note that this is done automatically by the `to_super` function when given `type='oper'` input.

```
S2 = to_super(X)

np.testing.assert_almost_equal((S - S2).norm(), 0)
```



Quantum objects representing superoperators are denoted by `type='super'`:

```
print(S)
```

Output:

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪= True
Qobj data =
[[0. 0. 0. 1.]
 [0. 0. 1. 0.]
 [0. 1. 0. 0.]
 [1. 0. 0. 0.]
```

Information about superoperators, such as whether they represent completely positive maps, is exposed through the `Qobj.iscp`, `Qobj.istp` and `Qobj.iscftp` attributes:

```
print(S.iscp, S.istp, S.iscftp)
```

Output:

```
True True True
```

In addition, dynamical generators on this extended space, often called *Liouvillian superoperators*, can be created using the `liouvillian` function. Each of these takes a Hamiltonian along with a list of collapse operators, and returns a `type="super"` object that can be exponentiated to find the superoperator for that evolution.

```
H = 10 * sigmaz()
c1 = destroy(2)
L = liouvillian(H, [c1])
print(L)
S = (12 * L).expm()
```

Output:

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪= False
Qobj data =
[[ 0. +0.j  0. +0.j  0. +0.j  1. +0.j]
 [ 0. +0.j -0.5+20.j  0. +0.j  0. +0.j]
 [ 0. +0.j  0. +0.j -0.5-20.j  0. +0.j]
 [ 0. +0.j  0. +0.j  0. +0.j -1. +0.j]]
```

For qubits, a particularly useful way to visualize superoperators is to plot them in the Pauli basis, such that  $S_{\mu,\nu} = \langle\langle\sigma_\mu|S[\sigma_\nu]\rangle\rangle$ . Because the Pauli basis is Hermitian,  $S_{\mu,\nu}$  is a real number for all Hermitian-preserving superoperators  $S$ , allowing us to plot the elements of  $S$  as a [Hinton diagram](#). In such diagrams, positive elements are indicated by white squares, and negative elements by black squares. The size of each element is indicated by the size of the corresponding square. For instance, let  $S[\rho] = \sigma_x \rho \sigma_x^\dagger$ . Then  $S[\sigma_\mu] = \sigma_\mu \cdot \begin{cases} +1 & \mu = 0, x \\ -1 & \mu = y, z \end{cases}$ . We can quickly see this by noting that the  $Y$  and  $Z$  elements of the Hinton diagram for  $S$  are negative:

```
from qutip import *
settings.colorblind_safe = True
```

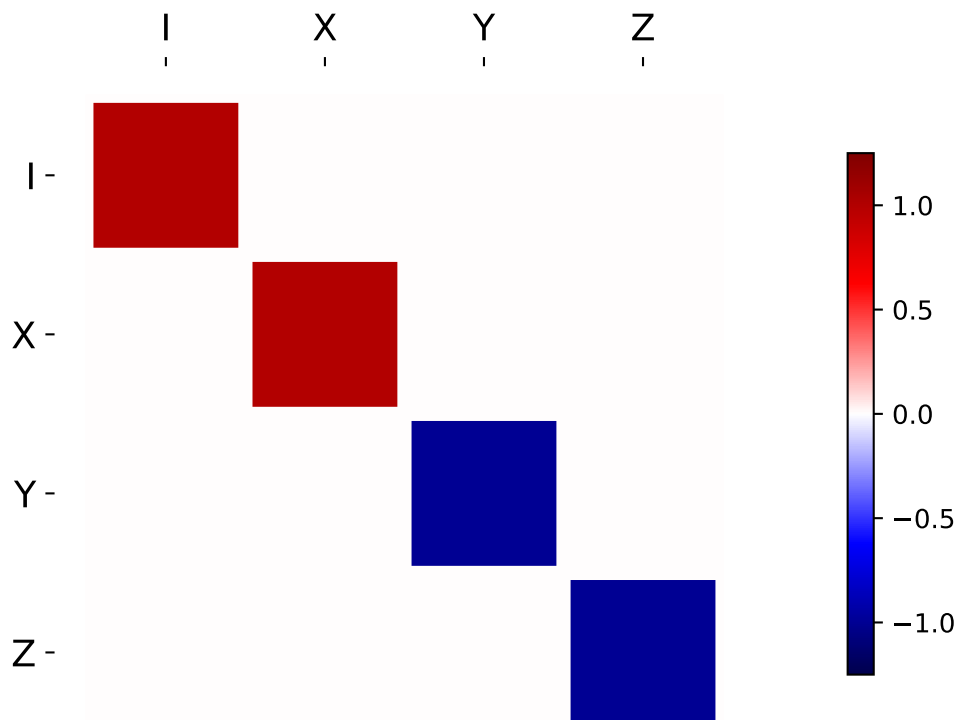
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```
import matplotlib.pyplot as plt
plt.rcParams['savefig.transparent'] = True

X = sigmax()
S = spre(X) * spost(X.dag())

hinton(S)
```



### 3.3.7 Choi, Kraus, Stinespring and $\chi$ Representations

In addition to the superoperator representation of quantum maps, QuTiP supports several other useful representations. First, the Choi matrix  $J(\Lambda)$  of a quantum map  $\Lambda$  is useful for working with ancilla-assisted process tomography (AAPT), and for reasoning about properties of a map or channel. Up to normalization, the Choi matrix is defined by acting  $\Lambda$  on half of an entangled pair. In the column-stacking convention,

$$J(\Lambda) = (\mathbb{I} \otimes \Lambda)[|\mathcal{H}\rangle\rangle\langle\langle\mathcal{H}|].$$

In QuTiP,  $J(\Lambda)$  can be found by calling the `to_choi` function on a `type="super"` *Qobj*.

```
X = sigmax()

S = sprepost(X, X)

J = to_choi(S)

print(J)
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪= True, superrep = choi
Qobj data =
[[0. 0. 0. 0.]
 [0. 1. 1. 0.]
 [0. 1. 1. 0.]
 [0. 0. 0. 0.]
```

```
print(to_choi(spre(qeye(2))))
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪= True, superrep = choi
Qobj data =
[[1. 0. 0. 1.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [1. 0. 0. 1.]
```

If a *Qobj* instance is already in the Choi *Qobj*.*superrep*, then calling *to\_choi* does nothing:

```
print(to_choi(J))
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪= True, superrep = choi
Qobj data =
[[0. 0. 0. 0.]
 [0. 1. 1. 0.]
 [0. 1. 1. 0.]
 [0. 0. 0. 0.]
```

To get back to the superoperator representation, simply use the *to\_super* function. As with *to\_choi*, *to\_super* is idempotent:

```
print(to_super(J) - S)
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪= True
Qobj data =
[[0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
```

```
print(to_super(S))
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪= True
```

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```
Qobj data =
[[0. 0. 0. 1.]
 [0. 0. 1. 0.]
 [0. 1. 0. 0.]
 [1. 0. 0. 0.]]
```

We can quickly obtain another useful representation from the Choi matrix by taking its eigendecomposition. In particular, let  $\{A_i\}$  be a set of operators such that  $J(\Lambda) = \sum_i |A_i\rangle\rangle\langle\langle A_i|$ . We can write  $J(\Lambda)$  in this way for any hermicity-preserving map; that is, for any map  $\Lambda$  such that  $J(\Lambda) = J^\dagger(\Lambda)$ . These operators then form the Kraus representation of  $\Lambda$ . In particular, for any input  $\rho$ ,

$$\Lambda(\rho) = \sum_i A_i \rho A_i^\dagger.$$

Notice using the column-stacking identity that  $(C^T \otimes A)|B\rangle\rangle = |ABC\rangle\rangle$ , we have that

$$\sum_i (\mathcal{K} \otimes A_i)(\mathcal{K} \otimes A_i)^\dagger |\mathcal{K}\rangle\rangle\langle\langle \mathcal{K}| = \sum_i |A_i\rangle\rangle\langle\langle A_i| = J(\Lambda).$$

The Kraus representation of a hermicity-preserving map can be found in QuTiP using the `to_kraus` function.

```
del sum # np.sum overwrote sum and caused a bug.
```

```
I, X, Y, Z = qeye(2), sigmax(), sigmay(), sigmaz()
```

```
S = sum([sprepost(P, P) for P in (I, X, Y, Z)]) / 4
print(S)
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪ = True
Qobj data =
[[0.5 0. 0. 0.5]
 [0. 0. 0. 0. ]
 [0. 0. 0. 0. ]
 [0.5 0. 0. 0.5]]
```

```
J = to_choi(S)
print(J)
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪ = True, superrep = choi
Qobj data =
[[0.5 0. 0. 0. ]
 [0. 0.5 0. 0. ]
 [0. 0. 0.5 0. ]
 [0. 0. 0. 0.5]]
```

```
print(J.eigenstates()[1])
```

**Output:**

```

[Quantum object: dims = [[[2], [2]], [1, 1]], shape = (4, 1), type = operator-ket
Qobj data =
[[1.]
 [0.]
 [0.]
 [0.]]
Quantum object: dims = [[[2], [2]], [1, 1]], shape = (4, 1), type = operator-ket
Qobj data =
[[0.]
 [1.]
 [0.]
 [0.]]
Quantum object: dims = [[[2], [2]], [1, 1]], shape = (4, 1), type = operator-ket
Qobj data =
[[0.]
 [0.]
 [1.]
 [0.]]
Quantum object: dims = [[[2], [2]], [1, 1]], shape = (4, 1), type = operator-ket
Qobj data =
[[0.]
 [0.]
 [0.]
 [1.]]

```

```

K = to_kraus(S)
print(K)

```

**Output:**

```

[Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0.70710678 0.          ]
 [0.          0.          ]], Quantum object: dims = [[2], [2]], shape = (2, 2), type =
↪oper, isherm = False
Qobj data =
[[0.          0.          ]
 [0.70710678 0.          ]], Quantum object: dims = [[2], [2]], shape = (2, 2), type =
↪oper, isherm = False
Qobj data =
[[0.          0.70710678]
 [0.          0.          ]], Quantum object: dims = [[2], [2]], shape = (2, 2), type =
↪oper, isherm = True
Qobj data =
[[0.          0.          ]
 [0.          0.70710678]]

```

As with the other representation conversion functions, `to_kraus` checks the `Qobj.superrep` attribute of its input, and chooses an appropriate conversion method. Thus, in the above example, we can also call `to_kraus` on `J`.

```

KJ = to_kraus(J)
print(KJ)

```

**Output:**

```

[Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =

```

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```
[[0.70710678 0.          ]
 [0.          0.          ]], Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper
↳ oper, isherm = False
Qobj data =
[[0.          0.          ]
 [0.70710678 0.          ]], Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper
↳ oper, isherm = False
Qobj data =
[[0.          0.70710678]
 [0.          0.          ]], Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper
↳ oper, isherm = True
Qobj data =
[[0.          0.          ]
 [0.          0.70710678]]]
```

```
for A, AJ in zip(K, KJ):
    print(A - AJ)
```

**Output:**

```
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0. 0.]
 [0. 0.]]
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0. 0.]
 [0. 0.]]
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0. 0.]
 [0. 0.]]
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0. 0.]
 [0. 0.]]
```

The Stinespring representation is closely related to the Kraus representation, and consists of a pair of operators  $A$  and  $B$  such that for all operators  $X$  acting on  $\mathcal{H}$ ,

$$\Lambda(X) = \text{Tr}_2(AXB^\dagger),$$

where the partial trace is over a new index that corresponds to the index in the Kraus summation. Conversion to Stinespring is handled by the `to_stinespring` function.

```
a = create(2).dag()

S_ad = sprepost(a * a.dag(), a * a.dag()) + sprepost(a, a.dag())
S = 0.9 * sprepost(I, I) + 0.1 * S_ad

print(S)
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm = False
↳ = False
```

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```
Qobj data =
[[1.  0.  0.  0.1]
 [0.  0.9 0.  0. ]
 [0.  0.  0.9 0. ]
 [0.  0.  0.  0.9]]
```

```
A, B = to_stinespring(S)
print(A)
```

**Output:**

```
Quantum object: dims = [[2, 3], [2]], shape = (6, 2), type = oper, isherm = False
Qobj data =
[[-0.98845443  0.          ]
 [ 0.          0.31622777]
 [ 0.15151842  0.          ]
 [ 0.          -0.93506452]
 [ 0.          0.          ]
 [ 0.          -0.16016975]]
```

```
print(B)
```

**Output:**

```
Quantum object: dims = [[2, 3], [2]], shape = (6, 2), type = oper, isherm = False
Qobj data =
[[-0.98845443  0.          ]
 [ 0.          0.31622777]
 [ 0.15151842  0.          ]
 [ 0.          -0.93506452]
 [ 0.          0.          ]
 [ 0.          -0.16016975]]
```

Notice that a new index has been added, such that  $A$  and  $B$  have dimensions  $[[2, 3], [2]]$ , with the length-3 index representing the fact that the Choi matrix is rank-3 (alternatively, that the map has three Kraus operators).

```
to_kraus(S)
print(to_choi(S).eigenenergies())
```

**Output:**

```
[0.          0.04861218 0.1          1.85138782]
```

Finally, the last superoperator representation supported by QuTiP is the  $\chi$ -matrix representation,

$$\Lambda(\rho) = \sum_{\alpha,\beta} \chi_{\alpha,\beta} B_{\alpha} \rho B_{\beta}^{\dagger},$$

where  $\{B_{\alpha}\}$  is a basis for the space of matrices acting on  $\mathcal{H}$ . In QuTiP, this basis is taken to be the Pauli basis  $B_{\alpha} = \sigma_{\alpha}/\sqrt{2}$ . Conversion to the  $\chi$  formalism is handled by the `to_chi` function.

```
chi = to_chi(S)
print(chi)
```

**Output:**

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪ = True, superrep = chi
Qobj data =
[[3.7+0.j  0. +0.j  0. +0.j  0.1+0.j ]
 [0. +0.j  0.1+0.j  0. +0.1j  0. +0.j ]
 [0. +0.j  0. -0.1j  0.1+0.j  0. +0.j ]
 [0.1+0.j  0. +0.j  0. +0.j  0.1+0.j ]]
```

One convenient property of the  $\chi$  matrix is that the average gate fidelity with the identity map can be read off directly from the  $\chi_{00}$  element:

```
np.testing.assert_almost_equal(average_gate_fidelity(S), 0.9499999999999998)

print(chi[0, 0] / 4)
```

**Output:**

```
(0.925+0j)
```

Here, the factor of 4 comes from the dimension of the underlying Hilbert space  $\mathcal{H}$ . As with the superoperator and Choi representations, the  $\chi$  representation is denoted by the `Qobj.superrep`, such that `to_super`, `to_choi`, `to_kraus`, `to_stinespring` and `to_chi` all convert from the  $\chi$  representation appropriately.

### 3.3.8 Properties of Quantum Maps

In addition to converting between the different representations of quantum maps, QuTiP also provides attributes to make it easy to check if a map is completely positive, trace preserving and/or hermicity preserving. Each of these attributes uses `Qobj.superrep` to automatically perform any needed conversions.

In particular, a quantum map is said to be positive (but not necessarily completely positive) if it maps all positive operators to positive operators. For instance, the transpose map  $\Lambda(\rho) = \rho^T$  is a positive map. We run into problems, however, if we tensor  $\Lambda$  with the identity to get a partial transpose map.

```
rho = ket2dm(bell_state())
rho_out = partial_transpose(rho, [0, 1])
print(rho_out.eigenenergies())
```

**Output:**

```
[-0.5  0.5  0.5  0.5]
```

Notice that even though we started with a positive map, we got an operator out with negative eigenvalues. Complete positivity addresses this by requiring that a map returns positive operators for all positive operators, and does so even under tensoring with another map. The Choi matrix is very useful here, as it can be shown that a map is completely positive if and only if its Choi matrix is positive [Wat13]. QuTiP implements this check with the `Qobj.iscp` attribute. As an example, notice that the snippet above already calculates the Choi matrix of the transpose map by acting it on half of an entangled pair. We simply need to manually set the `dims` and `superrep` attributes to reflect the structure of the underlying Hilbert space and the chosen representation.

```
J = rho_out
J.dims = [[[2], [2]], [[2], [2]]]
J.superrep = 'choi'
print(J.iscp)
```

**Output:**

```
False
```



This confirms that the transpose map is not completely positive. On the other hand, the transpose map does satisfy a weaker condition, namely that it is hermicity preserving. That is,  $\Lambda(\rho) = (\Lambda(\rho))^{\dagger}$  for all  $\rho$  such that  $\rho = \rho^{\dagger}$ . To see this, we note that  $(\rho^T)^{\dagger} = \rho^*$ , the complex conjugate of  $\rho$ . By assumption,  $\rho = \rho^{\dagger} = (\rho^*)^T$ , though, such that  $\Lambda(\rho) = \Lambda(\rho^{\dagger}) = \rho^*$ . We can confirm this by checking the `Qobj.ishp` attribute:

```
print(J.ishp)
```

Output:

```
True
```

Next, we note that the transpose map does preserve the trace of its inputs, such that  $\text{Tr}(\Lambda[\rho]) = \text{Tr}(\rho)$  for all  $\rho$ . This can be confirmed by the `Qobj.istp` attribute:

```
print(J.istp)
```

Output:

```
False
```

Finally, a map is called a quantum channel if it always maps valid states to valid states. Formally, a map is a channel if it is both completely positive and trace preserving. Thus, QuTiP provides a single attribute to quickly check that this is true.

```
>>> print(J.iscstp)
False

>>> print(to_super(qeye(2)).iscstp)
True
```

## 3.4 Using Tensor Products and Partial Traces

### 3.4.1 Tensor products

To describe the states of multipartite quantum systems - such as two coupled qubits, a qubit coupled to an oscillator, etc. - we need to expand the Hilbert space by taking the tensor product of the state vectors for each of the system components. Similarly, the operators acting on the state vectors in the combined Hilbert space (describing the coupled system) are formed by taking the tensor product of the individual operators.

In QuTiP the function `tensor` is used to accomplish this task. This function takes as argument a collection:

```
>>> tensor(op1, op2, op3)
```

or a list:

```
>>> tensor([op1, op2, op3])
```

of state vectors *or* operators and returns a composite quantum object for the combined Hilbert space. The function accepts an arbitrary number of states or operators as argument. The type returned quantum object is the same as that of the input(s).

For example, the state vector describing two qubits in their ground states is formed by taking the tensor product of the two single-qubit ground state vectors:

```
print(tensor(basis(2, 0), basis(2, 0)))
```

Output:

```
Quantum object: dims = [[2, 2], [1, 1]], shape = (4, 1), type = ket
Qobj data =
[[1.]
 [0.]
 [0.]
 [0.]]
```

or equivalently using the list format:

```
print(tensor([basis(2, 0), basis(2, 0)]))
```

**Output:**

```
Quantum object: dims = [[2, 2], [1, 1]], shape = (4, 1), type = ket
Qobj data =
[[1.]
 [0.]
 [0.]
 [0.]]
```

This is straightforward to generalize to more qubits by adding more component state vectors in the argument list to the `tensor` function, as illustrated in the following example:

```
print(tensor((basis(2, 0) + basis(2, 1)).unit(), (basis(2, 0) + basis(2, 1)).unit(),
↪ basis(2, 0)))
```

**Output:**

```
Quantum object: dims = [[2, 2, 2], [1, 1, 1]], shape = (8, 1), type = ket
Qobj data =
[[0.5]
 [0. ]
 [0.5]
 [0. ]
 [0.5]
 [0. ]
 [0.5]
 [0. ]]
```

This state is slightly more complicated, describing two qubits in a superposition between the up and down states, while the third qubit is in its ground state.

To construct operators that act on an extended Hilbert space of a combined system, we similarly pass a list of operators for each component system to the `tensor` function. For example, to form the operator that represents the simultaneous action of the  $\sigma_x$  operator on two qubits:

```
print(tensor(sigmax(), sigmax()))
```

**Output:**

```
Quantum object: dims = [[2, 2], [2, 2]], shape = (4, 4), type = oper, isherm = True
Qobj data =
[[0. 0. 0. 1.]
 [0. 0. 1. 0.]
 [0. 1. 0. 0.]
 [1. 0. 0. 0.]]
```

To create operators in a combined Hilbert space that only act on a single component, we take the tensor product of the operator acting on the subspace of interest, with the identity operators corresponding to the components that

are to be unchanged. For example, the operator that represents  $\sigma_z$  on the first qubit in a two-qubit system, while leaving the second qubit unaffected:

```
print(tensor(sigmaz(), identity(2)))
```

Output:

```
Quantum object: dims = [[2, 2], [2, 2]], shape = (4, 4), type = oper, isherm = True
Qobj data =
[[ 1.  0.  0.  0.]
 [ 0.  1.  0.  0.]
 [ 0.  0. -1.  0.]
 [ 0.  0.  0. -1.]]
```

### 3.4.2 Example: Constructing composite Hamiltonians

The `tensor` function is extensively used when constructing Hamiltonians for composite systems. Here we'll look at some simple examples.

#### Two coupled qubits

First, let's consider a system of two coupled qubits. Assume that both the qubits have equal energy splitting, and that the qubits are coupled through a  $\sigma_x \otimes \sigma_x$  interaction with strength  $g = 0.05$  (in units where the bare qubit energy splitting is unity). The Hamiltonian describing this system is:

```
H = tensor(sigmaz(), identity(2)) + tensor(identity(2), sigmaz()) + 0.05 *
    tensor(sigmax(), sigmax())
print(H)
```

Output:

```
Quantum object: dims = [[2, 2], [2, 2]], shape = (4, 4), type = oper, isherm = True
Qobj data =
[[ 2.  0.  0.  0.05]
 [ 0.  0.  0.05  0. ]
 [ 0.  0.05  0.  0. ]
 [ 0.05  0.  0. -2. ]]
```

#### Three coupled qubits

The two-qubit example is easily generalized to three coupled qubits:

```
H = (tensor(sigmaz(), identity(2), identity(2)) + tensor(identity(2), sigmaz(),
    identity(2)) + tensor(identity(2), identity(2), sigmaz()) + 0.5 * tensor(sigmax(),
    sigmax(), identity(2)) + 0.25 * tensor(identity(2), sigmax(), sigmax()))
print(H)
```

Output:

```
Quantum object: dims = [[2, 2, 2], [2, 2, 2]], shape = (8, 8), type = oper, isherm =
    True
Qobj data =
[[ 3.  0.  0.  0.25  0.  0.  0.5  0. ]
```

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```
[ 0.  1.  0.25  0.  0.  0.  0.  0.5 ]
[ 0.  0.25  1.  0.  0.5  0.  0.  0. ]
[ 0.25  0.  0.  -1.  0.  0.5  0.  0. ]
[ 0.  0.  0.5  0.  1.  0.  0.  0.25]
[ 0.  0.  0.  0.5  0.  -1.  0.25  0. ]
[ 0.5  0.  0.  0.  0.  0.25 -1.  0. ]
[ 0.  0.5  0.  0.  0.25  0.  0.  -3. ]]
```

### A two-level system coupled to a cavity: The Jaynes-Cummings model

The simplest possible quantum mechanical description for light-matter interaction is encapsulated in the Jaynes-Cummings model, which describes the coupling between a two-level atom and a single-mode electromagnetic field (a cavity mode). Denoting the energy splitting of the atom and cavity  $\omega_a$  and  $\omega_c$ , respectively, and the atom-cavity interaction strength  $g$ , the Jaynes-Cummings Hamiltonian can be constructed as:

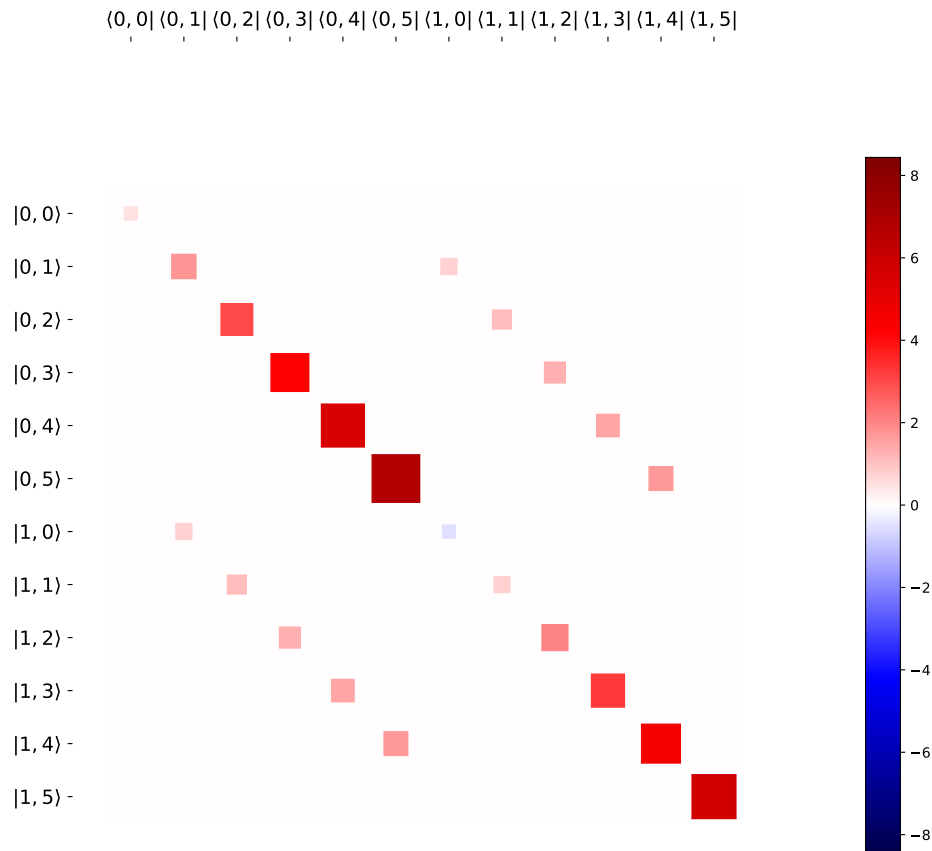
```
N = 6

omega_a = 1.0
omega_c = 1.25
g = 0.75

a = tensor(identity(2), destroy(N))
sm = tensor(destroy(2), identity(N))
sz = tensor(sigmaz(), identity(N))

H = 0.5 * omega_a * sz + omega_c * a.dag() * a + g * (a.dag() * sm + a * sm.dag())

hinton(H, fig=plt.figure(figsize=(12, 12)))
```



Here  $N$  is the number of Fock states included in the cavity mode.

### 3.4.3 Partial trace

The partial trace is an operation that reduces the dimension of a Hilbert space by eliminating some degrees of freedom by averaging (tracing). In this sense it is therefore the converse of the tensor product. It is useful when one is interested in only a part of a coupled quantum system. For open quantum systems, this typically involves tracing over the environment leaving only the system of interest. In QuTiP the class method `ptrace` is used to take partial traces. `ptrace` acts on the `Qobj` instance for which it is called, and it takes one argument `sel`, which is a list of integers that mark the component systems that should be **kept**. All other components are traced out.

For example, the density matrix describing a single qubit obtained from a coupled two-qubit system is obtained via:

```
>>> psi = tensor(basis(2, 0), basis(2, 1))
>>> psi.ptrace(0)
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
```

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```
Qobj data =
[[1. 0.]
 [0. 0.]]

>>> psi.ptrace(1)
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0. 0.]
 [0. 1.]]
```

Note that the partial trace always results in a density matrix (mixed state), regardless of whether the composite system is a pure state (described by a state vector) or a mixed state (described by a density matrix):

```
>>> psi = tensor((basis(2, 0) + basis(2, 1)).unit(), basis(2, 0))

>>> psi
Quantum object: dims = [[2, 2], [1, 1]], shape = (4, 1), type = ket
Qobj data =
[[0.70710678]
 [0.         ]
 [0.70710678]
 [0.         ]]

>>> psi.ptrace(0)
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0.5 0.5]
 [0.5 0.5]]

>>> rho = tensor(ket2dm((basis(2, 0) + basis(2, 1)).unit()), fock_dm(2, 0))

>>> rho
Quantum object: dims = [[2, 2], [2, 2]], shape = (4, 4), type = oper, isherm = True
Qobj data =
[[0.5 0. 0.5 0. ]
 [0. 0. 0. 0. ]
 [0.5 0. 0.5 0. ]
 [0. 0. 0. 0. ]]

>>> rho.ptrace(0)
Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
Qobj data =
[[0.5 0.5]
 [0.5 0.5]]
```

### 3.4.4 Superoperators and Tensor Manipulations

As described in *Superoperators and Vectorized Operators*, *superoperators* are operators that act on Liouville space, the vectorspace of linear operators. Superoperators can be represented using the isomorphism  $\text{vec} : \mathcal{L}(\mathcal{H}) \rightarrow \mathcal{H} \otimes \mathcal{H}$  [Hav03], [Wat13]. To represent superoperators acting on  $\mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$  thus takes some tensor rearrangement to get the desired ordering  $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_1 \otimes \mathcal{H}_2$ .

In particular, this means that *tensor* does not act as one might expect on the results of *to\_super*:

```
>>> A = qeye([2])

>>> B = qeye([3])

>>> to_super(tensor(A, B)).dims
[[[2, 3], [2, 3]], [[2, 3], [2, 3]]]

>>> tensor(to_super(A), to_super(B)).dims
[[[2], [2], [3], [3]], [[2], [2], [3], [3]]]
```

In the former case, the result correctly has four copies of the compound index with dims `[2, 3]`. In the latter case, however, each of the Hilbert space indices is listed independently and in the wrong order.

The `super_tensor` function performs the needed rearrangement, providing the most direct analog to `tensor` on the underlying Hilbert space. In particular, for any two `type="oper"` Qobjs A and B, `to_super(tensor(A, B)) == super_tensor(to_super(A), to_super(B))` and `operator_to_vector(tensor(A, B)) == super_tensor(operator_to_vector(A), operator_to_vector(B))`. Returning to the previous example:

```
>>> super_tensor(to_super(A), to_super(B)).dims
[[[2, 3], [2, 3]], [[2, 3], [2, 3]]]
```

The `composite` function automatically switches between `tensor` and `super_tensor` based on the `type` of its arguments, such that `composite(A, B)` returns an appropriate Qobj to represent the composition of two systems.

```
>>> composite(A, B).dims
[[2, 3], [2, 3]]

>>> composite(to_super(A), to_super(B)).dims
[[[2, 3], [2, 3]], [[2, 3], [2, 3]]]
```

QuTiP also allows more general tensor manipulations that are useful for converting between superoperator representations [WBC11]. In particular, the `tensor_contract` function allows for contracting one or more pairs of indices. This can be used to find superoperators that represent partial trace maps. Using this functionality, we can construct some quite exotic maps, such as a map from  $3 \times 3$  operators to  $2 \times 2$  operators:

```
>>> tensor_contract(composite(to_super(A), to_super(B)), (1, 3), (4, 6)).dims
[[[2], [2]], [[3], [3]]]
```

## 3.5 Superoperators, Pauli Basis and Channel Contraction

written by *Christopher Granade* <<http://www.cgranade.com>>, Institute for Quantum Computing

In this guide, we will demonstrate the `tensor_contract` function, which contracts one or more pairs of indices of a Qobj. This functionality can be used to find rectangular superoperators that implement the partial trace channel  $S(\rho) = \text{Tr}_2(\rho)$ , for instance. Using this functionality, we can quickly turn a system-environment representation of an open quantum process into a superoperator representation.

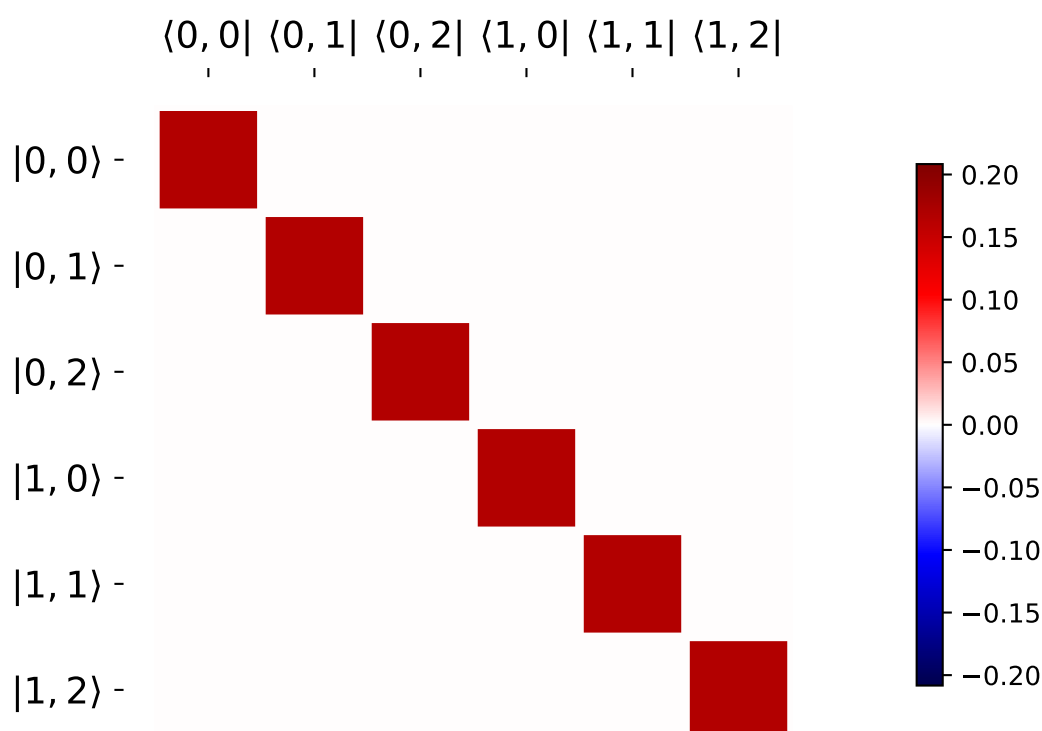
### 3.5.1 Superoperator Representations and Plotting

We start off by first demonstrating plotting of superoperators, as this will be useful to us in visualizing the results of a contracted channel.

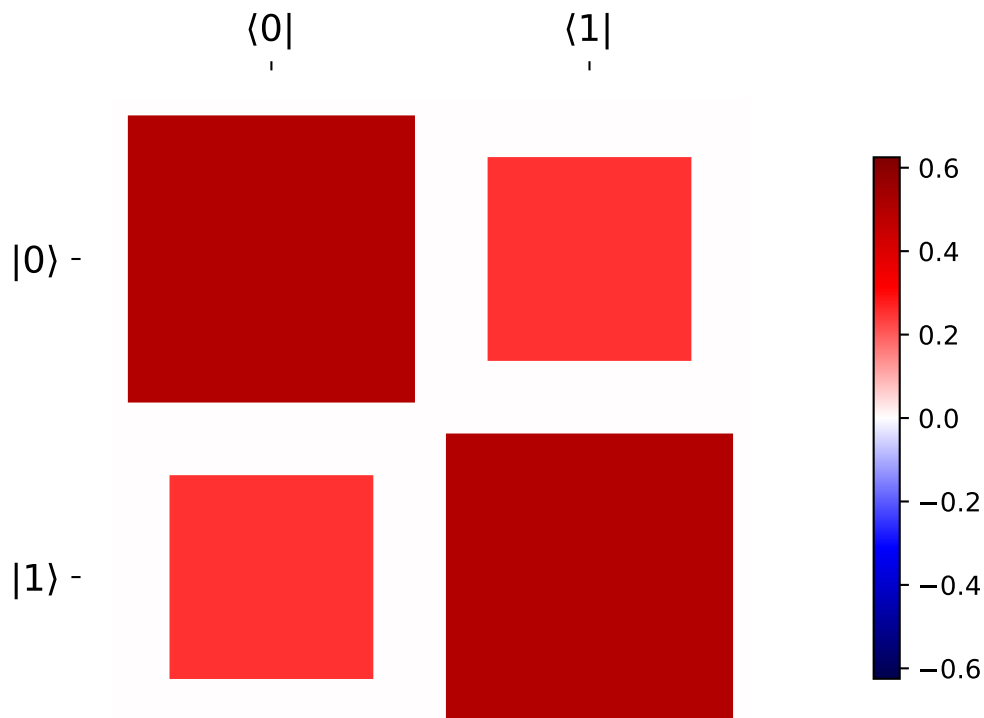
In particular, we will use Hinton diagrams as implemented by `hinton`, which show the real parts of matrix elements as squares whose size and color both correspond to the magnitude of each element. To illustrate, we first plot a few density operators.

```
from qutip import hinton, identity, Qobj, to_super, sigmaz, tensor, tensor_contract
from qutip.core.gates import cnot, hadamard_transform

hinton(identity([2, 3]).unit())
hinton(Qobj([[1, 0.5], [0.5, 1]]).unit())
```



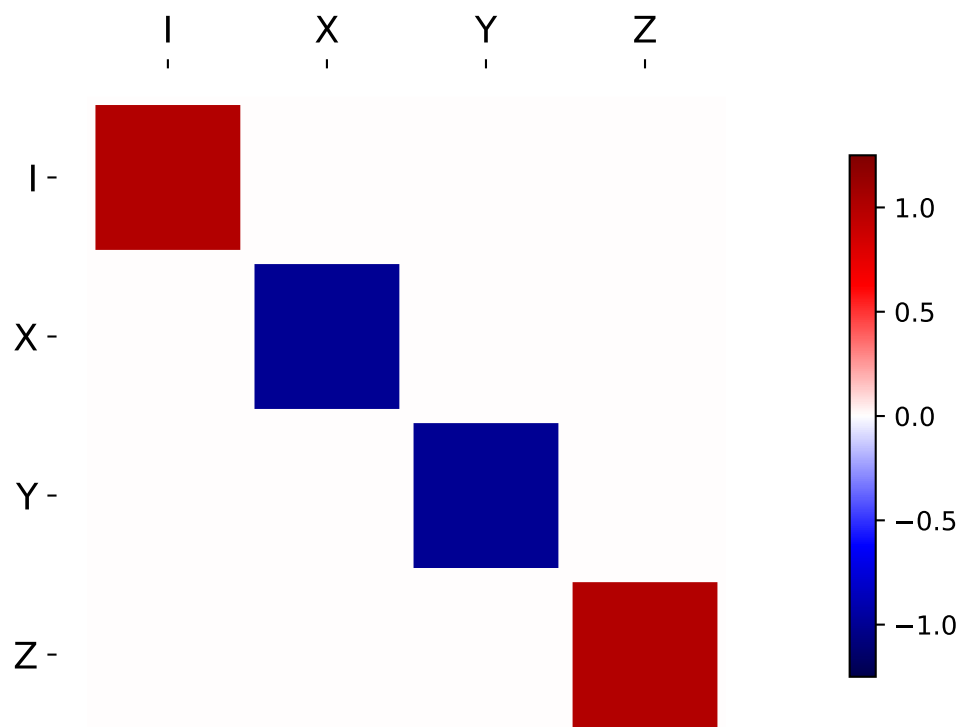




We show superoperators as matrices in the *Pauli basis*, such that any Hermiticity-preserving map is represented by a real-valued matrix. This is especially convenient for use with Hinton diagrams, as the plot thus carries complete information about the channel.

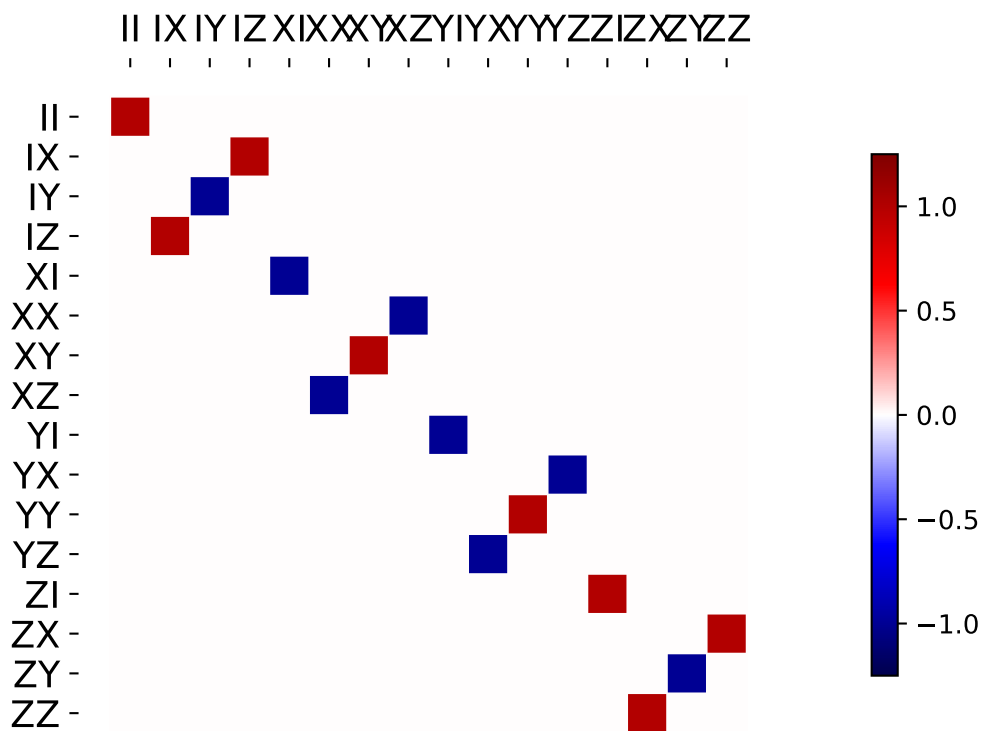
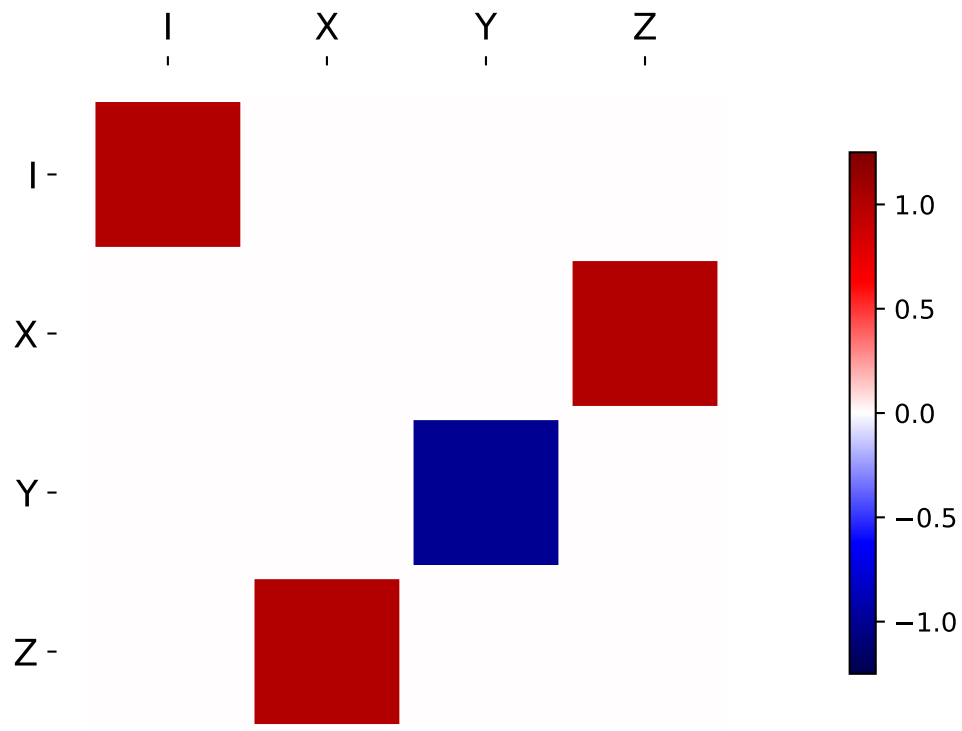
As an example, conjugation by  $\sigma_z$  leaves  $\mathbb{K}$  and  $\sigma_z$  invariant, but flips the sign of  $\sigma_x$  and  $\sigma_y$ . This is indicated in Hinton diagrams by a negative-valued square for the sign change and a positive-valued square for a +1 sign.

```
hinton(to_super(sigmaz()))
```



As a couple more examples, we also consider the supermatrix for a Hadamard transform and for  $\sigma_z \otimes H$ .

```
hinton(to_super(hadamard_transform()))
hinton(to_super(tensor(sigmaz(), hadamard_transform())))
```

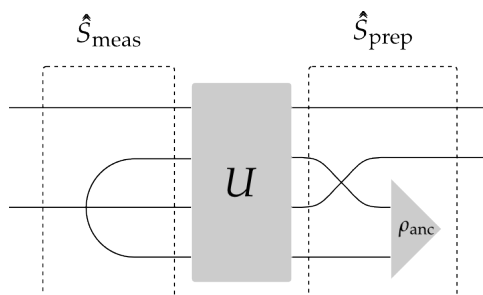


### 3.5.2 Reduced Channels

As an example of tensor contraction, we now consider the map

$$S(\rho) = \text{Tr}_2(\text{CNOT}(\rho \otimes |0\rangle\langle 0|)\text{CNOT}^\dagger)$$

We can think of the `CNOT` here as a system-environment representation of an open quantum process, in which an environment register is prepared in a state  $\rho_{\text{anc}}$ , then a unitary acts jointly on the system of interest and environment. Finally, the environment is traced out, leaving a *channel* on the system alone. In terms of *Wood diagrams* <<http://arxiv.org/abs/1111.6950>>, this can be represented as the composition of a preparation map, evolution under the system-environment unitary, and then a measurement map.



The two tensor wires on the left indicate where we must take a tensor contraction to obtain the measurement map. Numbering the tensor wires from 0 to 3, this corresponds to a `tensor_contract` argument of `(1, 3)`.

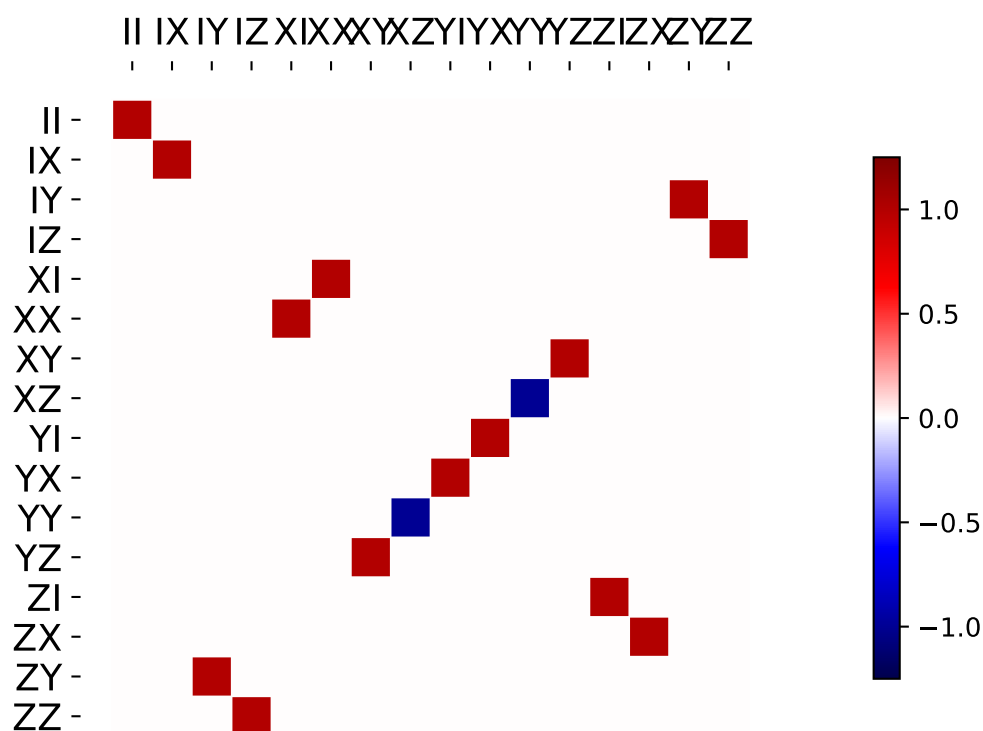
```
tensor_contract(to_super(identity([2, 2])), (1, 3))
```

Meanwhile, the `super_tensor` function implements the swap on the right, such that we can quickly find the preparation map.

```
q = tensor(identity(2), basis(2))
s_prep = sprepost(q, q.dag())
```

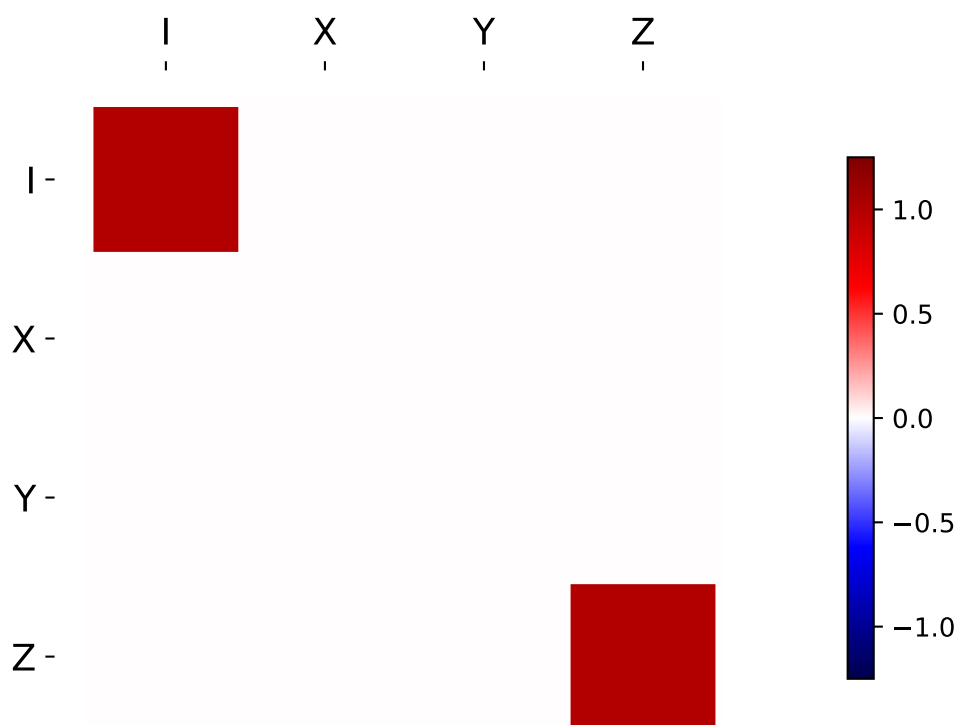
For a `CNOT` system-environment model, the composition of these maps should give us a completely dephasing channel. The channel on both qubits is just the superunitary `CNOT` channel:

```
hinton(to_super(cnot()))
```



We now complete by multiplying the superunitary `CNOT` by the preparation channel above, then applying the partial trace channel by contracting the second and fourth index indices. As expected, this gives us a dephasing map.

```
hinton(tensor_contract(to_super(cnot()), (1, 3)) * s_prep)
```



## 3.6 Time Evolution and Quantum System Dynamics

### 3.6.1 Introduction

Although in some cases, we want to find the stationary states of a quantum system, often we are interested in the dynamics: how the state of a system or an ensemble of systems evolves with time. QuTiP provides many ways to model dynamics.

There are two kinds of quantum systems: open systems that interact with a larger environment and closed systems that do not. In a closed system, the state can be described by a state vector. When we are modeling an open system, or an ensemble of systems, the use of the density matrix is mandatory.

The following table lists of the solvers QuTiP provides for dynamic quantum systems and indicates the type of object returned by the solver:

Table 1: QuTiP Solvers

Equation	Function	Class	Returns
Unitary evolution, Schrödinger equation.	<i>sesolve</i>	<i>SESolver</i>	<i>Result</i>
Periodic Schrödinger equation.	<i>fsesolve</i>	None	<i>Result</i>
Schrödinger equation using Krylov method	<i>krylovsolve</i>	None	<i>Result</i>
Lindblad master eqn. or Von Neuman eqn.	<i>mesolve</i>	<i>MESolver</i>	<i>Result</i>
Monte Carlo evolution	<i>mcsolve</i>	<i>MCSolver</i>	<i>McResult</i>
Non-Markovian Monte Carlo	<i>nm_mcsolve</i>	<i>NonMarkovianMCSO</i>	<i>NmmcResult</i>
Bloch-Redfield master equation	<i>brmesolve</i>	<i>BRSolver</i>	<i>Result</i>
Floquet-Markov master equation	<i>fmmsolve</i>	<i>FMESolver</i>	<i>FloquetResult</i>
Stochastic Schrödinger equation	<i>ssesolve</i>	<i>SSESolver</i>	<i>MultiTrajResult</i>
Stochastic master equation	<i>smesolve</i>	<i>SMESolver</i>	<i>MultiTrajResult</i>
Transfer Tensor Method time-evolution	<i>ttmsolve</i>	None	<i>Result</i>
Hierarchical Equations of Motion evolution	<i>heomsolve</i>	<i>HEOMSolver</i>	<i>HEOMResult</i>

## 3.6.2 Dynamics Simulation Results

### The solver.Result Class

Before embarking on simulating the dynamics of quantum systems, we will first look at the data structure used for returning the simulation results. This object is a *Result* class that stores all the crucial data needed for analyzing and plotting the results of a simulation. A generic *Result* object *result* contains the following properties for storing simulation data:

Property	Description
<i>result.solver</i>	String indicating which solver was used to generate the data.
<i>result.times</i>	List/array of times at which simulation data is calculated.
<i>result.expect</i>	List/array of expectation values, if requested.
<i>result.e_data</i>	Dictionary of expectation values, if requested.
<i>result.states</i>	List/array of state vectors/density matrices calculated at <i>times</i> , if requested.
<i>result.final_state</i>	State vector or density matrix at the last time of the evolution.
<i>result.stats</i>	Various statistics about the evolution.

### Accessing Result Data

To understand how to access the data in a *Result* object we will use an example as a guide, although we do not worry about the simulation details at this stage. Like all solvers, the Master Equation solver used in this example returns an *Result* object, here called simply *result*. To see what is contained inside *result* we can use the *print* function:

```
>>> print(result)
<Result
  Solver: mesolve
  Solver stats:
    method: 'scipy zvode adams'
    init time: 0.0001876354217529297
    preparation time: 0.007544517517089844
    run time: 0.001268625259399414
    solver: 'Master Equation Evolution'
    num_collapse: 1
  Time interval: [0, 1.0] (2 steps)
```

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```
Number of e_ops: 1
State not saved.
>
```

The first line tells us that this data object was generated from the Master Equation solver *mesolve*. Next we have the statistics including the ODE solver used, setup time, number of collapses. Then the integration interval is described, followed with the number of expectation value computed. Finally, it says whether the states are stored.

Now we have all the information needed to analyze the simulation results. To access the data for the two expectation values one can do:

```
expt0 = result.expect[0]
expt1 = result.expect[1]
```

Recall that Python uses C-style indexing that begins with zero (i.e., [0] => 1st collapse operator data). Alternatively, expectation values can be obtained as a dictionary:

```
e_ops = {"sx": sigmax(), "sy": sigmay(), "sz": sigmaz()}
...
expt_sx = result.e_data["sx"]
```

When *e\_ops* is a list, *e\_data* can be used with the list index. Together with the array of times at which these expectation values are calculated:

```
times = result.times
```

we can plot the resulting expectation values:

```
plot(times, expt0)
plot(times, expt1)
show()
```

State vectors, or density matrices, are accessed in a similar manner, although typically one does not need an index (i.e [0]) since there is only one list for each of these components. Some other solver can have other output, *heomsolve*'s results can have *ado\_states* output if the options *store\_ados* is set, similarly, *fmmsolve* can return *floquet\_states*.

## Multiple Trajectories Solver Results

Solver which compute multiple trajectories such as the Monte Carlo Equations Solvers or the Stochastics Solvers result will differ depending on whether the trajectories are flags to be saved. For example:

```
>>> mcsolve(H, psi, np.linspace(0, 1, 11), c_ops, e_ops=[num(N)], ntraj=25, options={
↳ "keep_runs_results": False})
>>> np.shape(result.expect)
(1, 11)

>>> mcsolve(H, psi, np.linspace(0, 1, 11), c_ops, e_ops=[num(N)], ntraj=25, options={
↳ "keep_runs_results": True})
>>> np.shape(result.expect)
(1, 25, 11)
```

When the runs are not saved, the expectation values and states are averaged over all trajectories, while a list over the runs are given when they are stored. For a fix output format, *average\_expect* return the average, while *runs\_states* return the list over trajectories. The *runs\_* output will return *None* when the trajectories are not saved. Standard derivation of the expectation values is also available:



Reduced result	Trajectories results	re-	Description
average_states	runs_states		State vectors or density matrices calculated at each times of tlist
average_final_state	runs_final_state		State vectors or density matrices calculated at the last time of tlist
average_expect	runs_expect		List/array of expectation values, if requested.
std_expect			List/array of standard derivation of the expectation values.
average_e_data	runs_e_data		Dictionary of expectation values, if requested.
std_e_data			Dictionary of standard derivation of the expectation values.

Multiple trajectories results also keep the trajectories seeds to allows recomputing the results.

```
seeds = result.seeds
```

One last feature specific to multi-trajectories results is the addition operation that can be used to merge sets of trajectories.

```
>>> run1 = smesolve(H, psi, np.linspace(0, 1, 11), c_ops, e_ops=[num(N)], ntraj=25)
>>> print(run1.num_trajectories)
25
>>> run2 = smesolve(H, psi, np.linspace(0, 1, 11), c_ops, e_ops=[num(N)], ntraj=25)
>>> print(run2.num_trajectories)
25
>>> merged = run1 + run2
>>> print(merged.num_trajectories)
50
```

This allows one to improve statistics while keeping previous computations.

### 3.6.3 Lindblad Master Equation Solver

#### Unitary evolution

The dynamics of a closed (pure) quantum system is governed by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi, \quad (3.1)$$

where  $\Psi$  is the wave function,  $\hat{H}$  the Hamiltonian, and  $\hbar$  is Planck's constant. In general, the Schrödinger equation is a partial differential equation (PDE) where both  $\Psi$  and  $\hat{H}$  are functions of space and time. For computational purposes it is useful to expand the PDE in a set of basis functions that span the Hilbert space of the Hamiltonian, and to write the equation in matrix and vector form

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle$$

where  $|\psi\rangle$  is the state vector and  $H$  is the matrix representation of the Hamiltonian. This matrix equation can, in principle, be solved by diagonalizing the Hamiltonian matrix  $H$ . In practice, however, it is difficult to perform this diagonalization unless the size of the Hilbert space (dimension of the matrix  $H$ ) is small. Analytically, it is a formidable task to calculate the dynamics for systems with more than two states. If, in addition, we consider dissipation due to the inevitable interaction with a surrounding environment, the computational complexity grows even larger, and we have to resort to numerical calculations in all realistic situations. This illustrates the importance of numerical calculations in describing the dynamics of open quantum systems, and the need for efficient and accessible tools for this task.

The Schrödinger equation, which governs the time-evolution of closed quantum systems, is defined by its Hamiltonian and state vector. In the previous section, *Using Tensor Products and Partial Traces*, we showed how Hamiltonians and state vectors are constructed in QuTiP. Given a Hamiltonian, we can calculate the unitary (non-dissipative) time-evolution of an arbitrary state vector  $|\psi_0\rangle$  (`psi0`) using the QuTiP solver *SESolver* or the function *sesolve*. It evolves the state vector and evaluates the expectation values for a set of operators `e_ops` at the points in time in the list `times`, using an ordinary differential equation solver.

For example, the time evolution of a quantum spin-1/2 system with tunneling rate 0.1 that initially is in the up state is calculated, and the expectation values of the  $\sigma_z$  operator evaluated, with the following code

```
>>> H = 2*np.pi * 0.1 * sigmax()
>>> psi0 = basis(2, 0)
>>> times = np.linspace(0.0, 10.0, 20)
>>> solver = SESolver(H)
>>> result = solver.run(psi0, times, e_ops=[sigmaz()])
>>> result.expect
[array([ 1.          ,  0.78914057,  0.24548543, -0.40169579, -0.87947417,
        -0.98636112, -0.67728018, -0.08257665,  0.54695111,  0.94581862,
         0.94581574,  0.54694361, -0.08258559, -0.67728679, -0.9863626 ,
        -0.87946979, -0.40168705,  0.24549517,  0.78914703,  1.          ])]
```

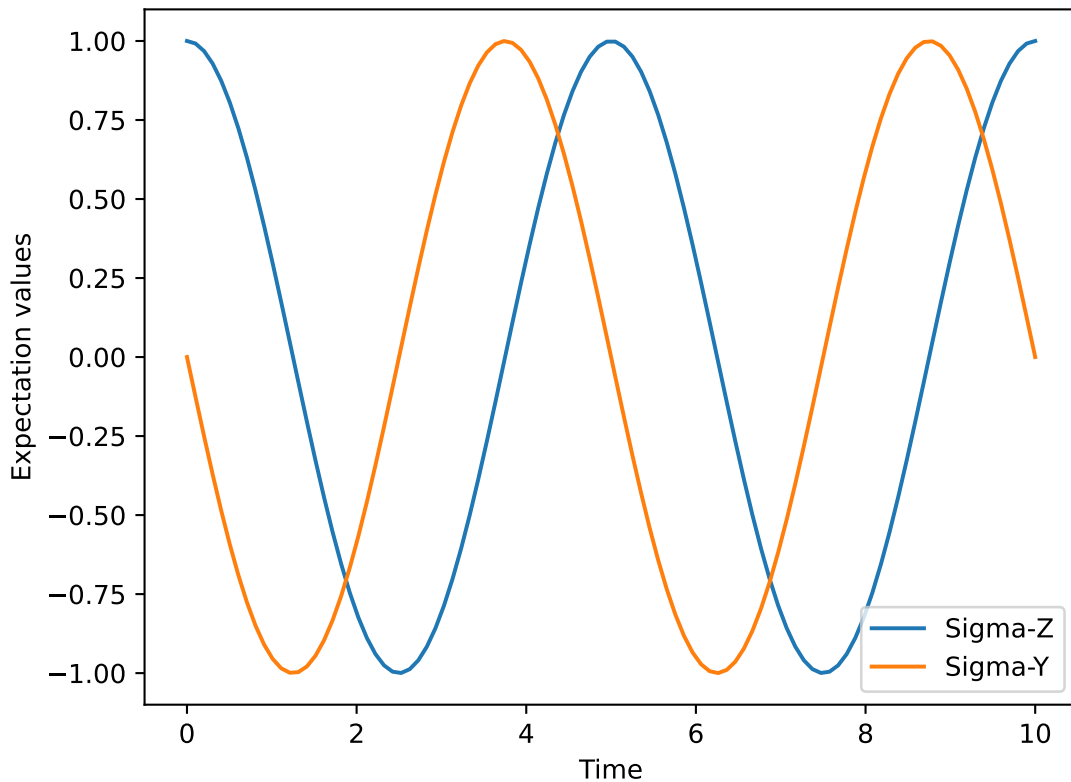
See the next section for examples on evolution with dissipation using *mesolve*.

The function returns an instance of *Result*, as described in the previous section *Dynamics Simulation Results*. The attribute `expect` in `result` is a list of expectation values for the operator(s) that are passed to the `e_ops` parameter. Passing multiple operators to `e_ops` as a list or dict results in a vector of expectation value for each operators. `result.e_data` present the expectation values as a dict of list of expect outputs, while `result.expect` coerce the values to numpy arrays.

```
>>> solver.run(psi0, times, e_ops={"s_z": sigmaz(), "s_y": sigmay()}).e_data
{'s_z': [1.0, 0.7891405656865187, 0.24548542861367784, -0.40169578982499127,
..., 0.24549516882108563, 0.7891470300925004, 0.999999999361128],
's_y': [0.0, -0.6142126403681064, -0.9694002807604085, -0.9157731664756708,
..., 0.9693978141534602, 0.6142043348073879, -1.1303742482923297e-05]}
```

The resulting expectation values can easily be visualized using matplotlib's plotting functions:

```
>>> H = 2*np.pi * 0.1 * sigmax()
>>> psi0 = basis(2, 0)
>>> times = np.linspace(0.0, 10.0, 100)
>>> result = sesolve(H, psi0, times, [sigmaz(), sigmay()])
>>> fig, ax = plt.subplots()
>>> ax.plot(result.times, result.expect[0])
>>> ax.plot(result.times, result.expect[1])
>>> ax.set_xlabel('Time')
>>> ax.set_ylabel('Expectation values')
>>> ax.legend(("Sigma-Z", "Sigma-Y"))
>>> plt.show()
```



If an empty list of operators is passed to the `e_ops` parameter, the `sesolve` and `mesolve` functions return a `Result` instance that contains a list of state vectors for the times specified in `times`

```
>>> times = [0.0, 1.0]
>>> result = sesolve(H, psi0, times, [])
>>> result.states
[Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
 Qobj data =
 [[1.]
 [0.]], Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
 Qobj data =
 [[0.80901699+0.j          ]
 [0.          -0.58778526j]]]
```

### Non-unitary evolution

While the evolution of the state vector in a closed quantum system is deterministic, open quantum systems are stochastic in nature. The effect of an environment on the system of interest is to induce stochastic transitions between energy levels, and to introduce uncertainty in the phase difference between states of the system. The state of an open quantum system is therefore described in terms of ensemble averaged states using the density matrix formalism. A density matrix  $\rho$  describes a probability distribution of quantum states  $|\psi_n\rangle$ , in a matrix representation  $\rho = \sum_n p_n |\psi_n\rangle \langle \psi_n|$ , where  $p_n$  is the classical probability that the system is in the quantum state  $|\psi_n\rangle$ . The time evolution of a density matrix  $\rho$  is the topic of the remaining portions of this section.

## The Lindblad Master equation

The standard approach for deriving the equations of motion for a system interacting with its environment is to expand the scope of the system to include the environment. The combined quantum system is then closed, and its evolution is governed by the von Neumann equation

$$\dot{\rho}_{\text{tot}}(t) = -\frac{i}{\hbar}[H_{\text{tot}}, \rho_{\text{tot}}(t)], \quad (3.2)$$

the equivalent of the Schrödinger equation (3.1) in the density matrix formalism. Here, the total Hamiltonian

$$H_{\text{tot}} = H_{\text{sys}} + H_{\text{env}} + H_{\text{int}},$$

includes the original system Hamiltonian  $H_{\text{sys}}$ , the Hamiltonian for the environment  $H_{\text{env}}$ , and a term representing the interaction between the system and its environment  $H_{\text{int}}$ . Since we are only interested in the dynamics of the system, we can at this point perform a partial trace over the environmental degrees of freedom in Eq. (3.2), and thereby obtain a master equation for the motion of the original system density matrix. The most general trace-preserving and completely positive form of this evolution is the Lindblad master equation for the reduced density matrix  $\rho = \text{Tr}_{\text{env}}[\rho_{\text{tot}}]$

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H(t), \rho(t)] + \sum_n \frac{1}{2} [2C_n \rho(t) C_n^\dagger - \rho(t) C_n^\dagger C_n - C_n^\dagger C_n \rho(t)] \quad (3.3)$$

where the  $C_n = \sqrt{\gamma_n} A_n$  are collapse operators, and  $A_n$  are the operators through which the environment couples to the system in  $H_{\text{int}}$ , and  $\gamma_n$  are the corresponding rates. The derivation of Eq. (3.3) may be found in several sources, and will not be reproduced here. Instead, we emphasize the approximations that are required to arrive at the master equation in the form of Eq. (3.3) from physical arguments, and hence perform a calculation in QuTiP:

- **Separability:** At  $t = 0$  there are no correlations between the system and its environment such that the total density matrix can be written as a tensor product  $\rho_{\text{tot}}^I(0) = \rho^I(0) \otimes \rho_{\text{env}}^I(0)$ .
- **Born approximation:** Requires: (1) that the state of the environment does not significantly change as a result of the interaction with the system; (2) The system and the environment remain separable throughout the evolution. These assumptions are justified if the interaction is weak, and if the environment is much larger than the system. In summary,  $\rho_{\text{tot}}(t) \approx \rho(t) \otimes \rho_{\text{env}}$ .
- **Markov approximation** The time-scale of decay for the environment  $\tau_{\text{env}}$  is much shorter than the smallest time-scale of the system dynamics  $\tau_{\text{sys}} \gg \tau_{\text{env}}$ . This approximation is often deemed a “short-memory environment” as it requires that environmental correlation functions decay on a time-scale fast compared to those of the system.
- **Secular approximation** Stipulates that elements in the master equation corresponding to transition frequencies satisfy  $|\omega_{ab} - \omega_{cd}| \ll 1/\tau_{\text{sys}}$ , i.e., all fast rotating terms in the interaction picture can be neglected. It also ignores terms that lead to a small renormalization of the system energy levels. This approximation is not strictly necessary for all master-equation formalisms (e.g., the Block-Redfield master equation), but it is required for arriving at the Lindblad form (3.3) which is used in *mesolve*.

For systems with environments satisfying the conditions outlined above, the Lindblad master equation (3.3) governs the time-evolution of the system density matrix, giving an ensemble average of the system dynamics. In order to ensure that these approximations are not violated, it is important that the decay rates  $\gamma_n$  be smaller than the minimum energy splitting in the system Hamiltonian. Situations that demand special attention therefore include, for example, systems strongly coupled to their environment, and systems with degenerate or nearly degenerate energy levels.

For non-unitary evolution of a quantum systems, i.e., evolution that includes incoherent processes such as relaxation and dephasing, it is common to use master equations. In QuTiP, the function *mesolve* is used for both: the evolution according to the Schrödinger equation and to the master equation, even though these two equations of motion are very different. The *mesolve* function automatically determines if it is sufficient to use the Schrödinger equation (if no collapse operators were given) or if it has to use the master equation (if collapse operators were given). Note that to calculate the time evolution according to the Schrödinger equation is easier and much faster (for large systems) than using the master equation, so if possible the solver will fall back on using the Schrödinger equation.

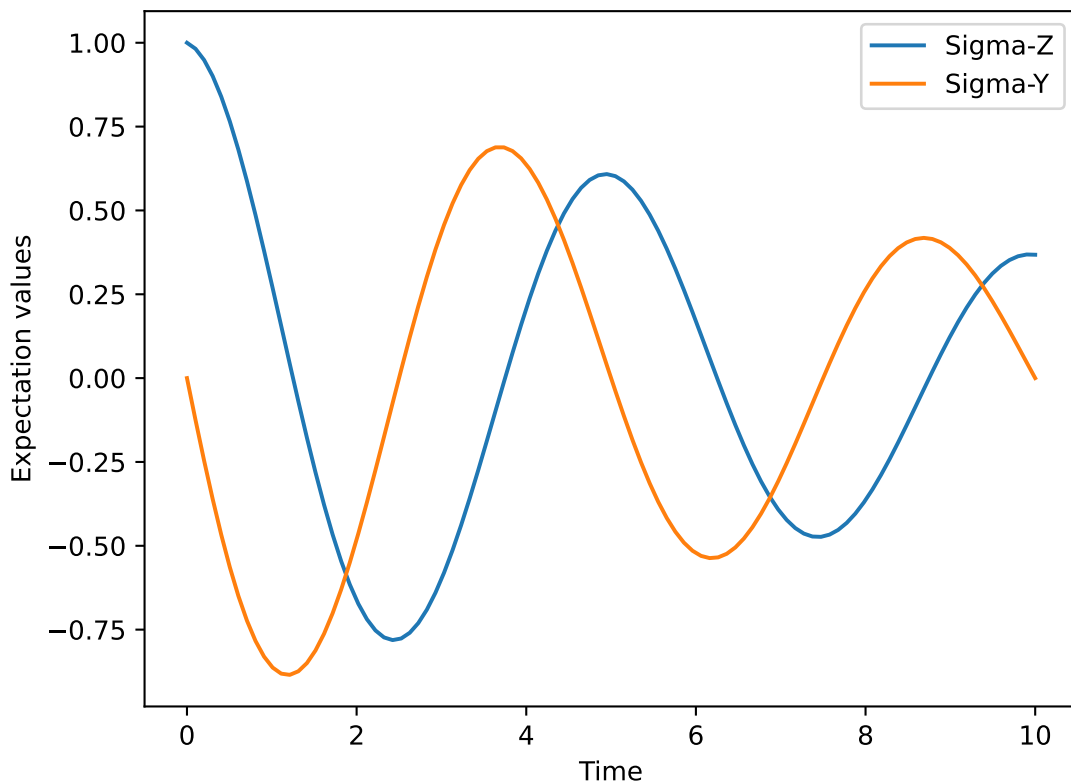
What is new in the master equation compared to the Schrödinger equation are processes that describe dissipation in the quantum system due to its interaction with an environment. These environmental interactions are defined

by the operators through which the system couples to the environment, and rates that describe the strength of the processes.

In QuTiP, the product of the square root of the rate and the operator that describe the dissipation process is called a collapse operator. A list of collapse operators (`c_ops`) is passed as the fourth argument to the `mesolve` function in order to define the dissipation processes in the master equation. When the `c_ops` isn't empty, the `mesolve` function will use the master equation instead of the unitary Schrödinger equation.

Using the example with the spin dynamics from the previous section, we can easily add a relaxation process (describing the dissipation of energy from the spin to its environment), by adding `np.sqrt(0.05) * sigmax()` in the fourth parameter to the `mesolve` function.

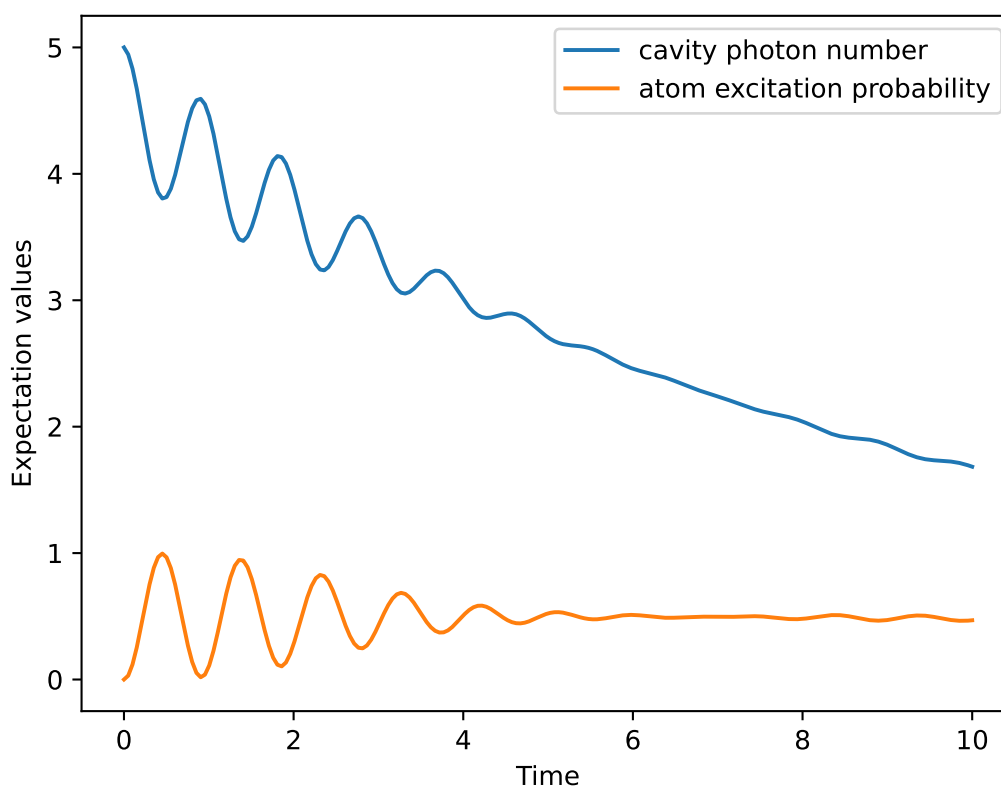
```
>>> times = np.linspace(0.0, 10.0, 100)
>>> result = mesolve(H, psi0, times, [np.sqrt(0.05) * sigmax()], e_ops=[sigmaz(),
↳ sigmay()])
>>> fig, ax = plt.subplots()
>>> ax.plot(times, result.expect[0])
>>> ax.plot(times, result.expect[1])
>>> ax.set_xlabel('Time')
>>> ax.set_ylabel('Expectation values')
>>> ax.legend(("Sigma-Z", "Sigma-Y"))
>>> plt.show()
```



Here, 0.05 is the rate and the operator  $\sigma_x$  (`sigmax`) describes the dissipation process.

Now a slightly more complex example: Consider a two-level atom coupled to a leaky single-mode cavity through a dipole-type interaction, which supports a coherent exchange of quanta between the two systems. If the atom initially is in its groundstate and the cavity in a 5-photon Fock state, the dynamics is calculated with the lines following code

```
>>> times = np.linspace(0.0, 10.0, 200)
>>> psi0 = tensor(fock(2,0), fock(10, 5))
>>> a = tensor(qeye(2), destroy(10))
>>> sm = tensor(destroy(2), qeye(10))
>>> H = 2 * np.pi * a.dag() * a + 2 * np.pi * sm.dag() * sm + 2 * np.pi * 0.25 * (sm_
↳ * a.dag() + sm.dag() * a)
>>> result = mesolve(H, psi0, times, [np.sqrt(0.1)*a], e_ops=[a.dag()*a, sm.dag()*sm])
>>> plt.figure()
>>> plt.plot(times, result.expect[0])
>>> plt.plot(times, result.expect[1])
>>> plt.xlabel('Time')
>>> plt.ylabel('Expectation values')
>>> plt.legend(("cavity photon number", "atom excitation probability"))
>>> plt.show()
```



### 3.6.4 Monte Carlo Solver

#### Introduction

Whereas the density matrix formalism describes the ensemble average over many identical realizations of a quantum system, the Monte Carlo (MC), or quantum-jump approach to wave function evolution, allows for simulating an individual realization of the system dynamics. Here, the environment is continuously monitored, resulting in a series of quantum jumps in the system wave function, conditioned on the increase in information gained about the state of the system via the environmental measurements. In general, this evolution is governed by the Schrödinger

equation with a **non-Hermitian** effective Hamiltonian

$$H_{\text{eff}} = H_{\text{sys}} - \frac{i\hbar}{2} \sum_n C_n^\dagger C_n, \quad (3.4)$$

where again, the  $C_n$  are collapse operators, each corresponding to a separate irreversible process with rate  $\gamma_n$ . Here, the strictly negative non-Hermitian portion of Eq. (3.4) gives rise to a reduction in the norm of the wave function, that to first-order in a small time  $\delta t$ , is given by  $\langle \psi(t + \delta t) | \psi(t + \delta t) \rangle = 1 - \delta p$  where

$$\delta p = \delta t \sum_n \langle \psi(t) | C_n^\dagger C_n | \psi(t) \rangle, \quad (3.5)$$

and  $\delta t$  is such that  $\delta p \ll 1$ . With a probability of remaining in the state  $|\psi(t + \delta t)\rangle$  given by  $1 - \delta p$ , the corresponding quantum jump probability is thus Eq. (3.5). If the environmental measurements register a quantum jump, say via the emission of a photon into the environment, or a change in the spin of a quantum dot, the wave function undergoes a jump into a state defined by projecting  $|\psi(t)\rangle$  using the collapse operator  $C_n$  corresponding to the measurement

$$|\psi(t + \delta t)\rangle = C_n |\psi(t)\rangle / \langle \psi(t) | C_n^\dagger C_n | \psi(t) \rangle^{1/2}. \quad (3.6)$$

If more than a single collapse operator is present in Eq. (3.4), the probability of collapse due to the  $i$ th-operator  $C_i$  is given by

$$P_i(t) = \langle \psi(t) | C_i^\dagger C_i | \psi(t) \rangle / \delta p. \quad (3.7)$$

Evaluating the MC evolution to first-order in time is quite tedious. Instead, QuTiP uses the following algorithm to simulate a single realization of a quantum system. Starting from a pure state  $|\psi(0)\rangle$ :

- **Ia:** Choose a random number  $r_1$  between zero and one, representing the probability that a quantum jump occurs.
- **Ib:** Choose a random number  $r_2$  between zero and one, used to select which collapse operator was responsible for the jump.
- **II:** Integrate the Schrödinger equation, using the effective Hamiltonian (3.4) until a time  $\tau$  such that the norm of the wave function satisfies  $\langle \psi(\tau) | \psi(\tau) \rangle = r_1$ , at which point a jump occurs.
- **III:** The resultant jump projects the system at time  $\tau$  into one of the renormalized states given by Eq. (3.6). The corresponding collapse operator  $C_n$  is chosen such that  $n$  is the smallest integer satisfying:

$$\sum_{i=1}^n P_i(\tau) \geq r_2 \quad (3.8)$$

where the individual  $P_n$  are given by Eq. (3.7). Note that the left hand side of Eq. (3.8) is, by definition, normalized to unity.

- **IV:** Using the renormalized state from step III as the new initial condition at time  $\tau$ , draw a new random number, and repeat the above procedure until the final simulation time is reached.

### Monte Carlo in QuTiP

In QuTiP, Monte Carlo evolution is implemented with the `mcsolve` function. It takes nearly the same arguments as the `mesolve` function for master-equation evolution, except that the initial state must be a ket vector, as oppose to a density matrix, and there is an optional keyword parameter `ntraj` that defines the number of stochastic trajectories to be simulated. By default, `ntraj=500` indicating that 500 Monte Carlo trajectories will be performed.

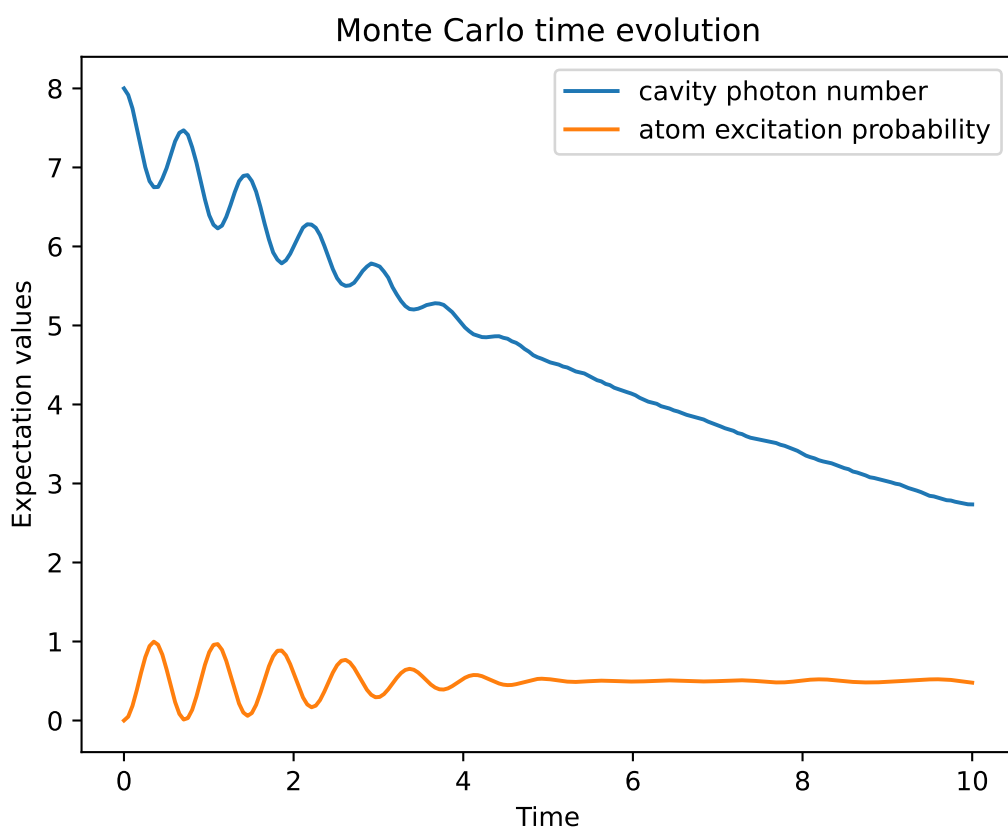
To illustrate the use of the Monte Carlo evolution of quantum systems in QuTiP, let's again consider the case of a two-level atom coupled to a leaky cavity. The only differences to the master-equation treatment is that in this case we invoke the `mcsolve` function instead of `mesolve`

```

times = np.linspace(0.0, 10.0, 200)
psi0 = tensor(fock(2, 0), fock(10, 8))
a = tensor(qeye(2), destroy(10))
sm = tensor(destroy(2), qeye(10))
H = 2*np.pi*a.dag()*a + 2*np.pi*sm.dag()*sm + 2*np.pi*0.25*(sm*a.dag() + sm.dag()*a)
data = mcsolve(H, psi0, times, [np.sqrt(0.1) * a], e_ops=[a.dag() * a, sm.dag() * sm])

plt.figure()
plt.plot(times, data.expect[0], times, data.expect[1])
plt.title('Monte Carlo time evolution')
plt.xlabel('Time')
plt.ylabel('Expectation values')
plt.legend(("cavity photon number", "atom excitation probability"))
plt.show()

```



The advantage of the Monte Carlo method over the master equation approach is that only the state vector is required to be kept in the computers memory, as opposed to the entire density matrix. For large quantum system this becomes a significant advantage, and the Monte Carlo solver is therefore generally recommended for such systems. For example, simulating a Heisenberg spin-chain consisting of 10 spins with random parameters and initial states takes almost 7 times longer using the master equation rather than Monte Carlo approach with the default number of trajectories running on a quad-CPU machine. Furthermore, it takes about 7 times the memory as well. However, for small systems, the added overhead of averaging a large number of stochastic trajectories to obtain the open system dynamics, as well as starting the multiprocessing functionality, outweighs the benefit of the minor (in this case) memory saving. Master equation methods are therefore generally more efficient when Hilbert space sizes are on the order of a couple of hundred states or smaller.



## Monte Carlo Solver Result

The Monte Carlo solver returns a `McResult` object consisting of expectation values and/or states. The main difference with `mesolve`'s `Result` is that it optionally stores the result of each trajectory together with their averages. When trajectories are stored, `result.runs_expect` is a list over the expectation operators, trajectories and times in that order. The averages are stored in `result.average_expect` and the standard derivation of the expectation values in `result.std_expect`. When the states are returned, `result.runs_states` will be an array of length `ntraj`. Each element contains an array of "Qobj" type ket with the same number of elements as `times`. `result.average_states` is a list of density matrices computed as the average of the states at each time step. Furthermore, the output will also contain a list of times at which the collapse occurred, and which collapse operators did the collapse. These can be obtained in `result.col_times` and `result.col_which` respectively.

## Changing the Number of Trajectories

By default, the `mcsolve` function runs 500 trajectories. This value was chosen because it gives good accuracy, Monte Carlo errors scale as  $1/n$  where  $n$  is the number of trajectories, and simultaneously does not take an excessive amount of time to run. However, you can change the number of trajectories to fit your needs. In order to run 1000 trajectories in the above example, we can simply modify the call to `mcsolve` like:

```
data = mcsolve(H, psi0, times, c_ops, e_ops=e_ops, ntraj=1000)
```

where we have added the keyword argument `ntraj=1000` at the end of the inputs. Now, the Monte Carlo solver will calculate expectation values for both operators, `a.dag() * a`, `sm.dag() * sm` averaging over 1000 trajectories.

Other than a target number of trajectories, it is possible to use a computation time or errors bars as condition to stop computing trajectories.

`timeout` is quite simple as `mcsolve` will stop starting the computation of new trajectories when it is reached. Thus:

```
data = mcsolve(H, psi0, times, [np.sqrt(0.1) * a], e_ops=e_ops, ntraj=1000,
↳ timeout=60)
```

Will compute 60 seconds of trajectories or 1000, which ever is reached first. The solver will finish any trajectory started when the timeout is reached. Therefore if the computation time of a single trajectory is quite long, the overall computation time can be much longer than the provided timeout.

Lastly, `mcsolve` can be instructed to stop when the statistical error of the expectation values get under a certain value. When computing the average over trajectories, the error on these are computed using [jackknife resampling](#) for each expect and each time and the computation will be stopped when all these values are under the tolerance passed to `target_tol`. Therefore:

```
data = mcsolve(H, psi0, times, [np.sqrt(0.1) * a], e_ops=e_ops,
ntraj=1000, target_tol=0.01, timeout=600)
```

will stop either after all errors bars on expectation values are under 0.01, 1000 trajectories are computed or 10 minutes have passed, whichever comes first. When a single values is passed, it is used as the absolute value of the tolerance. When a pair of values is passed, it is understood as an absolute and relative tolerance pair. For even finer control, one such pair can be passed for each `e_ops`. For example:

```
data = mcsolve(H, psi0, times, c_ops, e_ops=e_ops, target_tol=[
    (1e-5, 0.1),
    (0, 0),
])
```

will stop when the error bars on the expectation values of the first `e_ops` are under 10% of their average values.

If after computation of some trajectories, it is determined that more are needed, it is possible to add trajectories to existing result by adding result together:

```
>>> run1 = mcsolve(H, psi, times, c_ops, e_ops=e_ops, ntraj=25)
>>> print(run1.num_trajectories)
25
>>> run2 = mcsolve(H, psi, times, c_ops, e_ops=e_ops, ntraj=25)
>>> print(run2.num_trajectories)
25
>>> merged = run1 + run2
>>> print(merged.num_trajectories)
50
```

Note that this merging operation only checks that the results are compatible – i.e. that the `e_ops` and `tlist` are the same. It does not check that the same initial state or Hamiltonian were used.

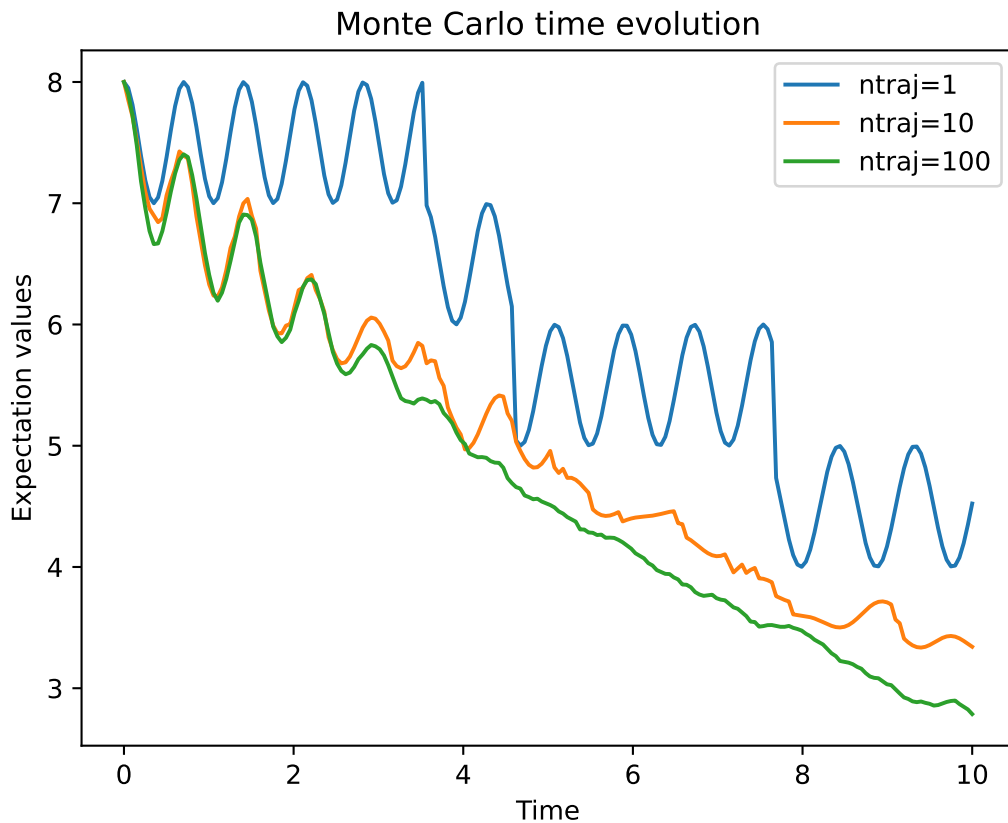
This can be used to explore the convergence of the Monte Carlo solver. For example, the following code block plots expectation values for 1, 10 and 100 trajectories:

```
solver = MCSolver(H, c_ops=[np.sqrt(0.1) * a])
c_ops=[np.sqrt(0.1) * a]
e_ops = [a.dag() * a, sm.dag() * sm]

data1 = mcsolve(H, psi0, times, c_ops, e_ops=e_ops, ntraj=1)
data10 = data1 + mcsolve(H, psi0, times, c_ops, e_ops=e_ops, ntraj=9)
data100 = data10 + mcsolve(H, psi0, times, c_ops, e_ops=e_ops, ntraj=90)

expt1 = data1.expect
expt10 = data10.expect
expt100 = data100.expect

plt.figure()
plt.plot(times, expt1[0], label="ntraj=1")
plt.plot(times, expt10[0], label="ntraj=10")
plt.plot(times, expt100[0], label="ntraj=100")
plt.title('Monte Carlo time evolution')
plt.xlabel('Time')
plt.ylabel('Expectation values')
plt.legend()
plt.show()
```



### Using the Improved Sampling Algorithm

Oftentimes, quantum jumps are rare. This is especially true in the context of simulating gates for quantum information purposes, where typical gate times are orders of magnitude smaller than typical timescales for decoherence. In this case, using the standard monte-carlo sampling algorithm, we often repeatedly sample the no-jump trajectory. We can thus reduce the number of required runs by only sampling the no-jump trajectory once. We then extract the no-jump probability  $p$ , and for all future runs we only sample random numbers  $r_1$  where  $r_1 > p$ , thus ensuring that a jump will occur. When it comes time to compute expectation values, we weight the no-jump trajectory by  $p$  and the jump trajectories by  $1 - p$ . This algorithm is described in [Abd19] and can be utilized by setting the option "improved\_sampling" in the call to `mcsolve`:

```
data = mcsolve(H, psi0, times, [np.sqrt(0.1) * a], options={"improved_sampling": True})
```

where in this case the first run samples the no-jump trajectory, and the remaining 499 trajectories are all guaranteed to include (at least) one jump.

The power of this algorithm is most obvious when considering systems that rarely undergo jumps. For instance, consider the following T1 simulation of a qubit with a lifetime of 10 microseconds (assuming time is in units of nanoseconds)

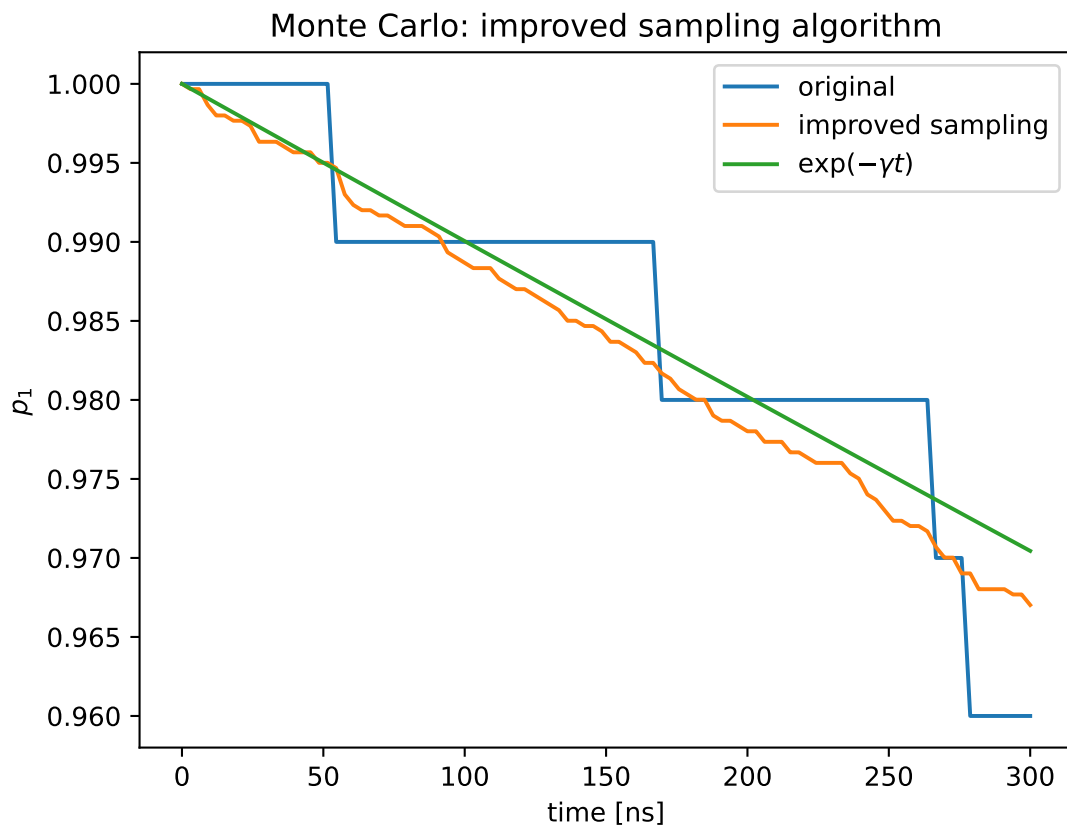
```
times = np.linspace(0.0, 300.0, 100)
psi0 = fock(2, 1)
sm = fock(2, 0) * fock(2, 1).dag()
omega = 2.0 * np.pi * 1.0
H0 = -0.5 * omega * sigmaz()
gamma = 1/10000
data = mcsolve(
```

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```
[H0], psi0, times, [np.sqrt(gamma) * sm], [sm.dag() * sm], ntraj=100
)
data_imp = mcsolve(
    [H0], psi0, times, [np.sqrt(gamma) * sm], [sm.dag() * sm], ntraj=100,
    options={"improved_sampling": True}
)

plt.figure()
plt.plot(times, data.expect[0], label="original")
plt.plot(times, data_imp.expect[0], label="improved sampling")
plt.plot(times, np.exp(-gamma * times), label=r"$\exp(-\gamma t)$")
plt.title('Monte Carlo: improved sampling algorithm')
plt.xlabel("time [ns]")
plt.ylabel(r"$p_{1}$")
plt.legend()
plt.show()
```



The original sampling algorithm samples the no-jump trajectory on average 96.7% of the time, while the improved sampling algorithm only does so once.

## Reproducibility

For reproducibility of Monte-Carlo computations it is possible to set the seed of the random number generator:

```
>>> res1 = mcsolve(H, psi0, tlist, c_ops, e_ops=e_ops, seeds=1, ntraj=1)
>>> res2 = mcsolve(H, psi0, tlist, c_ops, e_ops=e_ops, seeds=1, ntraj=1)
>>> res3 = mcsolve(H, psi0, tlist, c_ops, e_ops=e_ops, seeds=2, ntraj=1)
>>> np.allclose(res1, res2)
True
>>> np.allclose(res1, res3)
False
```

The `seeds` parameter can either be an integer or a numpy `SeedSequence`, which will then be used to create seeds for each trajectory. Alternatively it may be a list of integers or `SeedSequence`s with one seed for each trajectories. Seeds available in the result object can be used to redo the same evolution:

```
>>> res1 = mcsolve(H, psi0, tlist, c_ops, e_ops=e_ops, ntraj=10)
>>> res2 = mcsolve(H, psi0, tlist, c_ops, e_ops=e_ops, seeds=res1.seeds, ntraj=10)
>>> np.allclose(res1, res2)
True
```

## Running trajectories in parallel

Monte-Carlo evolutions often need hundreds of trajectories to obtain sufficient statistics. Since all trajectories are independent of each other, they can be computed in parallel. The option `map` can take "serial", "parallel" or "loky". Both "parallel" and "loky" compute trajectories on multiple CPUs using respectively the `multiprocessing` and `loky` python modules.

```
>>> res_par = mcsolve(H, psi0, tlist, c_ops, e_ops=e_ops, options={"map": "parallel"},
↳ seeds=1)
>>> res_ser = mcsolve(H, psi0, tlist, c_ops, e_ops=e_ops, options={"map": "serial"},
↳ seeds=1)
>>> np.allclose(res_par.average_expect, res_ser.average_expect)
True
```

Note that when running in parallel, the order in which the trajectories are added to the result can differ. Therefore

```
>>> print(res_par.seeds[:3])
[SeedSequence(entropy=1,spawn_key=(1,),),
 SeedSequence(entropy=1,spawn_key=(0,),),
 SeedSequence(entropy=1,spawn_key=(2,),)]

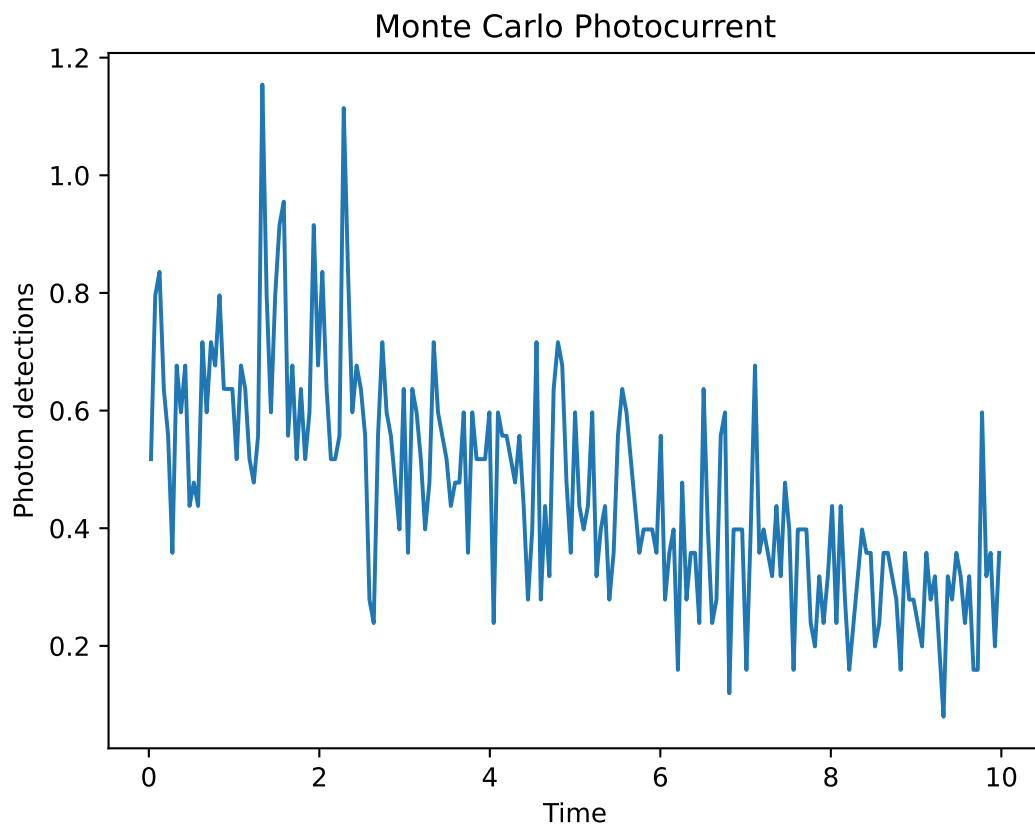
>>> print(res_ser.seeds[:3])
[SeedSequence(entropy=1,spawn_key=(0,),),
 SeedSequence(entropy=1,spawn_key=(1,),),
 SeedSequence(entropy=1,spawn_key=(2,),)]
```

## Photocurrent

The photocurrent, previously computed using the `photocurrent_sesolve` and `photocurrent_sesolve` functions, are now included in the output of `mcsolve` as `result.photocurrent`.

```
times = np.linspace(0.0, 10.0, 200)
psi0 = tensor(fock(2, 0), fock(10, 8))
a = tensor(qeye(2), destroy(10))
sm = tensor(destroy(2), qeye(10))
e_ops = [a.dag() * a, sm.dag() * sm]
H = 2*np.pi*a.dag()*a + 2*np.pi*sm.dag()*sm + 2*np.pi*0.25*(sm*a.dag() + sm.dag()*a)
data = mcsolve(H, psi0, times, [np.sqrt(0.1) * a], e_ops=e_ops)

plt.figure()
plt.plot((times[:-1] + times[1:])/2, data.photocurrent[0])
plt.title('Monte Carlo Photocurrent')
plt.xlabel('Time')
plt.ylabel('Photon detections')
plt.show()
```

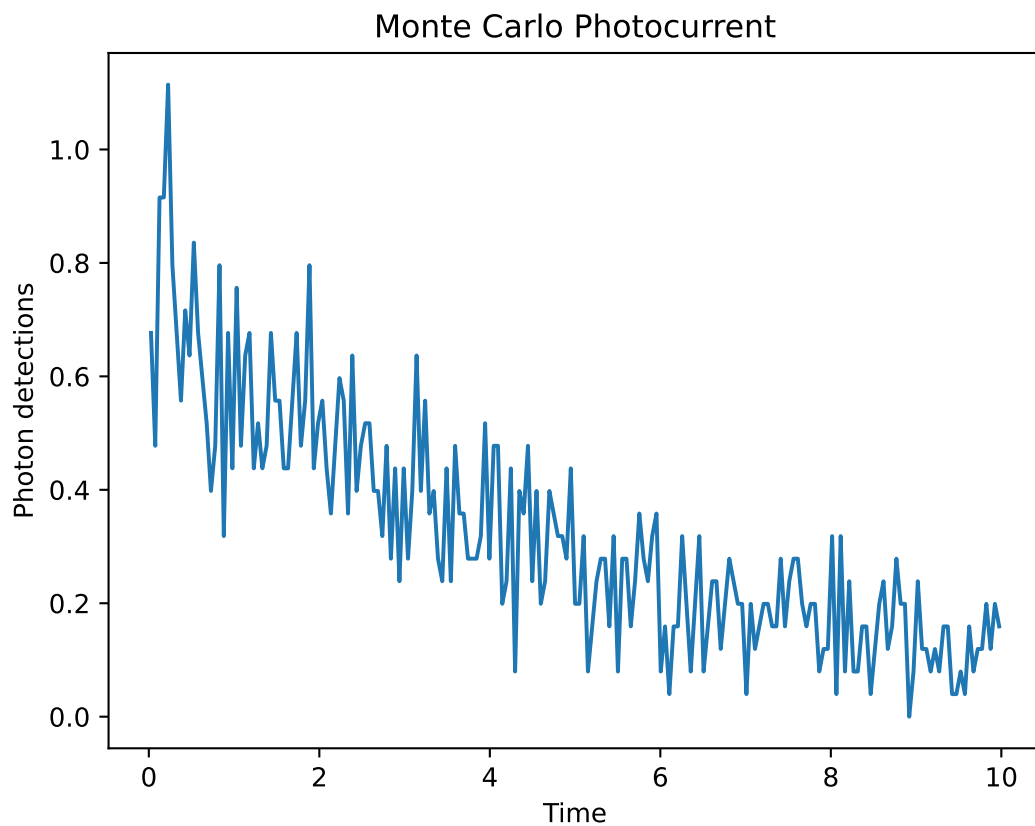


## Open Systems

mcsolve can be used to study systems which have measurement and dissipative interactions with their environment. This is done by passing a Liouvillian including the dissipative interaction to the solver instead of a Hamiltonian.

```
times = np.linspace(0.0, 10.0, 200)
psi0 = tensor(fock(2, 0), fock(10, 8))
a = tensor(qeye(2), destroy(10))
sm = tensor(destroy(2), qeye(10))
H = 2*np.pi*a.dag()*a + 2*np.pi*sm.dag()*sm + 2*np.pi*0.25*(sm*a.dag() + sm.dag()*a)
L = liouvillian(H, [0.01 * sm, np.sqrt(0.1) * a])
data = mcsolve(L, psi0, times, [np.sqrt(0.1) * a], e_ops=[a.dag() * a, sm.dag() * sm])

plt.figure()
plt.plot((times[:-1] + times[1:])/2, data.photocurrent[0])
plt.title('Monte Carlo Photocurrent')
plt.xlabel('Time')
plt.ylabel('Photon detections')
plt.show()
```



## 3.6.5 Krylov Solver

### Introduction

The Krylov-subspace method is a standard method to approximate quantum dynamics. Let  $|\psi\rangle$  be a state in a  $D$ -dimensional complex Hilbert space that evolves under a time-independent Hamiltonian  $H$ . Then, the  $N$ -dimensional Krylov subspace associated with that state and Hamiltonian is given by

$$\mathcal{K}_N = \text{span} \{ |\psi\rangle, H|\psi\rangle, \dots, H^{N-1}|\psi\rangle \}, \quad (3.9)$$

where the dimension  $N < D$  is a parameter of choice. To construct an orthonormal basis  $B_N$  for  $\mathcal{K}_N$ , the simplest algorithm is the well-known Lanczos algorithm, which provides a sort of Gram-Schmidt procedure that harnesses the fact that orthonormalization needs to be imposed only for the last two vectors in the basis. Written in this basis the time-evolved state can be approximated as

$$|\psi(t)\rangle = e^{-iHt}|\psi\rangle \approx \mathbb{P}_N e^{-iHt} \mathbb{P}_N |\psi\rangle = \mathbb{V}_N^\dagger e^{-iT_N t} \mathbb{V}_N |\psi\rangle \equiv |\psi_N(t)\rangle, \quad (3.10)$$

where  $T_N = \mathbb{V}_N H \mathbb{V}_N^\dagger$  is the Hamiltonian reduced to the Krylov subspace (which takes a tridiagonal matrix form), and  $\mathbb{V}_N^\dagger$  is the matrix containing the vectors of the Krylov basis as columns.

With the above approximation, the time-evolution is calculated only with a smaller square matrix of the desired size. Therefore, the Krylov method provides huge speed-ups in computation of short-time evolutions when the dimension of the Hamiltonian is very large, a point at which exact calculations on the complete subspace are practically impossible.

One of the biggest problems with this type of method is the control of the error. After a short time, the error starts to grow exponentially. However, this can be easily corrected by restarting the subspace when the error reaches a certain threshold. Therefore, a series of  $M$  Krylov-subspace time evolutions provides accurate solutions for the complete time evolution. Within this scheme, the magic of Krylov resides not only in its ability to capture complex time evolutions from very large Hilbert spaces with very small dimensions  $M$ , but also in the computing speed-up it presents.

For exceptional cases, the Lanczos algorithm might arrive at the exact evolution of the initial state at a dimension  $M_{hb} < M$ . This is called a happy breakdown. For example, if a Hamiltonian has a symmetry subspace  $D_{\text{sim}} < M$ , then the algorithm will optimize using the value `math:M_{\{hb\}}<M;`, at which the evolution is not only exact but also cheap.

### Krylov Solver in QuTiP

In QuTiP, Krylov-subspace evolution is implemented as the function `krylovsolve`. Arguments are nearly the same as `sesolve` function for master-equation evolution, except that the Hamiltonian cannot depend on time, the initial state must always be a ket vector, (it cannot be used to compute propagators) and an additional parameter `krylov_dim` is needed. `krylov_dim` defines the maximum allowed Krylov-subspace dimension.

Let's solve a simple example using the algorithm in QuTiP to get familiar with the method.

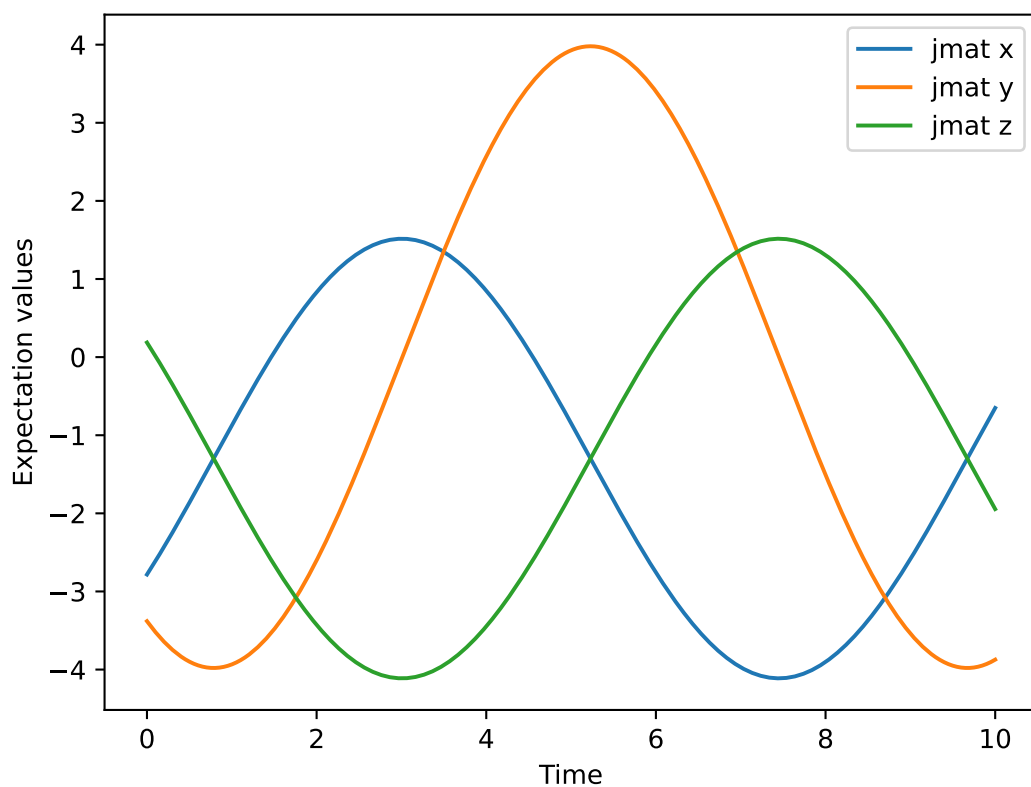
```
>>> dim = 100
>>> jx = jmat((dim - 1) / 2.0, "x")
>>> jy = jmat((dim - 1) / 2.0, "y")
>>> jz = jmat((dim - 1) / 2.0, "z")
>>> e_ops = [jx, jy, jz]
>>> H = (jz + jx) / 2
>>> psi0 = rand_ket(dim, seed=1)
>>> tlist = np.linspace(0.0, 10.0, 200)
>>> results = krylovsolve(H, psi0, tlist, krylov_dim=20, e_ops=e_ops)
>>> plt.figure()
>>> for expect in results.expect:
>>>     plt.plot(tlist, expect)
>>> plt.legend(('jmat x', 'jmat y', 'jmat z'))
```

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```
>>> plt.xlabel('Time')
>>> plt.ylabel('Expectation values')
>>> plt.show()
```



### 3.6.6 Stochastic Solver

When a quantum system is subjected to continuous measurement, through homodyne detection for example, it is possible to simulate the conditional quantum state using stochastic Schrodinger and master equations. The solution of these stochastic equations are quantum trajectories, which represent the conditioned evolution of the system given a specific measurement record.

In general, the stochastic evolution of a quantum state is calculated in QuTiP by solving the general equation

$$d\rho(t) = d_1\rho dt + \sum_n d_{2,n}\rho dW_n, \quad (3.11)$$

where  $dW_n$  is a Wiener increment, which has the expectation values  $E[dW] = 0$  and  $E[dW^2] = dt$ .

## Stochastic Schrodinger Equation

The stochastic Schrodinger equation is given by (see section 4.4, [Wis09])

$$d\psi(t) = -iH\psi(t)dt - \sum_n \left( \frac{S_n^\dagger S_n}{2} - \frac{e_n}{2} S_n + \frac{e_n^2}{8} \right) \psi(t)dt + \sum_n \left( S_n - \frac{e_n}{2} \right) \psi(t)dW_n, \quad (3.12)$$

where  $H$  is the Hamiltonian,  $S_n$  are the stochastic collapse operators, and  $e_n$  is

$$e_n = \langle \psi(t) | S_n + S_n^\dagger | \psi(t) \rangle \quad (3.13)$$

In QuTiP, this equation can be solved using the function `ssesolve`, which is implemented by defining  $d_1$  and  $d_{2,n}$  from Equation (3.11) as

$$d_1 = -iH - \frac{1}{2} \sum_n \left( S_n^\dagger S_n - e_n S_n + \frac{e_n^2}{4} \right), \quad (3.14)$$

and

$$d_{2,n} = S_n - \frac{e_n}{2}. \quad (3.15)$$

The solver `ssesolve` will construct the operators  $d_1$  and  $d_{2,n}$  once the user passes the Hamiltonian ( $H$ ) and the stochastic operator list (`sc_ops`). As with the `msolve`, the number of trajectories and the seed for the noise realisation can be fixed using the arguments: `ntraj` and `seeds`, respectively. If the user also requires the measurement output, the options entry `{"store_measurement": True}` should be included.

Per default, homodyne is used. Heterodyne detections can be easily simulated by passing the arguments `'heterodyne=True'` to `ssesolve`.

## Stochastic Master Equation

When the initial state of the system is a density matrix  $\rho$ , the stochastic master equation solver `qutip.stochastic.smesolve` must be used. The stochastic master equation is given by (see section 4.4, [Wis09])

$$d\rho(t) = -i[H, \rho(t)]dt + D[A]\rho(t)dt + \mathcal{H}[A]\rho dW(t) \quad (3.16)$$

where

$$D[A]\rho = \frac{1}{2} [2A\rho A^\dagger - \rho A^\dagger A - A^\dagger A\rho], \quad (3.17)$$

and

$$\mathcal{H}[A]\rho = A\rho(t) + \rho(t)A^\dagger - \text{tr}[A\rho(t) + \rho(t)A^\dagger]. \quad (3.18)$$

In QuTiP, solutions for the stochastic master equation are obtained using the solver `smesolve`. The implementation takes into account 2 types of collapse operators.  $C_i$  (`c_ops`) represent the dissipation in the environment, while  $S_n$  (`sc_ops`) are monitored operators. The deterministic part of the evolution, described by the  $d_1$  in Equation (3.11), takes into account all operators  $C_i$  and  $S_n$ :

$$d_1 = -i[H(t), \rho(t)] + \sum_i D[C_i]\rho + \sum_n D[S_n]\rho, \quad (3.19)$$

The stochastic part,  $d_{2,n}$ , is given solely by the operators  $S_n$

$$d_{2,n} = S_n\rho(t) + \rho(t)S_n^\dagger - \text{tr}(S_n\rho(t) + \rho(t)S_n^\dagger) \rho(t). \quad (3.20)$$

As in the stochastic Schrodinger equation, heterodyne detection can be chosen by passing `heterodyne=True`.

## Example

Below, we solve the dynamics for an optical cavity at OK whose output is monitored using homodyne detection. The cavity decay rate is given by  $\kappa$  and the  $\Delta$  is the cavity detuning with respect to the driving field. The measurement operators can be passed using the option `m_ops`. The homodyne current  $J_x$  is calculated using

$$J_x = \langle x \rangle + dW/dt, \quad (3.21)$$

where  $x$  is the operator passed using `m_ops`. The results are available in `result.measurements`.

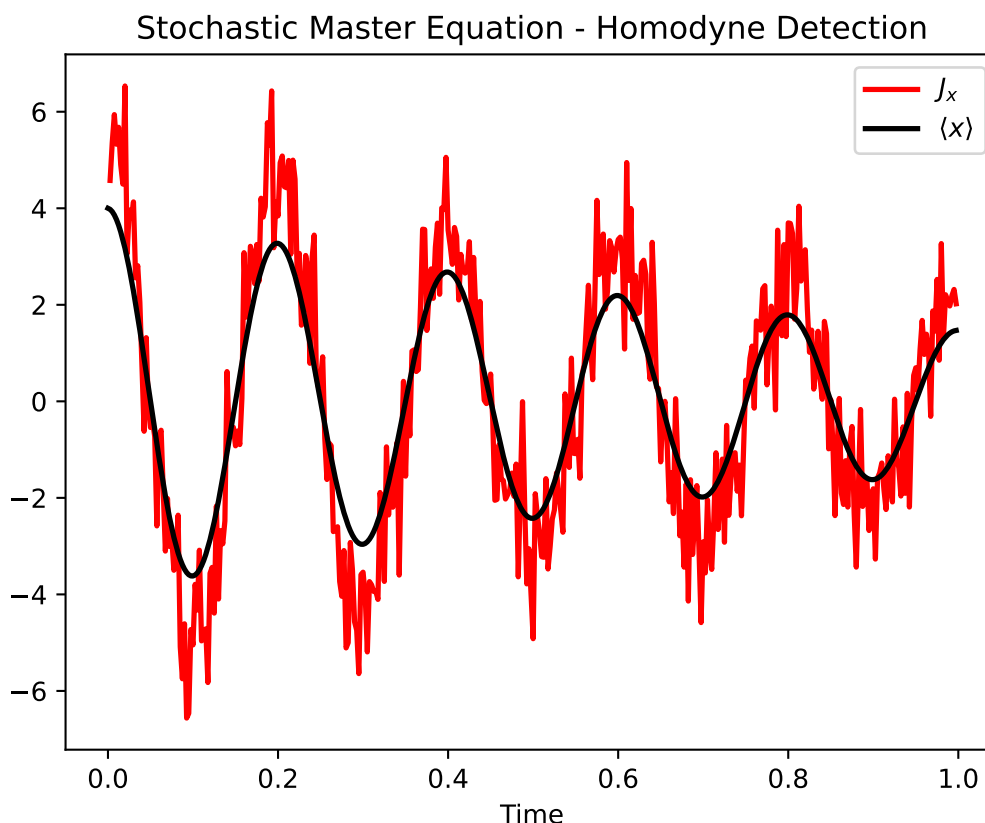
```
# parameters
DIM = 20 # Hilbert space dimension
DELTA = 5 * 2 * np.pi # cavity detuning
KAPPA = 2 # cavity decay rate
INTENSITY = 4 # intensity of initial state
NUMBER_OF_TRAJECTORIES = 500

# operators
a = destroy(DIM)
x = a + a.dag()
H = DELTA * a.dag() * a

rho_0 = coherent(DIM, np.sqrt(INTENSITY))
times = np.arange(0, 1, 0.0025)

stoc_solution = smesolve(
    H, rho_0, times,
    c_ops=[],
    sc_ops=[np.sqrt(KAPPA) * a],
    e_ops=[x],
    ntraj=NUMBER_OF_TRAJECTORIES,
    options={"dt": 0.00125, "store_measurement": True},
)

fig, ax = plt.subplots()
ax.set_title('Stochastic Master Equation - Homodyne Detection')
ax.plot(times[1:], np.array(stoc_solution.measurement).mean(axis=0)[0, :].real,
        'r', lw=2, label=r'$J_x$')
ax.plot(times, stoc_solution.expect[0], 'k', lw=2,
        label=r'$\langle x \rangle$')
ax.set_xlabel('Time')
ax.legend()
```



The stochastic solvers share many features with *mcsolve*, such as end conditions, seed control and running in parallel. See the sections *Changing the Number of Trajectories*, *Reproducibility* and *Running trajectories in parallel* for details.

### 3.6.7 Solving Problems with Time-dependent Hamiltonians

#### Time-Dependent Operators

In the previous examples of quantum evolution, we assumed that the systems under consideration were described by time-independent Hamiltonians. However, many systems have explicit time dependence in either the Hamiltonian, or the collapse operators describing coupling to the environment, and sometimes both components might depend on time. The time-evolutions solvers such as *sesolve*, *brmesolve*, etc. are all capable of handling time-dependent Hamiltonians and collapse terms. QuTiP use *QobjEvo* to represent time-dependent quantum operators. There are three different ways to build a *QobjEvo*:

1. **Function based:** Build the time dependent operator from a function returning a *Qobj*:

```
def oper(t):
    return num(N) + (destroy(N) + create(N)) * np.sin(t)

H_t = QobjEvo(oper)
```

1. **List based:** The time dependent quantum operator is represented as a list of *qobj* and [*qobj*, coefficient] pairs:

```
H_t = QobjEvo([num(N), [create(N), lambda t: np.sin(t)], [destroy(N), lambda t: np.
    ↪ sin(t)]]])
```

3. **coefficient based**: The product of a *Qobj* with a Coefficient, created by the *coefficient* function, result in a *QobjEvo*:

```
coeff = coefficient(lambda t: np.sin(t))
H_t = num(N) + (destroy(N) + create(N)) * coeff
```

These 3 examples will create the same time dependent operator, however the function based method will usually be slower when used in solver.

Most solvers accept a *QobjEvo* when an operator is expected: this include the Hamiltonian  $H$ , collapse operators, expectation values operators, the operator of *brmesolve*'s *a\_ops*, etc. Exception are *krylovsolve*'s Hamiltonian and HEOM's Bath operators.

Most solvers will accept any format that could be made into a *QobjEvo* for the Hamiltonian. All of the following are equivalent:

```
result = mesolve(H_t, ...)
result = mesolve([num(N), [destroy(N) + create(N), lambda t: np.sin(t)]], ...)
result = mesolve(oper, ...)
```

Collapse operator also accept a list of object that could be made into *QobjEvo*. However one needs to be careful about not confusing the list nature of the *c\_ops* parameter with list format quantum system. In the following call:

```
result = mesolve(H_t, ..., c_ops=[num(N), [destroy(N) + create(N), lambda t: np.
    ↪ sin(t)]])
```

*mesolve* will see 2 collapses operators: *num(N)* and *[destroy(N) + create(N), lambda t: np.sin(t)]*. It is therefore preferred to pass each collapse operator as either a *Qobj* or a *QobjEvo*.

As an example, we will look at a case with a time-dependent Hamiltonian of the form  $H = H_0 + f(t)H_1$  where  $f(t)$  is the time-dependent driving strength given as  $f(t) = A \exp[-(t/\sigma)^2]$ . The following code sets up the problem

```
ustate = basis(3, 0)
excited = basis(3, 1)
ground = basis(3, 2)

N = 2 # Set where to truncate Fock state for cavity
sigma_ge = tensor(qeye(N), ground * excited.dag()) # |g><e|
sigma_ue = tensor(qeye(N), ustate * excited.dag()) # |u><e|
a = tensor(destroy(N), qeye(3))
ada = tensor(num(N), qeye(3))

c_ops = [] # Build collapse operators
kappa = 1.5 # Cavity decay rate
c_ops.append(np.sqrt(kappa) * a)
gamma = 6 # Atomic decay rate
c_ops.append(np.sqrt(5*gamma/9) * sigma_ue) # Use Rb branching ratio of 5/9 e->u
c_ops.append(np.sqrt(4*gamma/9) * sigma_ge) # 4/9 e->g

t = np.linspace(-15, 15, 100) # Define time vector
psi0 = tensor(basis(N, 0), ustate) # Define initial state

state_GG = tensor(basis(N, 1), ground) # Define states onto which to project
sigma_GG = state_GG * state_GG.dag()
state_UU = tensor(basis(N, 0), ustate)
sigma_UU = state_UU * state_UU.dag()

g = 5 # coupling strength
```

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```
H0 = -g * (sigma_ge.dag() * a + a.dag() * sigma_ge) # time-independent term
H1 = (sigma_ue.dag() + sigma_ue) # time-dependent term
```

Given that we have a single time-dependent Hamiltonian term, and constant collapse terms, we need to specify a single Python function for the coefficient  $f(t)$ . In this case, one can simply do

```
def H1_coeff(t):
    return 9 * np.exp(-(t / 5.) ** 2)
```

In this case, the return value depends only on time. However it is possible to add optional arguments to the call, see [Using arguments](#). Having specified our coefficient function, we can now specify the Hamiltonian in list format and call the solver (in this case *mesolve*)

```
H = [H0, [H1, H1_coeff]]
output = mesolve(H, psi0, t, c_ops, [ada, sigma_UU, sigma_GG])
```

We can call the Monte Carlo solver in the exact same way (if using the default `ntraj=500`):

```
output = mcsolve(H, psi0, t, c_ops, [ada, sigma_UU, sigma_GG])
```

The output from the master equation solver is identical to that shown in the examples, the Monte Carlo however will be noticeably off, suggesting we should increase the number of trajectories for this example. In addition, we can also consider the decay of a simple Harmonic oscillator with time-varying decay rate

```
kappa = 0.5

def col_coeff(t, args): # coefficient function
    return np.sqrt(kappa * np.exp(-t))

N = 10 # number of basis states
a = destroy(N)
H = a.dag() * a # simple HO
psi0 = basis(N, 9) # initial state
c_ops = [QobjEvo([a, col_coeff])] # time-dependent collapse term
times = np.linspace(0, 10, 100)
output = mesolve(H, psi0, times, c_ops, [a.dag() * a])
```

## Qobjevo

*QobjEvo* as a time dependent quantum system, as it's main functionality create a *Qobj* at a time:

```
>>> print(H_t(np.pi / 2))
Quantum object: dims=[[2], [2]], shape=(2, 2), type='oper', isherm=True
Qobj data =
[[0. 1.]
 [1. 1.]]
```

*QobjEvo* shares a lot of properties with the *Qobj*.

Property	Attribute	Description
Dimensions	<code>Q.dims</code>	Shapes the tensor structure.
Shape	<code>Q.shape</code>	Dimensions of underlying data matrix.
Type	<code>Q.type</code>	Is object of type 'ket', 'bra', 'oper', or 'super'?
Representation	<code>Q.superrep</code>	Representation used if <i>type</i> is 'super'?
Is constant	<code>Q.isconstant</code>	Does the <i>QobjEvo</i> depend on time.

*QobjEvo*'s follow the same mathematical operations rules than *Qobj*. They can be added, subtracted and multiplied with scalar, *Qobj* and *QobjEvo*. They also support the `dag` and `trans` and `conj` method and can be used for tensor operations and super operator transformation:

```
H = tensor(H_t, qeye(2))
c_op = tensor(QobjEvo([destroy(N), lambda t: np.exp(-t)]), sigmax())

L = -1j * (spre(H) - spost(H.dag()))
L += spre(c_op) * spost(c_op.dag()) - 0.5 * spre(c_op.dag() * c_op) - 0.5 * spost(c_
    op.dag() * c_op)
```

Or equivalently:

```
L = liouvillian(H, [c_op])
```

## Using arguments

Until now, the coefficients were only functions of time. In the definition of `H1_coeff`, the driving amplitude `A` and width `sigma` were hardcoded with their numerical values. This is fine for problems that are specialized, or that we only want to run once. However, in many cases, we would like study the same problem with a range of parameters and not have to worry about manually changing the values on each run. QuTiP allows you to accomplish this using by adding extra arguments to coefficients function that make the *QobjEvo*. For instance, instead of explicitly writing 9 for the amplitude and 5 for the width of the gaussian driving term, we can add an *args* positional variable:

```
>>> def H1_coeff(t, args):
>>>     return args['A'] * np.exp(-(t/args['sigma'])**2)
```

or, new from v5, add the extra parameter directly:

```
>>> def H1_coeff(t, A, sigma):
>>>     return A * np.exp(-(t / sigma)**2)
```

When the second positional input of the coefficient function is named *args*, the arguments are passed as a Python dictionary of key: value pairs. Otherwise the coefficient function is called as `coeff(t, **args)`. In the last example, `args = {'A': a, 'sigma': b}` where `a` and `b` are the two parameters for the amplitude and width, respectively. This *args* dictionary need to be given at creation of the *QobjEvo* when function using then are included:

```
>>> system = [sigmaz(), [sigmax(), H1_coeff]]
>>> args={'A': 9, 'sigma': 5}
>>> qevo = QobjEvo(system, args=args)
```

But without *args*, the *QobjEvo* creation will fail:

```
>>> QobjEvo(system)
TypeError: H1_coeff() missing 2 required positional arguments: 'A' and 'sigma'
```

When evaluation the *QobjEvo* at a time, new arguments can be passed either with the *args* dictionary positional arguments, or with specific keywords arguments:

```
>>> print(qevo(1))
Quantum object: dims=[[2], [2]], shape=(2, 2), type='oper', isherm=True
Qobj data =
[[ 1.          8.64710495]
 [ 8.64710495 -1.          ]]
>>> print(qevo(1, {"A": 5, "sigma": 0.2}))
Quantum object: dims=[[2], [2]], shape=(2, 2), type='oper', isherm=True
```

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```
Qobj data =
[[ 1.00000000e+00  6.94397193e-11]
 [ 6.94397193e-11 -1.00000000e+00]]
>>> print(qevo(1, A=5))
Quantum object: dims=[[2], [2]], shape=(2, 2), type='oper', isherm=True
Qobj data =
[[ 1.          4.8039472]
 [ 4.8039472 -1.          ]]
```

Whether the original coefficient used the `args` or specific input does not matter. It is fine to mix the different signatures.

Solver calls take an `args` input that is used to build the time dependent system. If the Hamiltonian or collapse operators are already *QobjEvo*, their arguments will be overwritten.

```
def system(t, A, sigma):
    return H0 + H1 * (A * np.exp(-(t / sigma)**2))

mesolve(system, ..., args=args)
```

To update arguments of an existing time dependent quantum system, you can pass the previous object as the input of a *QobjEvo* with new `args`:

```
>>> new_qevo = QobjEvo(qevo, args={"A": 5, "sigma": 0.2})
>>> new_qevo(1) == qevo(1, {"A": 5, "sigma": 0.2})
True
```

*QobjEvo* created from a monolithic function can also use arguments:

```
def oper(t, w):
    return num(N) + (destroy(N) + create(N)) * np.sin(t*w)

H_t = QobjEvo(oper, args={"w": np.pi})
```

When merging two or more *QobjEvo*, each will keep its arguments, but calling it with updated arguments will affect all parts:

```
>>> qevo1 = QobjEvo([sigmap(), lambda t, a: a], args={"a": 1})
>>> qevo2 = QobjEvo([sigmam(), lambda t, a: a], args={"a": 2})
>>> summed_evo = qevo1 + qevo2
>>> print(summed_evo(0))
Quantum object: dims=[[2], [2]], shape=(2, 2), type='oper', isherm=False
Qobj data =
[[0. 1.]
 [2. 0.]]
>>> print(summed_evo(0, a=3, b=1))
Quantum object: dims=[[2], [2]], shape=(2, 2), type='oper', isherm=True
Qobj data =
[[0. 3.]
 [3. 0.] ]]
```



## Coefficients

To build time dependent quantum system we often use a list of *Qobj* and Coefficient. These Coefficient represent the strength of the corresponding quantum object a function that of time. Up to now, we used functions for these, but QuTiP support multiple formats: callable, strings, array.

**Function coefficients** : Use a callable with the signature `f(t: double, ...) -> double` as coefficient. Any function or method that can be called by `f(t, args)`, `f(t, **args)` is accepted.

```
def coeff(t, A, sigma):
    return A * np.exp(-(t / sigma)**2)

H = QobjEvo([H0, [H1, coeff]], args=args)
```

**String coefficients** : Use a string containing a simple Python expression. The variable `t`, common mathematical functions such as `sin` or `exp` an variable in `args` will be available. If available, the string will be compiled using cython, fixing variable type when possible, allowing slightly faster execution than function. While the speed up is usually very small, in long evolution, numerous calls to the functions are made and it's can accumulate. From version 5, compilation of the coefficient is done only once and saved between sessions. When either the cython or filelock modules are not available, the code will be executed in python using `exec` with the same environment . This, however, as no advantage over using python function.

```
coeff = "A * exp(-(t / sigma)**2)"

H = QobjEvo([H0, [H1, coeff]], args=args)
```

**Here is a list of defined variables:**

`sin`, `cos`, `tan`, `asin`, `acos`, `atan`, `pi`, `sinh`, `cosh`, `tanh`, `asinh`, `acosh`, `atanh`, `exp`, `log`, `log10`, `erf`, `zerf`, `sqrt`, `real`, `imag`, `conj`, `abs`, `norm`, `arg`, `proj`, `np` (numpy), `spe` (scipy.special) and `cython_special` (scipy cython interface).

**Array coefficients** : Use the spline interpolation of an array. Useful when the coefficient is hard to define as a function or obtained from experimental data. The times at which the array are defined must be passed as `tlist`:

```
times = np.linspace(-sigma*5, sigma*5, 500)
coeff = A * exp(-(times / sigma)**2)

H = QobjEvo([H0, [H1, coeff]], tlist=times)
```

Per default, a cubic spline interpolation is used, but the order of the interpolation can be controlled with the `order` input: Outside the interpolation range, the first or last value are used.

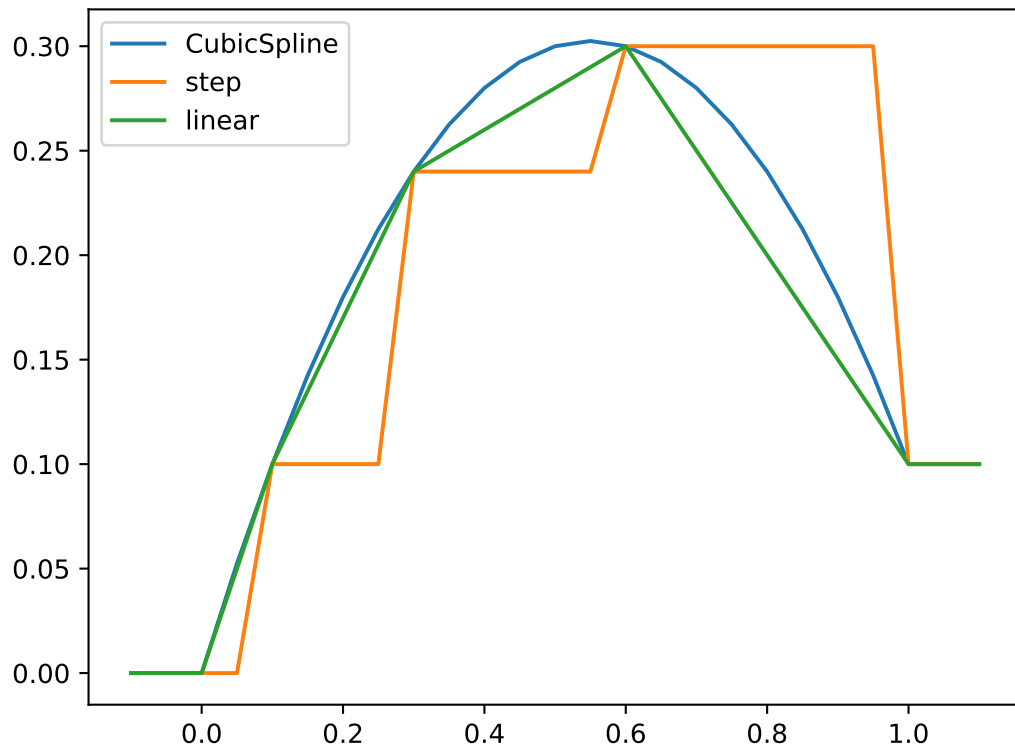
```
times = np.array([0, 0.1, 0.3, 0.6, 1.0])
coeff = times * (1.1 - times)
tlist = np.linspace(-0.1, 1.1, 25)

H = QobjEvo([qeye(1), coeff], tlist=times)
plt.plot(tlist, [H(t).norm() for t in tlist], label="CubicSpline")

H = QobjEvo([qeye(1), coeff], tlist=times, order=0)
plt.plot(tlist, [H(t).norm() for t in tlist], label="step")

H = QobjEvo([qeye(1), coeff], tlist=times, order=1)
plt.plot(tlist, [H(t).norm() for t in tlist], label="linear")

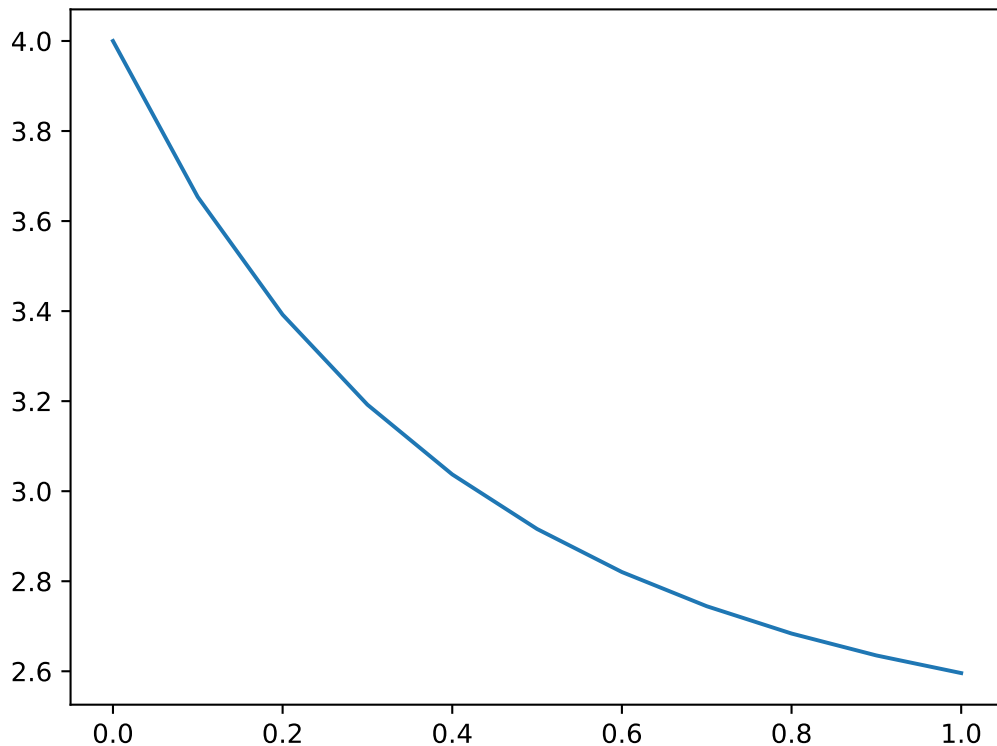
plt.legend()
```



When using array coefficients in solver, if the time dependent quantum system is in list format, the solver tlist is used as times of the array. This is often not ideal as the interpolation is usually less precise close the extremities of the range. It is therefore better to create the QobjEvo using an extended range prior to the solver:

```
N = 5
times = np.linspace(-0.1, 1.1, 13)
coeff = np.exp(-times)

c_ops = [QobjEvo([destroy(N), coeff], tlist=times)]
tlist = np.linspace(0, 1, 11)
data = mesolve(qeye(N), basis(N, N-1), tlist, c_ops=c_ops, e_ops=[num(N)]).expect[0]
plt.plot(tlist, data)
```



Different coefficient types can be mixed in a *QobjEvo*.

Given the multiple choices of input style, the first question that arises is which option to choose? In short, the function based method (first option) is the most general, allowing for essentially arbitrary coefficients expressed via user defined functions. However, by automatically compiling your system into C++ code, the second option (string based) tends to be more efficient and run faster. Of course, for small system sizes and evolution times, the difference will be minor. Lastly the spline method is usually as fast the string method, but it cannot be modified once created.

### Working with pulses

Special care is needed when working with pulses. ODE solvers select the step length automatically and can miss thin pulses when not properly warned. Integrations methods with variable step sizes have the `max_step` option that control the maximum length of a single internal integration step. This value should be set to under half the pulse width to be certain they are not missed.

For example, the following pulse is missed without fixing the maximum step length.

```
def pulse(t):
    return 10 * np.pi * (0.7 < t < 0.75)

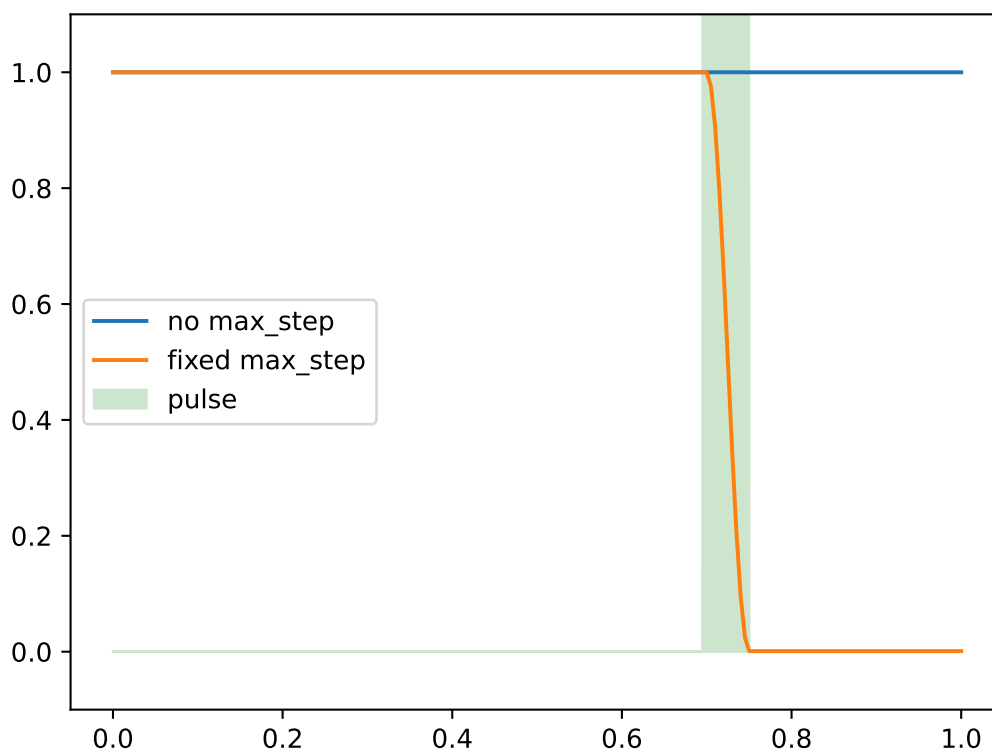
tlist = np.linspace(0, 1, 201)
H = [sigmaz(), [sigmax(), pulse]]
psi0 = basis(2,1)

data1 = sesolve(H, psi0, tlist, e_ops=num(2)).expect[0]
data2 = sesolve(H, psi0, tlist, e_ops=num(2), options={"max_step": 0.01}).expect[0]
```

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```
plt.plot(tlist, data1, label="no max_step")
plt.plot(tlist, data2, label="fixed max_step")
plt.fill_between(tlist, [pulse(t) for t in tlist], color="g", alpha=0.2, label="pulse
↪")
plt.ylim([-0.1, 1.1])
plt.legend(loc="center left")
```



### 3.6.8 Solver Class Interface

In QuTiP version 5 and later, solvers such as [mesolve](#), [mcsolve](#) also have a class interface. The class interface allows reusing the Hamiltonian and fine tuning many details of how the solver is run.

Examples of some of the solver class features are given below.

#### Reusing Hamiltonian Data

There are many cases where one would like to study multiple evolutions of the same quantum system, whether by changing the initial state or other parameters. In order to evolve a given system as fast as possible, the solvers in QuTiP take the given input operators (Hamiltonian, collapse operators, etc) and prepare them for use with the selected ODE solver.

These operations are usually reasonably fast, but for some solvers, such as [brmesolve](#) or [fmmesolve](#), the overhead can be significant. Even for simpler solvers, the time spent organizing data can become appreciable when repeatedly solving a system.

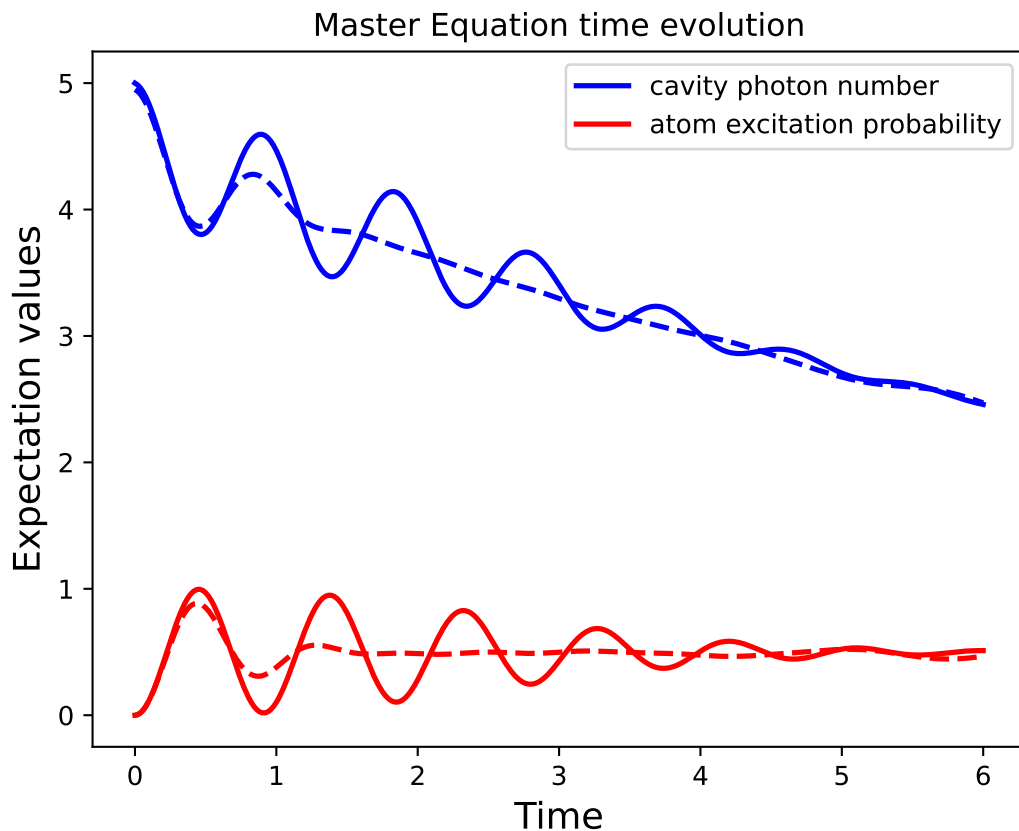
The class interface allows us to setup the system once and reuse it with various parameters. Most `...solve` function have a paired `...Solver` class, with a `...Solver.run` method to run the evolution. At class instance

creation, the physics (`H`, `c_ops`, `a_ops`, etc.) and options are passed. The initial state, times and expectation operators are only passed when calling `run`:

```
times = np.linspace(0.0, 6.0, 601)
a = tensor(qeye(2), destroy(10))
sm = tensor(destroy(2), qeye(10))
e_ops = [a.dag() * a, sm.dag() * sm]
H = QobjEvo(
    [a.dag()*a + sm.dag()*sm, [(sm*a.dag() + sm.dag()*a), lambda t, A: A]],
    args={"A": 0.5*np.pi}
)

solver = MESolver(H, c_ops=[np.sqrt(0.1) * a], options={"atol": 1e-8})
solver.options["normalize_output"] = True
psi0 = tensor(fock(2, 0), fock(10, 5))
data1 = solver.run(psi0, times, e_ops=e_ops)
psi1 = tensor(fock(2, 0), coherent(10, 2 - 1j))
data2 = solver.run(psi1, times, e_ops=e_ops)

plt.figure()
plt.plot(times, data1.expect[0], "b", times, data1.expect[1], "r", lw=2)
plt.plot(times, data2.expect[0], 'b--', times, data2.expect[1], 'r--', lw=2)
plt.title('Master Equation time evolution')
plt.xlabel('Time', fontsize=14)
plt.ylabel('Expectation values', fontsize=14)
plt.legend(("cavity photon number", "atom excitation probability"))
plt.show()
```

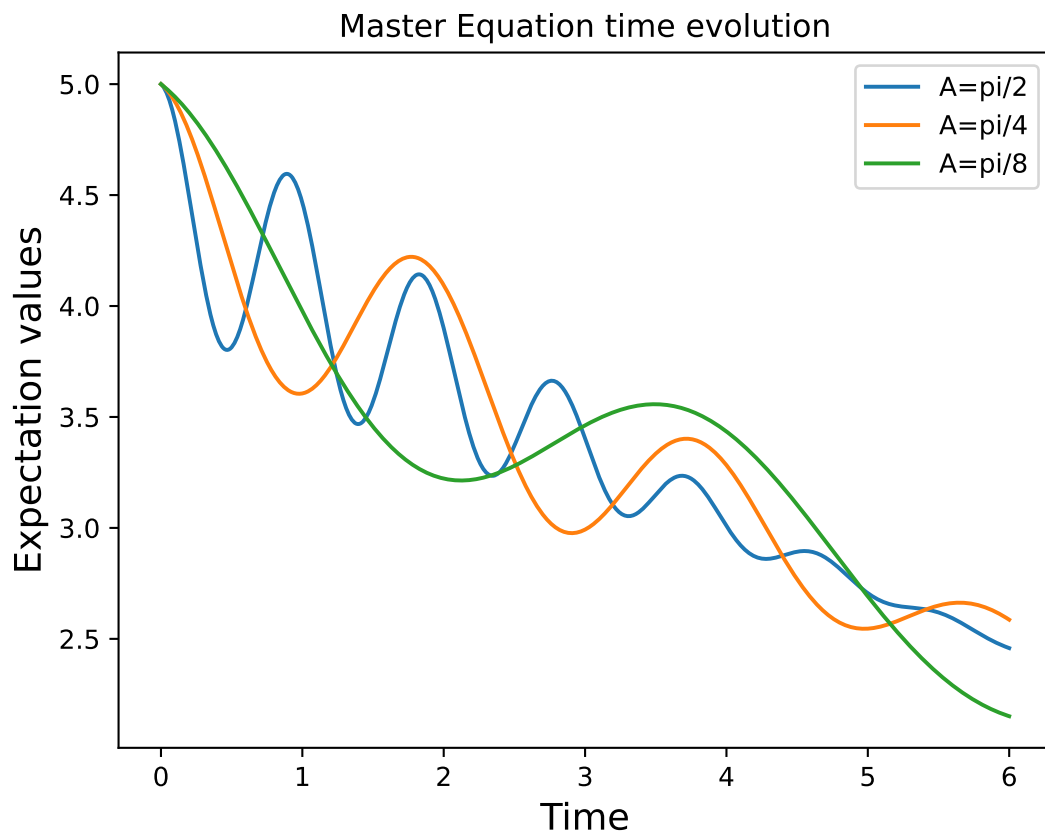


Note that as shown, options can be set at initialization or with the `options` property.

The simulation parameters, the args of the `QobjEvo` passed as system operators, can be updated at the start of a run:

```
data1 = solver.run(psi0, times, e_ops=e_ops)
data2 = solver.run(psi0, times, e_ops=e_ops, args={"A": 0.25*np.pi})
data3 = solver.run(psi0, times, e_ops=e_ops, args={"A": 0.125*np.pi})

plt.figure()
plt.plot(times, data1.expect[0], label="A=pi/2")
plt.plot(times, data2.expect[0], label="A=pi/4")
plt.plot(times, data3.expect[0], label="A=pi/8")
plt.title('Master Equation time evolution')
plt.xlabel('Time', fontsize=14)
plt.ylabel('Expectation values', fontsize=14)
plt.legend()
plt.show()
```

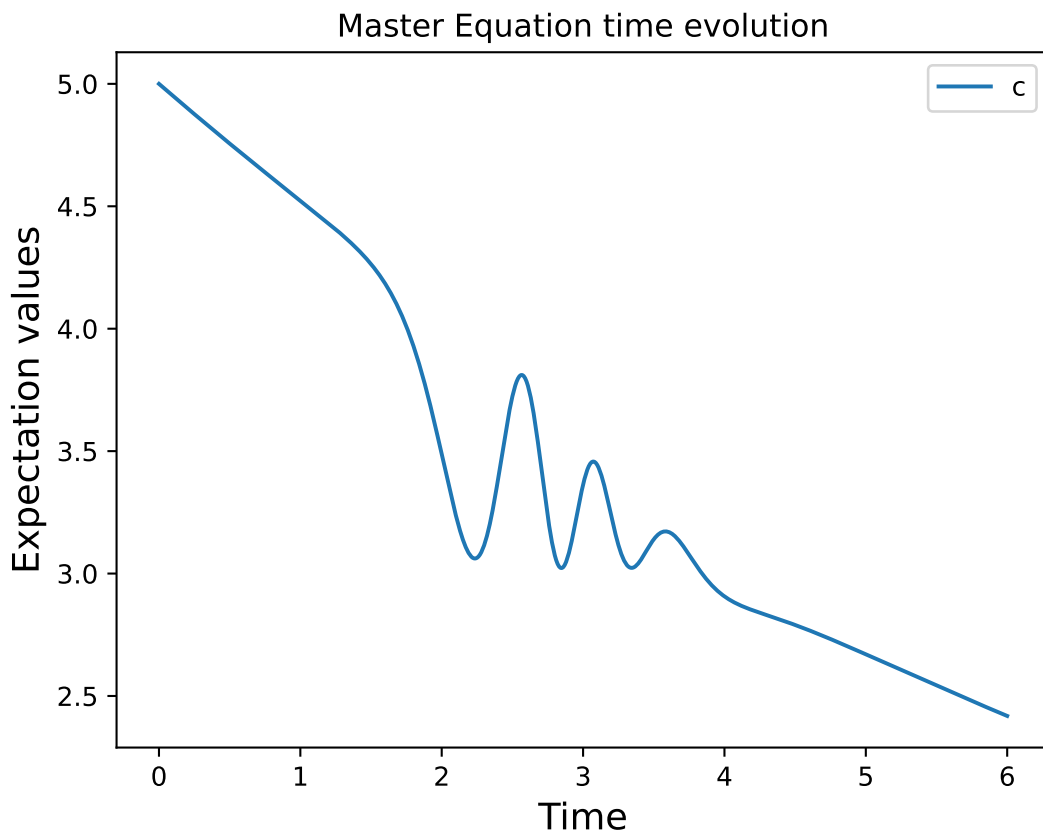


## Stepping through the run

The solver class also allows to run through a simulation one step at a time, updating args at each step:

```
data = [5.]
solver.start(state0=psi0, t0=times[0])
for t in times[1:]:
    psi_t = solver.step(t, args={"A": np.pi*np.exp(-(t-3)**2)})
    data.append(expect(e_ops[0], psi_t))

plt.figure()
plt.plot(times, data)
plt.title('Master Equation time evolution')
plt.xlabel('Time', fontsize=14)
plt.ylabel('Expectation values', fontsize=14)
plt.legend(("cavity photon number"))
plt.show()
```



**Note:** This is an example only, updating a constant args parameter between step should not replace using a function as QobjEvo's coefficient.

**Note:** It is possible to create multiple solvers and to advance them using step in parallel. However, many ODE solver, including the default adams method, only allow one instance at a time per process. QuTiP supports using multiple solver instances of these ODE solvers but with a performance cost. In these situations, using dop853 or vern9 integration method is recommended instead.

## Feedback: Accessing the solver state from evolution operators

The state of the system during the evolution is accessible via properties of the solver classes.

Each solver has a `StateFeedback` and `ExpectFeedback` class method that can be passed as arguments to time dependent systems. For example, `ExpectFeedback` can be used to create a system which uncouples when there are 5 or fewer photons in the cavity.

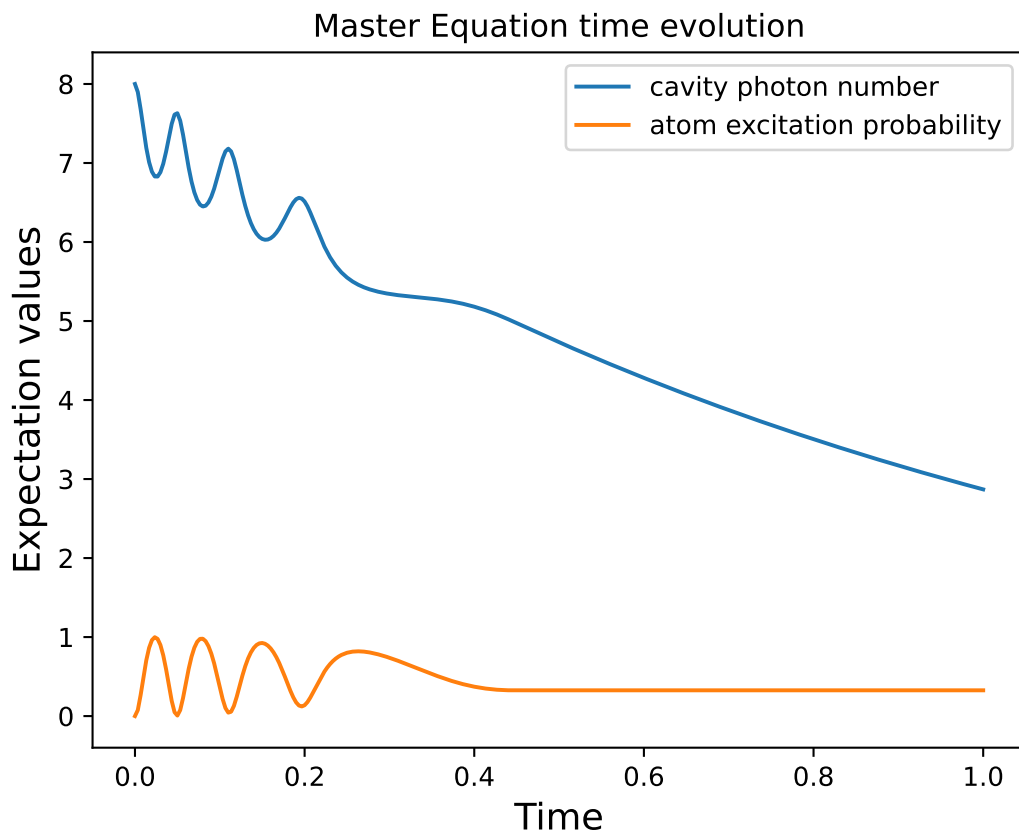
```
def f(t, e1):
    ex = (e1.real - 5)
    return (ex > 0) * ex * 10

times = np.linspace(0.0, 1.0, 301)
a = tensor(qeye(2), destroy(10))
sm = tensor(destroy(2), qeye(10))
e_ops = [a.dag() * a, sm.dag() * sm]
psi0 = tensor(fock(2, 0), fock(10, 8))
e_ops = [a.dag() * a, sm.dag() * sm]

H = [a*a.dag(), [sm*a.dag() + sm.dag()*a, f]]
data = mesolve(H, psi0, times, c_ops=[a], e_ops=e_ops,
               args={"e1": MESolver.ExpectFeedback(a.dag() * a)}
               ).expect

plt.figure()
plt.plot(times, data[0])
plt.plot(times, data[1])
plt.title('Master Equation time evolution')
plt.xlabel('Time', fontsize=14)
plt.ylabel('Expectation values', fontsize=14)
plt.legend(("cavity photon number", "atom excitation probability"))
plt.show()
```





### 3.6.9 Bloch-Redfield master equation

#### Introduction

The Lindblad master equation introduced earlier is constructed so that it describes a physical evolution of the density matrix (i.e., trace and positivity preserving), but it does not provide a connection to any underlying microscopic physical model. The Lindblad operators (collapse operators) describe phenomenological processes, such as for example dephasing and spin flips, and the rates of these processes are arbitrary parameters in the model. In many situations the collapse operators and their corresponding rates have clear physical interpretation, such as dephasing and relaxation rates, and in those cases the Lindblad master equation is usually the method of choice.

However, in some cases, for example systems with varying energy biases and eigenstates and that couple to an environment in some well-defined manner (through a physically motivated system-environment interaction operator), it is often desirable to derive the master equation from more fundamental physical principles, and relate it to for example the noise-power spectrum of the environment.

The Bloch-Redfield formalism is one such approach to derive a master equation from a microscopic system. It starts from a combined system-environment perspective, and derives a perturbative master equation for the system alone, under the assumption of weak system-environment coupling. One advantage of this approach is that the dissipation processes and rates are obtained directly from the properties of the environment. On the downside, it does not intrinsically guarantee that the resulting master equation unconditionally preserves the physical properties of the density matrix (because it is a perturbative method). The Bloch-Redfield master equation must therefore be used with care, and the assumptions made in the derivation must be honored. (The Lindblad master equation is in a sense more robust – it always results in a physical density matrix – although some collapse operators might not be physically justified). For a full derivation of the Bloch Redfield master equation, see e.g. [Coh92] or [Bre02]. Here we present only a brief version of the derivation, with the intention of introducing the notation and how it relates to the implementation in QuTiP.

## Brief Derivation and Definitions

The starting point of the Bloch-Redfield formalism is the total Hamiltonian for the system and the environment (bath):  $H = H_S + H_B + H_I$ , where  $H$  is the total system+bath Hamiltonian,  $H_S$  and  $H_B$  are the system and bath Hamiltonians, respectively, and  $H_I$  is the interaction Hamiltonian.

The most general form of a master equation for the system dynamics is obtained by tracing out the bath from the von-Neumann equation of motion for the combined system ( $\dot{\rho} = -i\hbar^{-1}[H, \rho]$ ). In the interaction picture the result is

$$\frac{d}{dt}\rho_S(t) = -\hbar^{-2} \int_0^t d\tau \text{Tr}_B[H_I(t), [H_I(\tau), \rho_S(\tau) \otimes \rho_B]], \quad (3.22)$$

where the additional assumption that the total system-bath density matrix can be factorized as  $\rho(t) \approx \rho_S(t) \otimes \rho_B$ . This assumption is known as the Born approximation, and it implies that there never is any entanglement between the system and the bath, neither in the initial state nor at any time during the evolution. *It is justified for weak system-bath interaction.*

The master equation (3.22) is non-Markovian, i.e., the change in the density matrix at a time  $t$  depends on states at all times  $\tau < t$ , making it intractable to solve both theoretically and numerically. To make progress towards a manageable master equation, we now introduce the Markovian approximation, in which  $\rho_S(\tau)$  is replaced by  $\rho_S(t)$  in Eq. (3.22). The result is the Redfield equation

$$\frac{d}{dt}\rho_S(t) = -\hbar^{-2} \int_0^t d\tau \text{Tr}_B[H_I(t), [H_I(\tau), \rho_S(t) \otimes \rho_B]], \quad (3.23)$$

which is local in time with respect the density matrix, but still not Markovian since it contains an implicit dependence on the initial state. By extending the integration to infinity and substituting  $\tau \rightarrow t - \tau$ , a fully Markovian master equation is obtained:

$$\frac{d}{dt}\rho_S(t) = -\hbar^{-2} \int_0^\infty d\tau \text{Tr}_B[H_I(t), [H_I(t - \tau), \rho_S(t) \otimes \rho_B]]. \quad (3.24)$$

The two Markovian approximations introduced above are valid if the time-scale with which the system dynamics changes is large compared to the time-scale with which correlations in the bath decays (corresponding to a “short-memory” bath, which results in Markovian system dynamics).

The master equation (3.24) is still on a too general form to be suitable for numerical implementation. We therefore assume that the system-bath interaction takes the form  $H_I = \sum_\alpha A_\alpha \otimes B_\alpha$  and where  $A_\alpha$  are system operators and  $B_\alpha$  are bath operators. This allows us to write master equation in terms of system operators and bath correlation functions:

$$\begin{aligned} \frac{d}{dt}\rho_S(t) = -\hbar^{-2} \sum_{\alpha\beta} \int_0^\infty d\tau \{ & g_{\alpha\beta}(\tau) [A_\alpha(t)A_\beta(t-\tau)\rho_S(t) - A_\alpha(t-\tau)\rho_S(t)A_\beta(t)] \\ & g_{\alpha\beta}(-\tau) [\rho_S(t)A_\alpha(t-\tau)A_\beta(t) - A_\alpha(t)\rho_S(t)A_\beta(t-\tau)] \}, \end{aligned}$$

where  $g_{\alpha\beta}(\tau) = \text{Tr}_B [B_\alpha(t)B_\beta(t-\tau)\rho_B] = \langle B_\alpha(\tau)B_\beta(0) \rangle$ , since the bath state  $\rho_B$  is a steady state.

In the eigenbasis of the system Hamiltonian, where  $A_{mn}(t) = A_{mn}e^{i\omega_{mn}t}$ ,  $\omega_{mn} = \omega_m - \omega_n$  and  $\omega_m$  are the eigenfrequencies corresponding the eigenstate  $|m\rangle$ , we obtain in matrix form in the Schrödinger picture

$$\begin{aligned} \frac{d}{dt}\rho_{ab}(t) = & -i\omega_{ab}\rho_{ab}(t) \\ & -\hbar^{-2} \sum_{\alpha,\beta} \sum_{c,d}^{\text{sec}} \int_0^\infty d\tau \left\{ g_{\alpha\beta}(\tau) \left[ \delta_{bd} \sum_n A_{an}^\alpha A_{nc}^\beta e^{i\omega_{cn}\tau} - A_{ac}^\alpha A_{db}^\beta e^{i\omega_{ca}\tau} \right] \right. \\ & \left. + g_{\alpha\beta}(-\tau) \left[ \delta_{ac} \sum_n A_{dn}^\alpha A_{nb}^\beta e^{i\omega_{nd}\tau} - A_{ac}^\alpha A_{db}^\beta e^{i\omega_{bd}\tau} \right] \right\} \rho_{cd}(t), \end{aligned}$$

where the “sec” above the summation symbol indicate summation of the secular terms which satisfy  $|\omega_{ab} - \omega_{cd}| \ll \tau_{\text{decay}}$ . This is an almost-useful form of the master equation. The final step before arriving at the form of the Bloch-Redfield master equation that is implemented in QuTiP, involves rewriting the bath correlation function  $g(\tau)$  in

terms of the noise-power spectrum of the environment  $S(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} g(\tau)$ :

$$\int_0^{\infty} d\tau g_{\alpha\beta}(\tau) e^{i\omega\tau} = \frac{1}{2} S_{\alpha\beta}(\omega) + i\lambda_{\alpha\beta}(\omega), \quad (3.25)$$

where  $\lambda_{ab}(\omega)$  is an energy shift that is neglected here. The final form of the Bloch-Redfield master equation is

$$\frac{d}{dt} \rho_{ab}(t) = -i\omega_{ab} \rho_{ab}(t) + \sum_{c,d}^{\text{sec}} R_{abcd} \rho_{cd}(t), \quad (3.26)$$

where

$$R_{abcd} = -\frac{\hbar^{-2}}{2} \sum_{\alpha,\beta} \left\{ \delta_{bd} \sum_n A_{an}^{\alpha} A_{nc}^{\beta} S_{\alpha\beta}(\omega_{cn}) - A_{ac}^{\alpha} A_{db}^{\beta} S_{\alpha\beta}(\omega_{ca}) \right. \\ \left. + \delta_{ac} \sum_n A_{dn}^{\alpha} A_{nb}^{\beta} S_{\alpha\beta}(\omega_{dn}) - A_{ac}^{\alpha} A_{db}^{\beta} S_{\alpha\beta}(\omega_{db}) \right\},$$

is the Bloch-Redfield tensor.

The Bloch-Redfield master equation in the form Eq. (3.26) is suitable for numerical implementation. The input parameters are the system Hamiltonian  $H$ , the system operators through which the environment couples to the system  $A_{\alpha}$ , and the noise-power spectrum  $S_{\alpha\beta}(\omega)$  associated with each system-environment interaction term.

To simplify the numerical implementation we assume that  $A_{\alpha}$  are Hermitian and that cross-correlations between different environment operators vanish, so that the final expression for the Bloch-Redfield tensor that is implemented in QuTiP is

$$R_{abcd} = -\frac{\hbar^{-2}}{2} \sum_{\alpha} \left\{ \delta_{bd} \sum_n A_{an}^{\alpha} A_{nc}^{\alpha} S_{\alpha}(\omega_{cn}) - A_{ac}^{\alpha} A_{db}^{\alpha} S_{\alpha}(\omega_{ca}) \right. \\ \left. + \delta_{ac} \sum_n A_{dn}^{\alpha} A_{nb}^{\alpha} S_{\alpha}(\omega_{dn}) - A_{ac}^{\alpha} A_{db}^{\alpha} S_{\alpha}(\omega_{db}) \right\}.$$

### Bloch-Redfield master equation in QuTiP

In QuTiP, the Bloch-Redfield tensor Eq. (3.27) can be calculated using the function `bloch_redfield_tensor`. It takes two mandatory arguments: The system Hamiltonian  $H$ , a nested list of operator  $A_{\alpha}$ , spectral density functions  $S_{\alpha}(\omega)$  pairs that characterize the coupling between system and bath. The spectral density functions are Python callback functions that takes the (angular) frequency as a single argument.

To illustrate how to calculate the Bloch-Redfield tensor, let's consider a two-level atom

$$H = -\frac{1}{2} \Delta \sigma_x - \frac{1}{2} \epsilon_0 \sigma_z \quad (3.27)$$

```
delta = 0.2 * 2*np.pi
eps0 = 1.0 * 2*np.pi
gamma1 = 0.5

H = - delta/2.0 * sigmax() - eps0/2.0 * sigmaz()

def ohmic_spectrum(w):
    if w == 0.0: # dephasing inducing noise
        return gamma1
    else: # relaxation inducing noise
        return gamma1 / 2 * (w / (2 * np.pi)) * (w > 0.0)
```

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```
R, ekets = bloch_redfield_tensor(H, a_ops=[[sigmax(), ohmic_spectrum]])
print(R)
```

Output:

```
Quantum object: dims = [[[2], [2]], [[2], [2]]], shape = (4, 4), type = super, isherm_
↪ = False
Qobj data =
[[ 0.          +0.j          0.          +0.j          0.          +0.j
  0.24514517+0.j          ]
 [ 0.          +0.j         -0.16103412-6.4076169j  0.          +0.j
  0.          +0.j          ]
 [ 0.          +0.j          0.          +0.j         -0.16103412+6.4076169j
  0.          +0.j          ]
 [ 0.          +0.j          0.          +0.j          0.          +0.j
 -0.24514517+0.j          ]]
```

Note that it is also possible to add Lindblad dissipation superoperators in the Bloch-Redfield tensor by passing the operators via the `c_ops` keyword argument like you would in the `mesolve` or `mcsolve` functions. For convenience, the function `bloch_redfield_tensor` also returns the basis transformation operator, the eigen vector matrix, since they are calculated in the process of calculating the Bloch-Redfield tensor  $R$ , and the `ekets` are usually needed again later when transforming operators between the laboratory basis and the eigen basis. The tensor can be obtained in the laboratory basis by setting `fock_basis=True`, in that case, the transformation operator is not returned.

The evolution of a wavefunction or density matrix, according to the Bloch-Redfield master equation (3.26), can be calculated using the QuTiP function `mesolve` using Bloch-Redfield tensor in the laboratory basis instead of a liouvillian. For example, to evaluate the expectation values of the  $\sigma_x$ ,  $\sigma_y$ , and  $\sigma_z$  operators for the example above, we can use the following code:

```
delta = 0.2 * 2*np.pi
eps0 = 1.0 * 2*np.pi
gamma1 = 0.5

H = - delta/2.0 * sigmax() - eps0/2.0 * sigmaz()

def ohmic_spectrum(w):
    if w == 0.0: # dephasing inducing noise
        return gamma1
    else: # relaxation inducing noise
        return gamma1 / 2 * (w / (2 * np.pi)) * (w > 0.0)

R = bloch_redfield_tensor(H, [[sigmax(), ohmic_spectrum]], fock_basis=True)

tlist = np.linspace(0, 15.0, 1000)

psi0 = rand_ket(2, seed=1)

e_ops = [sigmax(), sigmay(), sigmaz()]

expt_list = mesolve(R, psi0, tlist, e_ops=e_ops).expect

sphere = Bloch()

sphere.add_points([expt_list[0], expt_list[1], expt_list[2]])
```

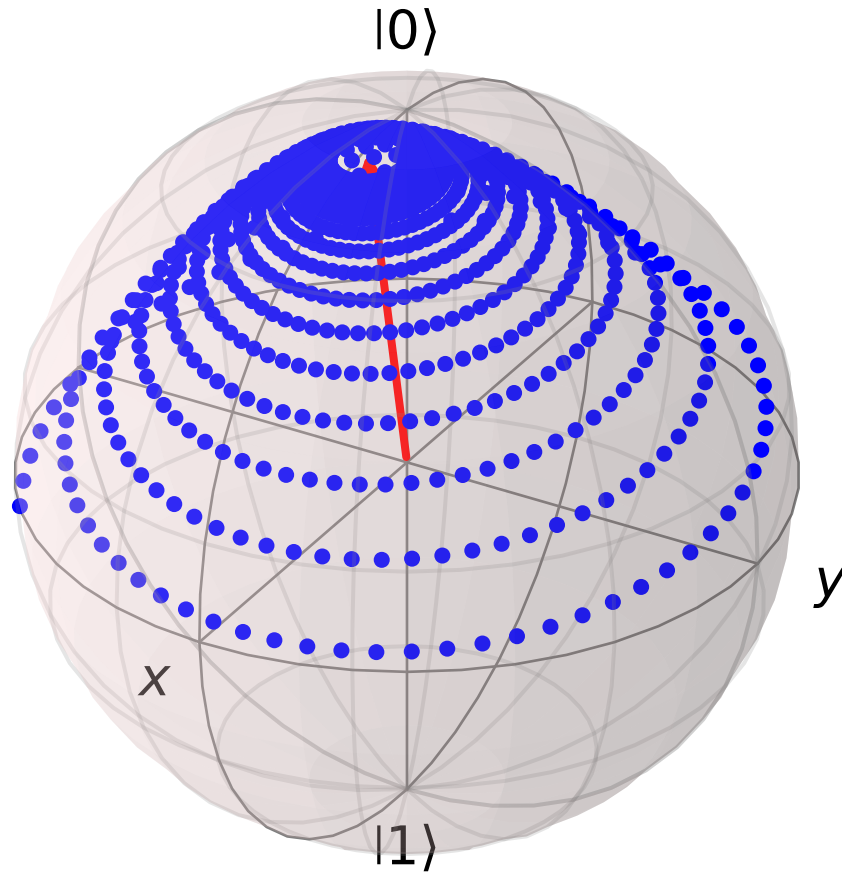
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```
sphere.vector_color = ['r']

sphere.add_vectors(np.array([delta, 0, eps0]) / np.sqrt(delta ** 2 + eps0 ** 2))

sphere.make_sphere()
```



The two steps of calculating the Bloch-Redfield tensor and evolving according to the corresponding master equation can be combined into one by using the function `brmesolve`, which takes same arguments as `mesolve` and `mcsolve`, save for the additional nested list of operator-spectrum pairs that is called `a_ops`.

```
output = brmesolve(H, psi0, tlist, a_ops=[[sigmax(), ohmic_spectrum]], e_ops=e_ops)
```

where the resulting `output` is an instance of the class `Result`.

**Note:** While the code example simulates the Bloch-Redfield equation in the secular approximation, QuTiP's implementation allows the user to simulate the non-secular version of the Bloch-Redfield equation by setting `sec_cutoff=-1`, as well as do a partial secular approximation by setting it to a float, this float will become the cutoff for the sum in (3.26) meaning terms with  $|\omega_{ab} - \omega_{cd}|$  greater than the cutoff will be neglected. Its default value is 0.1 which corresponds to the secular approximation. For example the command

```
output = brmesolve(H, psi0, tlist, a_ops=[[sigmax(), ohmic_spectrum]],
                  e_ops=e_ops, sec_cutoff=-1)
```

will simulate the same example as above without the secular approximation. Note that using the non-secular version

may lead to negativity issues.

---

## Time-dependent Bloch-Redfield Dynamics

If you have not done so already, please read the section: *Solving Problems with Time-dependent Hamiltonians*.

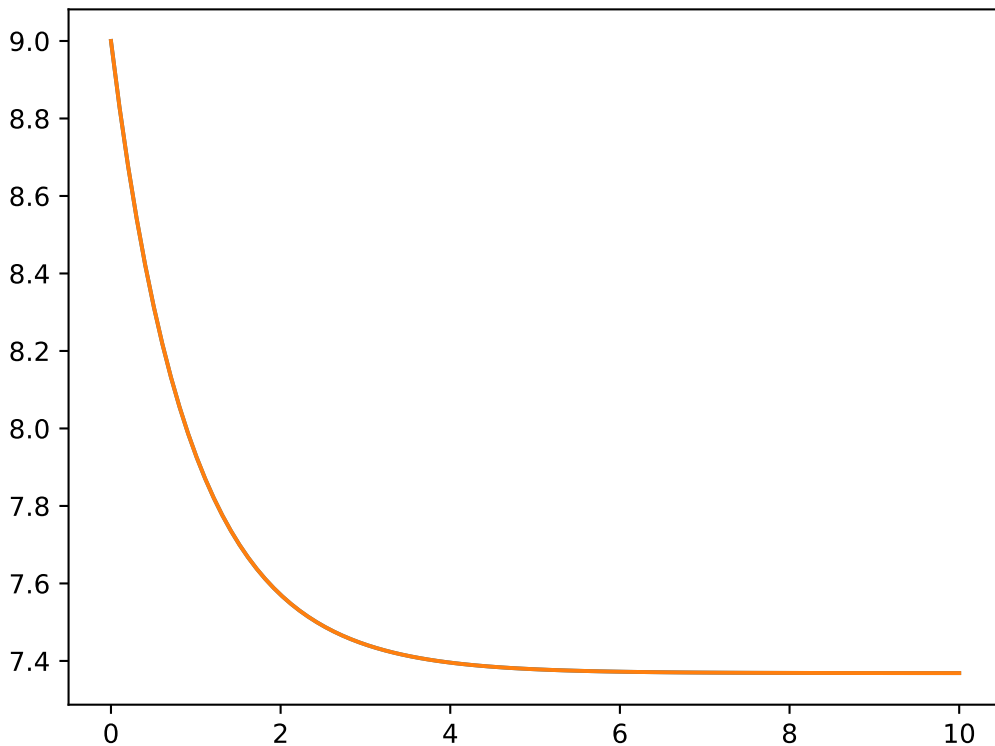
As we have already discussed, the Bloch-Redfield master equation requires transforming into the eigenbasis of the system Hamiltonian. For time-independent systems, this transformation need only be done once. However, for time-dependent systems, one must move to the instantaneous eigenbasis at each time-step in the evolution, thus greatly increasing the computational complexity of the dynamics. In addition, the requirement for computing all the eigenvalues severely limits the scalability of the method. Fortunately, this eigen decomposition occurs at the Hamiltonian level, as opposed to the super-operator level, and thus, with efficient programming, one can tackle many systems that are commonly encountered.

For time-dependent Hamiltonians, the Hamiltonian itself can be passed into the solver like any other time dependent Hamiltonian, as thus we will not discuss this topic further. Instead, here the focus is on time-dependent bath coupling terms. To this end, suppose that we have a dissipative harmonic oscillator, where the white-noise dissipation rate decreases exponentially with time  $\kappa(t) = \kappa(0) \exp(-t)$ . In the Lindblad or Monte Carlo solvers, this could be implemented as a time-dependent collapse operator list `c_ops = [[a, 'sqrt(kappa*exp(-t))']]`. In the Bloch-Redfield solver, the bath coupling terms must be Hermitian. As such, in this example, our coupling operator is the position operator `a+a.dag()`. The complete example, and comparison to the analytic expression is:

```
N = 10 # number of basis states to consider
a = destroy(N)
H = a.dag() * a
psi0 = basis(N, 9) # initial state
kappa = 0.2 # coupling to oscillator
a_ops = [
    ([a+a.dag(), f'sqrt({kappa}*exp(-t))'], '(w>=0)')
]
tlist = np.linspace(0, 10, 100)

out = brmesolve(H, psi0, tlist, a_ops, e_ops=[a.dag() * a])
actual_answer = 9.0 * np.exp(-kappa * (1.0 - np.exp(-tlist)))

plt.figure()
plt.plot(tlist, out.expect[0])
plt.plot(tlist, actual_answer)
plt.show()
```



In many cases, the bath-coupling operators can take the form  $A = f(t)a + f(t)^*a^\dagger$ . The operator parts of the  $a\_ops$  can be made of as many time-dependent terms as needed to construct such operator. For example consider a white-noise bath that is coupled to an operator of the form  $\exp(1j*t)*a + \exp(-1j*t)*a.dag()$ . In this example, the  $a\_ops$  list would be:

```
a_ops = [
    ([[a, 'exp(1j*t)'], [a.dag(), 'exp(-1j*t)']], f'{kappa} * (w >= 0)')
]
```

where the first tuple element  $[[a, 'exp(1j*t)'], [a.dag(), 'exp(-1j*t)']]$  tells the solver what is the time-dependent Hermitian coupling operator. The second tuple  $f'\{kappa\} * (w >= 0)'$ , gives the noise power spectrum. A full example is:

```
N = 10
w0 = 1.0 * 2 * np.pi
g = 0.05 * w0
kappa = 0.15
times = np.linspace(0, 25, 1000)

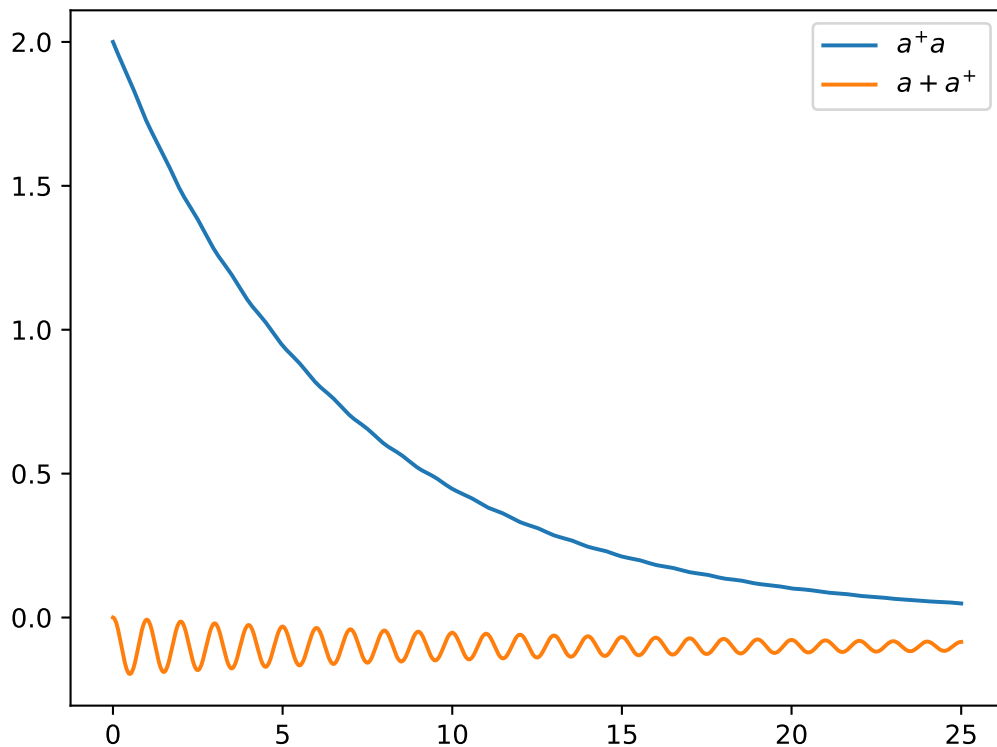
a = destroy(N)
H = w0 * a.dag() * a + g * (a + a.dag())
psi0 = ket2dm((basis(N, 4) + basis(N, 2) + basis(N, 0)).unit())
a_ops = [[
    QobjEvo([[a, 'exp(1j*t)'], [a.dag(), 'exp(-1j*t)']], (f'{kappa} * (w >= 0)')
]]
e_ops = [a.dag() * a, a + a.dag()]

res_brme = brmesolve(H, psi0, times, a_ops, e_ops)
```

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```
plt.figure()
plt.plot(times, res_brme.expect[0], label=r'$a^{\dagger}a$')
plt.plot(times, res_brme.expect[1], label=r'$a+a^{\dagger}$')
plt.legend()
plt.show()
```



Further examples on time-dependent Bloch-Redfield simulations can be found in the online tutorials.

### 3.6.10 Floquet Formalism

#### Introduction

Many time-dependent problems of interest are periodic. The dynamics of such systems can be solved for directly by numerical integration of the Schrödinger or Master equation, using the time-dependent Hamiltonian. But they can also be transformed into time-independent problems using the Floquet formalism. Time-independent problems can be solve much more efficiently, so such a transformation is often very desirable.

In the standard derivations of the Lindblad and Bloch-Redfield master equations the Hamiltonian describing the system under consideration is assumed to be time independent. Thus, strictly speaking, the standard forms of these master equation formalisms should not blindly be applied to system with time-dependent Hamiltonians. However, in many relevant cases, in particular for weak driving, the standard master equations still turns out to be useful for many time-dependent problems. But a more rigorous approach would be to rederive the master equation taking the time-dependent nature of the Hamiltonian into account from the start. The Floquet-Markov Master equation is one such a formalism, with important applications for strongly driven systems (see e.g., [Gri98]).



Here we give an overview of how the Floquet and Floquet-Markov formalisms can be used for solving time-dependent problems in QuTiP. To introduce the terminology and naming conventions used in QuTiP we first give a brief summary of quantum Floquet theory.

### Floquet theory for unitary evolution

The Schrödinger equation with a time-dependent Hamiltonian  $H(t)$  is

$$H(t)\Psi(t) = i\hbar \frac{\partial}{\partial t} \Psi(t), \quad (3.28)$$

where  $\Psi(t)$  is the wave function solution. Here we are interested in problems with periodic time-dependence, i.e., the Hamiltonian satisfies  $H(t) = H(t + T)$  where  $T$  is the period. According to the Floquet theorem, there exist solutions to (3.28) of the form

$$\Psi_\alpha(t) = \exp(-i\epsilon_\alpha t/\hbar) \Phi_\alpha(t), \quad (3.29)$$

where  $\Psi_\alpha(t)$  are the *Floquet states* (i.e., the set of wave function solutions to the Schrödinger equation),  $\Phi_\alpha(t) = \Phi_\alpha(t + T)$  are the periodic *Floquet modes*, and  $\epsilon_\alpha$  are the *quasienergy levels*. The quasienergy levels are constants in time, but only uniquely defined up to multiples of  $2\pi/T$  (i.e., unique value in the interval  $[0, 2\pi/T]$ ).

If we know the Floquet modes (for  $t \in [0, T]$ ) and the quasienergies for a particular  $H(t)$ , we can easily decompose any initial wavefunction  $\Psi(t = 0)$  in the Floquet states and immediately obtain the solution for arbitrary  $t$

$$\Psi(t) = \sum_\alpha c_\alpha \Psi_\alpha(t) = \sum_\alpha c_\alpha \exp(-i\epsilon_\alpha t/\hbar) \Phi_\alpha(t), \quad (3.30)$$

where the coefficients  $c_\alpha$  are determined by the initial wavefunction  $\Psi(0) = \sum_\alpha c_\alpha \Psi_\alpha(0)$ .

This formalism is useful for finding  $\Psi(t)$  for a given  $H(t)$  only if we can obtain the Floquet modes  $\Phi_\alpha(t)$  and quasienergies  $\epsilon_\alpha$  more easily than directly solving (3.28). By substituting (3.29) into the Schrödinger equation (3.28) we obtain an eigenvalue equation for the Floquet modes and quasienergies

$$\mathcal{H}(t)\Phi_\alpha(t) = \epsilon_\alpha \Phi_\alpha(t), \quad (3.31)$$

where  $\mathcal{H}(t) = H(t) - i\hbar \partial_t$ . This eigenvalue problem could be solved analytically or numerically, but in QuTiP we use an alternative approach for numerically finding the Floquet states and quasienergies [see e.g. Creffield et al., Phys. Rev. B 67, 165301 (2003)]. Consider the propagator for the time-dependent Schrödinger equation (3.28), which by definition satisfies

$$U(T + t, t)\Psi(t) = \Psi(T + t).$$

Inserting the Floquet states from (3.29) into this expression results in

$$U(T + t, t) \exp(-i\epsilon_\alpha t/\hbar) \Phi_\alpha(t) = \exp(-i\epsilon_\alpha (T + t)/\hbar) \Phi_\alpha(T + t),$$

or, since  $\Phi_\alpha(T + t) = \Phi_\alpha(t)$ ,

$$U(T + t, t) \Phi_\alpha(t) = \exp(-i\epsilon_\alpha T/\hbar) \Phi_\alpha(t) = \eta_\alpha \Phi_\alpha(t),$$

which shows that the Floquet modes are eigenstates of the one-period propagator. We can therefore find the Floquet modes and quasienergies  $\epsilon_\alpha = -\hbar \arg(\eta_\alpha)/T$  by numerically calculating  $U(T + t, t)$  and diagonalizing it. In particular this method is useful to find  $\Phi_\alpha(0)$  by calculating and diagonalize  $U(T, 0)$ .

The Floquet modes at arbitrary time  $t$  can then be found by propagating  $\Phi_\alpha(0)$  to  $\Phi_\alpha(t)$  using the wave function propagator  $U(t, 0)\Psi_\alpha(0) = \Psi_\alpha(t)$ , which for the Floquet modes yields

$$U(t, 0)\Phi_\alpha(0) = \exp(-i\epsilon_\alpha t/\hbar) \Phi_\alpha(t),$$

so that  $\Phi_\alpha(t) = \exp(i\epsilon_\alpha t/\hbar) U(t, 0)\Phi_\alpha(0)$ . Since  $\Phi_\alpha(t)$  is periodic we only need to evaluate it for  $t \in [0, T]$ , and from  $\Phi_\alpha(t \in [0, T])$  we can directly evaluate  $\Phi_\alpha(t)$ ,  $\Psi_\alpha(t)$  and  $\Psi(t)$  for arbitrary large  $t$ .

## Floquet formalism in QuTiP

QuTiP provides a family of functions to calculate the Floquet modes and quasi energies, Floquet state decomposition, etc., given a time-dependent Hamiltonian.

Consider for example the case of a strongly driven two-level atom, described by the Hamiltonian

$$H(t) = -\frac{1}{2}\Delta\sigma_x - \frac{1}{2}\epsilon_0\sigma_z + \frac{1}{2}A\sin(\omega t)\sigma_z. \quad (3.32)$$

In QuTiP we can define this Hamiltonian as follows:

```
>>> delta = 0.2 * 2*np.pi
>>> eps0 = 1.0 * 2*np.pi
>>> A = 2.5 * 2*np.pi
>>> omega = 1.0 * 2*np.pi
>>> H0 = - delta/2.0 * sigmax() - eps0/2.0 * sigmaz()
>>> H1 = A/2.0 * sigmaz()
>>> args = {'w': omega}
>>> H = [H0, [H1, 'sin(w * t)']]
```

The  $t = 0$  Floquet modes corresponding to the Hamiltonian (3.32) can then be calculated using the *FloquetBasis* class, which encapsulates the Floquet modes and the quasienergies:

```
>>> T = 2*np.pi / omega
>>> floquet_basis = FloquetBasis(H, T, args)
>>> f_energies = floquet_basis.e_quasi
>>> f_energies
array([-2.83131212,  2.83131212])
>>> f_modes_0 = floquet_basis.mode(0)
>>> f_modes_0
[Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[ 0.72964231+0.j          ]
 [-0.39993746+0.554682j]],
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[0.39993746+0.554682j]
 [0.72964231+0.j          ]]]
```

For some problems interesting observations can be drawn from the quasienergy levels alone. Consider for example the quasienergies for the driven two-level system introduced above as a function of the driving amplitude, calculated and plotted in the following example. For certain driving amplitudes the quasienergy levels cross. Since the quasienergies can be associated with the time-scale of the long-term dynamics due to the driving, degenerate quasienergies indicate a “freezing” of the dynamics (sometimes known as coherent destruction of tunneling).

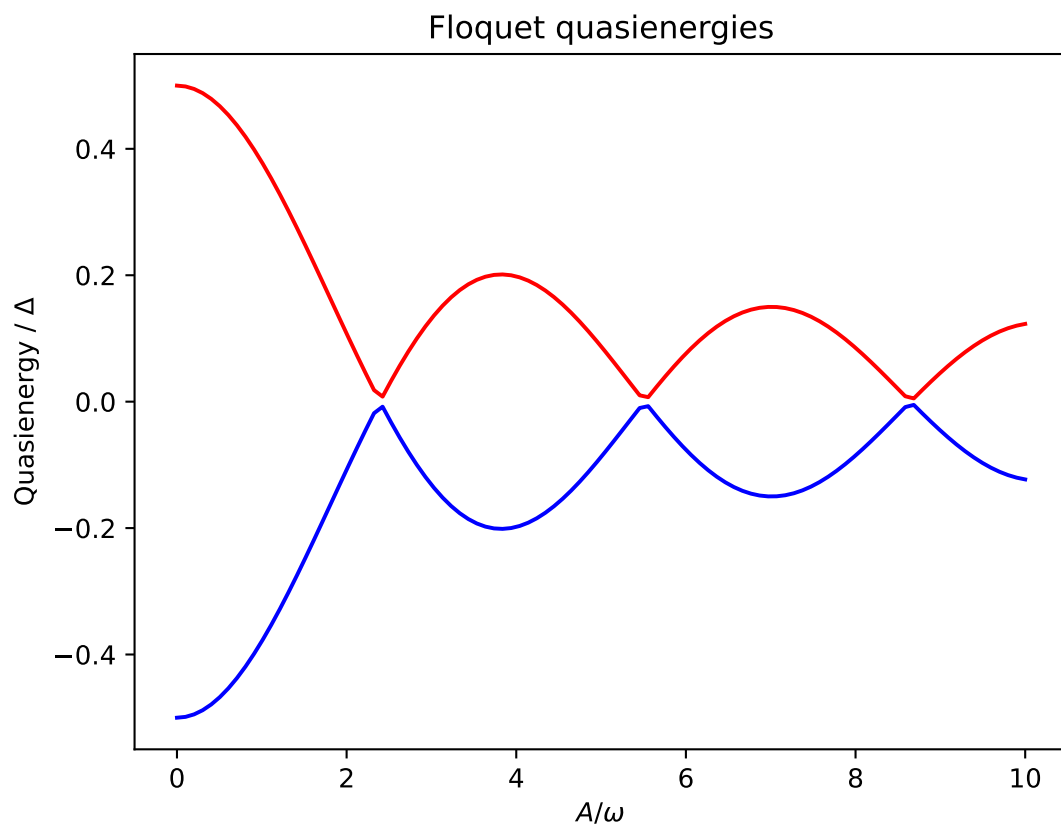
```
>>> delta = 0.2 * 2 * np.pi
>>> eps0 = 0.0 * 2 * np.pi
>>> omega = 1.0 * 2 * np.pi
>>> A_vec = np.linspace(0, 10, 100) * omega
>>> T = (2 * np.pi) / omega
>>> tlist = np.linspace(0.0, 10 * T, 101)
>>> spsi0 = basis(2, 0)
>>> q_energies = np.zeros((len(A_vec), 2))
>>> H0 = delta / 2.0 * sigmaz() - eps0 / 2.0 * sigmax()
>>> args = {'w': omega}
>>> for idx, A in enumerate(A_vec):
>>>     H1 = A / 2.0 * sigmax()
>>>     H = [H0, [H1, lambda t, args: np.sin(args['w'] * t)]]
```

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```

>>> floquet_basis = FloquetBasis(H, T, args)
>>> q_energies[idx,:] = floquet_basis.e_quasi
>>> plt.figure()
>>> plt.plot(A_vec/omega, q_energies[:,0] / delta, 'b', A_vec/omega, q_energies[:,1] /
↳ delta, 'r')
>>> plt.xlabel(r'$A/\omega$')
>>> plt.ylabel(r'Quasienergy / $\Delta$')
>>> plt.title(r'Floquet quasienergies')
>>> plt.show()
    
```



Given the Floquet modes at  $t = 0$ , we obtain the Floquet mode at some later time  $t$  using `FloquetBasis.mode`:

```

>>> f_modes_t = floquet_basis.mode(2.5)
>>> f_modes_t
[Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[-0.89630512-0.23191946j]
 [ 0.37793106-0.00431336j]],
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[-0.37793106-0.00431336j]
 [-0.89630512+0.23191946j]]]
    
```

The purpose of calculating the Floquet modes is to find the wavefunction solution to the original problem (3.32) given some initial state  $|\psi_0\rangle$ . To do that, we first need to decompose the initial state in the Floquet states, using the function `FloquetBasis.to_floquet_basis`

```
>>> psi0 = rand_ket(2)
>>> f_coeff = floquet_basis.to_floquet_basis(psi0)
>>> f_coeff
[(-0.645265993068382+0.7304552549315746j),
 (0.15517002114250228-0.1612116102238258j)]
```

and given this decomposition of the initial state in the Floquet states we can easily evaluate the wavefunction that is the solution to (3.32) at an arbitrary time  $t$  using the function `FloquetBasis.from_floquet_basis`:

```
>>> t = 10 * np.random.rand()
>>> psi_t = floquet_basis.from_floquet_basis(f_coeff, t)
```

The following example illustrates how to use the functions introduced above to calculate and plot the time-evolution of (3.32).

```
import numpy as np
from matplotlib import pyplot

import qutip

delta = 0.2 * 2*np.pi
eps0 = 1.0 * 2*np.pi
A = 0.5 * 2*np.pi
omega = 1.0 * 2*np.pi
T = (2*np.pi)/omega
tlist = np.linspace(0.0, 10 * T, 101)
psi0 = qutip.basis(2, 0)

H0 = - delta/2.0 * qutip.sigmaz() - eps0/2.0 * qutip.sigmaz()
H1 = A/2.0 * qutip.sigmaz()
args = {'w': omega}
H = [H0, [H1, lambda t, w: np.sin(w * t)]]

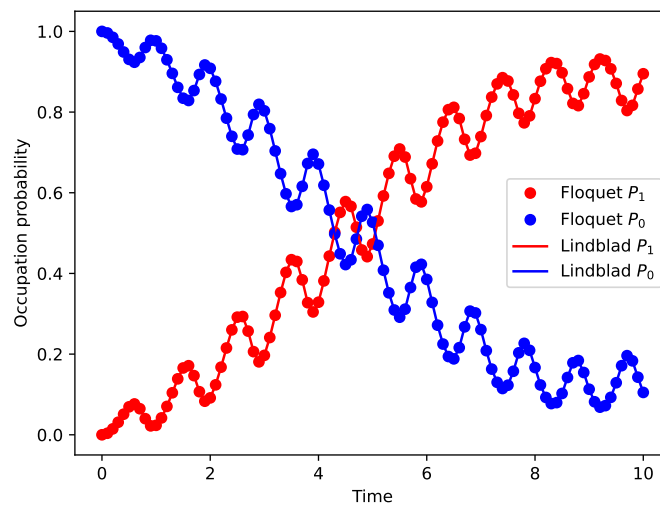
# Create the floquet system for the time-dependent hamiltonian
floquetbasis = qutip.FloquetBasis(H, T, args)

# decompose the initial state in the floquet modes
f_coeff = floquetbasis.to_floquet_basis(psi0)

# calculate the wavefunctions using the from the floquet modes coefficients
p_ex = np.zeros(len(tlist))
for n, t in enumerate(tlist):
    psi_t = floquetbasis.from_floquet_basis(f_coeff, t)
    p_ex[n] = qutip.expect(qutip.num(2), psi_t)

# For reference: calculate the same thing with mesolve
p_ex_ref = qutip.mesolve(H, psi0, tlist, [], [qutip.num(2)], args).expect[0]

# plot the results
pyplot.plot(tlist, np.real(p_ex), 'ro', tlist, 1-np.real(p_ex), 'bo')
pyplot.plot(tlist, np.real(p_ex_ref), 'r', tlist, 1-np.real(p_ex_ref), 'b')
pyplot.xlabel('Time')
pyplot.ylabel('Occupation probability')
pyplot.legend(("Floquet $P_1$", "Floquet $P_0$", "Lindblad $P_1$", "Lindblad $P_0$"))
pyplot.show()
```



### Pre-computing the Floquet modes for one period

When evaluating the Floquet states or the wavefunction at many points in time it is useful to pre-compute the Floquet modes for the first period of the driving with the required times. The list of times to pre-compute modes for may be passed to `FloquetBasis` using `precompute=tlist`, and then `FloquetBasis.from_floquet_basis` and `FloquetBasis.to_floquet_basis` can be used to efficiently retrieve the wave function at the pre-computed times. The following example illustrates how the example from the previous section can be solved more efficiently using these functions for pre-computing the Floquet modes:

```
import numpy as np
from matplotlib import pyplot
import qutip

delta = 0.0 * 2*np.pi
eps0 = 1.0 * 2*np.pi
A = 0.25 * 2*np.pi
omega = 1.0 * 2*np.pi
T = 2*np.pi / omega
tlist = np.linspace(0.0, 10 * T, 101)
psi0 = qutip.basis(2,0)

H0 = - delta/2.0 * qutip.sigmax() - eps0/2.0 * qutip.sigmaz()
H1 = A/2.0 * qutip.sigmax()
args = {'w': omega}
H = [H0, [H1, lambda t, w: np.sin(w * t)]]

# find the floquet modes for the time-dependent hamiltonian
floquetbasis = qutip.FloquetBasis(H, T, args, precompute=tlist)

# decompose the initial state in the floquet modes
f_coeff = floquetbasis.to_floquet_basis(psi0)

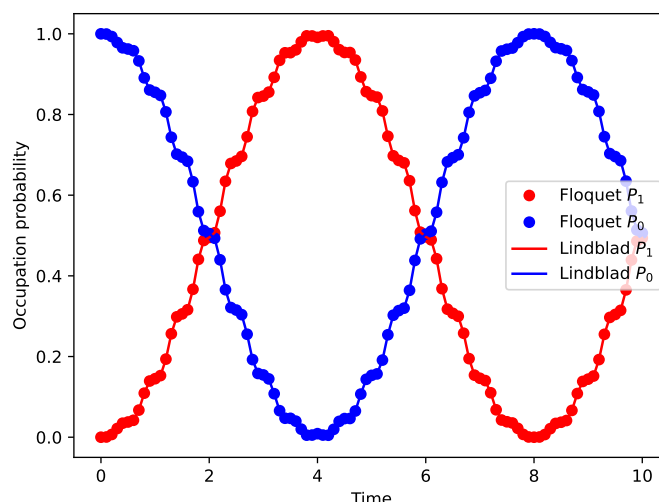
# calculate the wavefunctions using the from the floquet modes coefficients
p_ex = np.zeros(len(tlist))
for n, t in enumerate(tlist):
    psi_t = floquetbasis.from_floquet_basis(f_coeff, t)
    p_ex[n] = qutip.expect(qutip.num(2), psi_t)
```

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```
# For reference: calculate the same thing with mesolve
p_ex_ref = qutip.mesolve(H, psi0, tlist, [], [qutip.num(2)], args).expect[0]

# plot the results
pyplot.plot(tlist, np.real(p_ex), 'ro', tlist, 1-np.real(p_ex), 'bo')
pyplot.plot(tlist, np.real(p_ex_ref), 'r', tlist, 1-np.real(p_ex_ref), 'b')
pyplot.xlabel('Time')
pyplot.ylabel('Occupation probability')
pyplot.legend(("Floquet $P_1$", "Floquet $P_0$", "Lindblad $P_1$", "Lindblad $P_0$"))
pyplot.show()
```



Note that the parameters and the Hamiltonian used in this example is not the same as in the previous section, and hence the different appearance of the resulting figure.

For convenience, all the steps described above for calculating the evolution of a quantum system using the Floquet formalisms are encapsulated in the function `fsesolve`. Using this function, we could have achieved the same results as in the examples above using

```
output = fsesolve(H, psi0=psi0, tlist=tlist, e_ops=[qutip.num(2)], args=args)
p_ex = output.expect[0]
```

## Floquet theory for dissipative evolution

A driven system that is interacting with its environment is not necessarily well described by the standard Lindblad master equation, since its dissipation process could be time-dependent due to the driving. In such cases a rigorous approach would be to take the driving into account when deriving the master equation. This can be done in many different ways, but one way common approach is to derive the master equation in the Floquet basis. That approach results in the so-called Floquet-Markov master equation, see Grifoni et al., Physics Reports 304, 299 (1998) for details.

For a brief summary of the derivation, the important contents for the implementation in QuTiP are listed below.

The floquet mode  $|\phi_\alpha(t)\rangle$  refers to a full class of quasienergies defined by  $\epsilon_\alpha + k\Omega$  for arbitrary  $k$ . Hence, the quasienergy difference between two floquet modes is given by

$$\Delta_{\alpha\beta k} = \frac{\epsilon_\alpha - \epsilon_\beta}{\hbar} + k\Omega$$

For any coupling operator  $q$  (given by the user) the matrix elements in the floquet basis are calculated as:

$$X_{\alpha\beta k} = \frac{1}{T} \int_0^T dt e^{-ik\Omega t} \langle \phi_\alpha(t) | q | \phi_\beta(t) \rangle$$

From the matrix elements and the spectral density  $J(\omega)$ , the decay rate  $\gamma_{\alpha\beta k}$  is defined:

$$\gamma_{\alpha\beta k} = 2\pi J(\Delta_{\alpha\beta k}) |X_{\alpha\beta k}|^2$$

The master equation is further simplified by the RWA, which makes the following matrix useful:

$$A_{\alpha\beta} = \sum_{k=-\infty}^{\infty} [\gamma_{\alpha\beta k} + n_{th}(|\Delta_{\alpha\beta k}|)(\gamma_{\alpha\beta k} + \gamma_{\alpha\beta -k})]$$

The density matrix of the system then evolves according to:

$$\begin{aligned} \dot{\rho}_{\alpha\alpha}(t) &= \sum_{\nu} (A_{\alpha\nu} \rho_{\nu\nu}(t) - A_{\nu\alpha} \rho_{\alpha\alpha}(t)) \\ \dot{\rho}_{\alpha\beta}(t) &= -\frac{1}{2} \sum_{\nu} (A_{\nu\alpha} + A_{\nu\beta}) \rho_{\alpha\beta}(t) \quad \alpha \neq \beta \end{aligned}$$

### The Floquet-Markov master equation in QuTiP

The QuTiP function `fmmesolve` implements the Floquet-Markov master equation. It calculates the dynamics of a system given its initial state, a time-dependent Hamiltonian, a list of operators through which the system couples to its environment and a list of corresponding spectral-density functions that describes the environment. In contrast to the `mesolve` and `mcsolve`, and the `fmmesolve` does characterize the environment with dissipation rates, but extract the strength of the coupling to the environment from the noise spectral-density functions and the instantaneous Hamiltonian parameters (similar to the Bloch-Redfield master equation solver `brmesolve`).

**Note:** Currently the `fmmesolve` can only accept a single environment coupling operator and spectral-density function.

The noise spectral-density function of the environment is implemented as a Python callback function that is passed to the solver. For example:

```
gamma1 = 0.1
def noise_spectrum(omega):
    return (omega>0) * 0.5 * gamma1 * omega/(2*pi)
```

The other parameters are similar to the `mesolve` and `mcsolve`, and the same format for the return value is used `Result`. The following example extends the example studied above, and uses `fmmesolve` to introduce dissipation into the calculation

```
import numpy as np
from matplotlib import pyplot
import qutip

delta = 0.0 * 2*np.pi
eps0 = 1.0 * 2*np.pi
A = 0.25 * 2*np.pi
omega = 1.0 * 2*np.pi
T = 2*np.pi / omega
tlist = np.linspace(0.0, 20 * T, 301)
psi0 = qutip.basis(2,0)
```

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```
H0 = - delta/2.0 * qutip.sigmaz() - eps0/2.0 * qutip.sigmaz()
H1 = A/2.0 * qutip.sigmaz()
args = {'w': omega}
H = [H0, [H1, lambda t, w: np.sin(w * t)]]

# noise power spectrum
gamma1 = 0.1
def noise_spectrum(omega):
    return (omega>0) * 0.5 * gamma1 * omega/(2*np.pi)

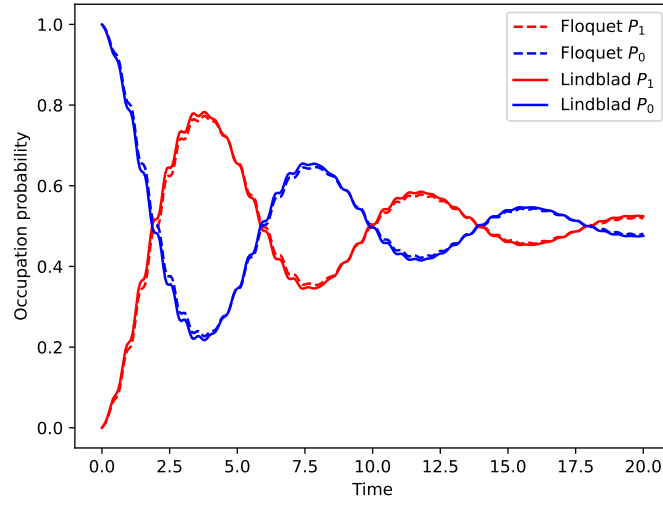
# solve the floquet-markov master equation
output = qutip.fmmsolve(
    H, psi0, tlist, [qutip.sigmaz()],
    spectra_cb=[noise_spectrum], T=T,
    args=args, options={"store_floquet_states": True}
)

# calculate expectation values in the computational basis
p_ex = np.zeros(tlist.shape, dtype=np.complex128)
for idx, t in enumerate(tlist):
    f_coeff_t = output.floquet_states[idx]
    psi_t = output.floquet_basis.from_floquet_basis(f_coeff_t, t)
    # Alternatively
    psi_t = output.states[idx]
    p_ex[idx] = qutip.expect(qutip.num(2), psi_t)

# For reference: calculate the same thing with mesolve
output = qutip.mesolve(H, psi0, tlist,
    [np.sqrt(gamma1) * qutip.sigmaz()], [qutip.num(2)],
    args)
p_ex_ref = output.expect[0]

# plot the results
pyplot.plot(tlist, np.real(p_ex), 'r--', tlist, 1-np.real(p_ex), 'b--')
pyplot.plot(tlist, np.real(p_ex_ref), 'r', tlist, 1-np.real(p_ex_ref), 'b')
pyplot.xlabel('Time')
pyplot.ylabel('Occupation probability')
pyplot.legend(("Floquet $P_1$", "Floquet $P_0$", "Lindblad $P_1$", "Lindblad $P_0$"))
pyplot.show()
```





Finally, `fmmsolve` always expects the `e_ops` to be specified in the laboratory basis (as for other solvers) and we can calculate expectation values using:

```
output = fmmsolve(H, psi0, tlist, [sigmax()], e_ops=[num(2)],
                  spectra_cb=[noise_spectrum], T=T, args=args)
p_ex = output.expect[0]
```

### 3.6.11 Monte Carlo for Non-Markovian Dynamics

The Monte Carlo solver of QuTiP can also be used to solve the dynamics of time-local non-Markovian master equations, i.e., master equations of the Lindblad form

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H, \rho(t)] + \sum_n \frac{\gamma_n(t)}{2} [2A_n \rho(t) A_n^\dagger - \rho(t) A_n^\dagger A_n - A_n^\dagger A_n \rho(t)] \quad (3.33)$$

with “rates”  $\gamma_n(t)$  that can take negative values. This can be done with the `nm_mcsolve` function. The function is based on the influence martingale formalism [Donvil22] and formally requires that the collapse operators  $A_n$  satisfy a completeness relation of the form

$$\sum_n A_n^\dagger A_n = \alpha \mathbb{I}, \quad (3.34)$$

where  $\mathbb{I}$  is the identity operator on the system Hilbert space and  $\alpha > 0$ . Note that when the collapse operators of a model don’t satisfy such a relation, `nm_mcsolve` automatically adds an extra collapse operator such that (3.34) is satisfied. The rate corresponding to this extra collapse operator is set to zero.

Technically, the influence martingale formalism works as follows. We introduce an influence martingale  $\mu(t)$ , which follows the evolution of the system state. When no jump happens, it evolves as

$$\mu(t) = \exp \left( \alpha \int_0^t K(\tau) d\tau \right) \quad (3.35)$$

where  $K(t)$  is for now an arbitrary function. When a jump corresponding to the collapse operator  $A_n$  happens, the influence martingale becomes

$$\mu(t + \delta t) = \mu(t) \left( \frac{K(t) - \gamma_n(t)}{\gamma_n(t)} \right) \quad (3.36)$$

Assuming that the state  $\bar{\rho}(t)$  computed by the Monte Carlo average

$$\bar{\rho}(t) = \frac{1}{N} \sum_{l=1}^N |\psi_l(t)\rangle \langle \psi_l(t)| \quad (3.37)$$

solves a Lindblad master equation with collapse operators  $A_n$  and rates  $\Gamma_n(t)$ , the state  $\rho(t)$  defined by

$$\rho(t) = \frac{1}{N} \sum_{l=1}^N \mu_l(t) |\psi_l(t)\rangle \langle \psi_l(t)| \quad (3.38)$$

solves a Lindblad master equation with collapse operators  $A_n$  and shifted rates  $\gamma_n(t) - K(t)$ . Thus, while  $\Gamma_n(t) \geq 0$ , the new “rates”  $\gamma_n(t) = \Gamma_n(t) - K(t)$  satisfy no positivity requirement.

The input of `nm_mcsolve` is almost the same as for `mcsolve`. The only difference is how the collapse operators and rate functions should be defined. `nm_mcsolve` requires collapse operators  $A_n$  and target “rates”  $\gamma_n$  (which are allowed to take negative values) to be given in list form `[[C_1, gamma_1], [C_2, gamma_2], ...]`. Note that we give the actual rate and not its square root, and that `nm_mcsolve` automatically computes associated jump rates  $\Gamma_n(t) \geq 0$  appropriate for simulation.

We conclude with a simple example demonstrating the usage of the `nm_mcsolve` function. For more elaborate, physically motivated examples, we refer to the [accompanying tutorial notebook](#).

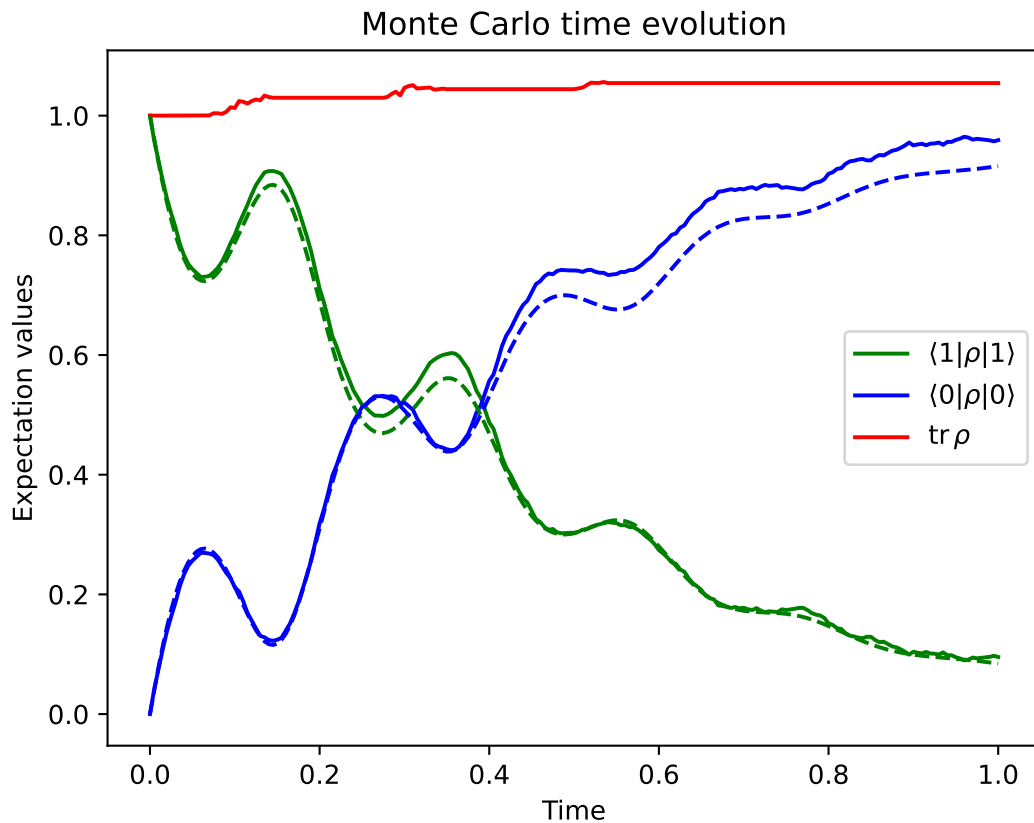
```
times = np.linspace(0, 1, 201)
psi0 = basis(2, 1)
a0 = destroy(2)
H = a0.dag() * a0

# Rate functions
gamma1 = "kappa * nth"
gamma2 = "kappa * (nth+1) + 12 * np.exp(-2*t**3) * (-np.sin(15*t)**2)"
# gamma2 becomes negative during some time intervals

# nm_mcsolve integration
ops_and_rates = []
ops_and_rates.append([a0.dag(), gamma1])
ops_and_rates.append([a0, gamma2])
MCSol = nm_mcsolve(H, psi0, times, ops_and_rates,
                  args={'kappa': 1.0 / 0.129, 'nth': 0.063},
                  e_ops=[a0.dag() * a0, a0 * a0.dag()],
                  options={'map': 'parallel'}, ntraj=2500)

# mesolve integration for comparison
d_ops = [[lindblad_dissipator(a0.dag(), a0.dag()), gamma1],
          [lindblad_dissipator(a0, a0), gamma2]]
MESol = mesolve(H, psi0, times, d_ops, e_ops=[a0.dag() * a0, a0 * a0.dag()],
               args={'kappa': 1.0 / 0.129, 'nth': 0.063})

plt.figure()
plt.plot(times, MCSol.expect[0], 'g',
         times, MCSol.expect[1], 'b',
         times, MCSol.trace, 'r')
plt.plot(times, MESol.expect[0], 'g--',
         times, MESol.expect[1], 'b--')
plt.title('Monte Carlo time evolution')
plt.xlabel('Time')
plt.ylabel('Expectation values')
plt.legend((r'$\langle 1 | \rho | 1 \rangle$',
            r'$\langle 0 | \rho | 0 \rangle$',
            r'$\operatorname{tr} \rho$'))
plt.show()
```



### 3.6.12 Setting Options for the Dynamics Solvers

Occasionally it is necessary to change the built in parameters of the dynamics solvers used by for example the *mesolve* and *mcsolve* functions. The options for all dynamics solvers may be changed by using the dictionaries.

```
options = {"store_states": True, "atol": 1e-12}
```

Supported items come from 2 sources, the solver and the ODE integration method. Supported solver options and their default can be seen using the class interface:

```
help(MESolver.options)
```

Options supported by the ODE integration depend on the “method” options of the solver, they can be listed through the integrator method of the solvers:

```
help(MESolver.integrator("adams").options)
```

See *Integrator* for a list of supported methods.

As an example, let us consider changing the integrator, turn the GUI off, and strengthen the absolute tolerance.

```
options = {method="bdf", "atol": 1e-10, "progress_bar": False}
```

To use these new settings we can use the keyword argument *options* in either the *mesolve* and *mcsolve* function:

```
>>> mesolve(H0, psi0, tlist, c_op_list, [sigmaz()], options=options)
```

or:

```
>>> MCSolver(H0, c_op_list, options=options)
```

### 3.6.13 Computing propagators

Sometime the evolution of a single state is not sufficient and the full propagator is desired. QuTiP has the *propagator* function to compute them:

```
>>> H = sigmaz() + np.pi * sigmax()
>>> psi_t = sesolve(H, basis(2, 1), [0, 0.5, 1]).states
>>> prop = propagator(H, [0, 0.5, 1])

>>> print((psi_t[1] - prop[1] @ basis(2, 1)).norm())
2.455965272327082e-06

>>> print((psi_t[2] - prop[2] @ basis(2, 1)).norm())
2.00719000004562142e-06
```

The first argument is the Hamiltonian, any time dependent system format is accepted. The function also accepts an optional *c\_ops* argument for collapse operators. When used, a propagator for density matrices is computed:  $\rho(t) = U(t)(\rho(0))$ :

```
>>> rho_t = mesolve(H, fock_dm(2, 1), [0, 0.5, 1], c_ops=[sigmam()]).states
>>> prop = propagator(H, [0, 0.5, 1], c_ops=[sigmam()])

>>> print((rho_t[1] - prop[1](fock_dm(2, 1))).norm())
7.23009476734681e-07

>>> print((rho_t[2] - prop[2](fock_dm(2, 1))).norm())
1.2666967766644768e-06
```

The propagator function is also available as a class:

```
>>> U = Propagator(H, c_ops=[sigmam()])

>>> state_0_5 = U(0.5)(fock_dm(2, 1))
>>> state_1 = U(1., t_start=0.5)(state_0_5)

>>> print((rho_t[1] - state_0_5).norm())
7.23009476734681e-07

>>> print((rho_t[2] - state_1).norm())
8.355518501351504e-07
```

The *Propagator* can take options and args as a solver instance.

#### Using a solver to compute a propagator

Many solvers accept an operator as the initial state. When an identity matrix is passed as the initial state, the propagator is computed. This can be used to compute a propagator for Bloch-Redfield or Floquet equations:

```
>>> delta = 0.2 * 2*np.pi
>>> eps0 = 1.0 * 2*np.pi
>>> gamma1 = 0.5

>>> H = - delta/2.0 * sigmax() - eps0/2.0 * sigmaz()
```

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```
>>> def ohmic_spectrum(w):
>>>     if w == 0.0: # dephasing inducing noise
>>>         return gamma1
>>>     else: # relaxation inducing noise
>>>         return gamma1 / 2 * (w / (2 * np.pi)) * (w > 0.0)

>>> prop = brmesolve(H, qeye(2), [0, 1], a_ops=[[sigmax(), ohmic_spectrum]]).final_
↪state
```

## 3.7 Hierarchical Equations of Motion

### 3.7.1 Introduction

The Hierarchical Equations of Motion (HEOM) method was originally developed by Tanimura and Kubo [TK89] in the context of physical chemistry to “exactly” solve a quantum system in contact with a bosonic environment, encapsulated in the Hamiltonian:

$$H = H_s + \sum_k \omega_k a_k^\dagger a_k + \hat{Q} \sum_k g_k (a_k + a_k^\dagger).$$

As in other solutions to this problem, the properties of the bath are encapsulated by its temperature and its spectral density,

$$J(\omega) = \pi \sum_k g_k^2 \delta(\omega - \omega_k).$$

In the HEOM, for bosonic baths, one typically chooses a Drude-Lorentz spectral density:

$$J_D = \frac{2\lambda\gamma\omega}{(\gamma^2 + \omega^2)},$$

or an under-damped Brownian motion spectral density:

$$J_U = \frac{\alpha^2 \Gamma \omega}{[(\omega_c^2 - \omega^2)^2 + \Gamma^2 \omega^2]}.$$

Given the spectral density, the HEOM requires a decomposition of the bath correlation functions in terms of exponentials. In *Bosonic Environments* we describe how this is done with code examples, and how these expansions are passed to the solver.

In addition to support for bosonic environments, QuTiP also provides support for fermionic environments which is described in *Fermionic Environments*.

Both bosonic and fermionic environments are supported via a single solver, *HEOMSolver*, that supports solving for both dynamics and steady-states.

### 3.7.2 Bosonic Environments

In this section we consider a simple two-level system coupled to a Drude-Lorentz bosonic bath. The system Hamiltonian,  $H_{sys}$ , and the bath spectral density,  $J_D$ , are

$$H_{sys} = \frac{\epsilon\sigma_z}{2} + \frac{\Delta\sigma_x}{2}$$

$$J_D = \frac{2\lambda\gamma\omega}{(\gamma^2 + \omega^2)},$$

We will demonstrate how to describe the bath using two different expansions of the spectral density correlation function (Matsubara's expansion and a Padé expansion), how to evolve the system in time, and how to calculate the steady state.

First we will do this in the simplest way, using the built-in implementations of the two bath expansions, `DrudeLorentzBath` and `DrudeLorentzPadeBath`. We will do this both with a truncated expansion and show how to include an approximation to all of the remaining terms in the bath expansion.

Afterwards, we will show how to calculate the bath expansion coefficients and to use those coefficients to construct your own bath description so that you can implement your own bosonic baths.

Finally, we will demonstrate how to simulate a system coupled to multiple independent baths, as occurs, for example, in certain photosynthesis processes.

A notebook containing a complete example similar to this one implemented in BoFiN can be found in [example notebook 1a](#).

## Describing the system and bath

First, let us construct the system Hamiltonian,  $H_{sys}$ , and the initial system state,  $\rho_{00}$ :

```
from qutip import basis, sigmax, sigmaz

# The system Hamiltonian:
eps = 0.5 # energy of the 2-level system
Del = 1.0 # tunnelling term
H_sys = 0.5 * eps * sigmaz() + 0.5 * Del * sigmax()

# Initial state of the system:
rho0 = basis(2,0) * basis(2,0).dag()
```

Now let us describe the bath properties:

```
# Bath properties:
gamma = 0.5 # cut off frequency
lam = 0.1 # coupling strength
T = 0.5 # temperature

# System-bath coupling operator:
Q = sigmaz()
```

where  $\gamma$  (gamma),  $\lambda$  (lam) and  $T$  are the parameters of a Drude-Lorentz bath, and  $Q$  is the coupling operator between the system and the bath.

We may then pass these parameters to either `DrudeLorentzBath` or `DrudeLorentzPadeBath` to construct an expansion of the bath correlations:

```
from qutip.solver.heom import DrudeLorentzBath
from qutip.solver.heom import DrudeLorentzPadeBath

# Number of expansion terms to retain:
Nk = 2

# Matsubara expansion:
bath = DrudeLorentzBath(Q, lam, gamma, T, Nk)

# Padé expansion:
bath = DrudeLorentzPadeBath(Q, lam, gamma, T, Nk)
```

Where  $N_k$  is the number of terms to retain within the expansion of the bath.

## System and bath dynamics

Now we are ready to construct a solver:

```
from qutip.solver.heom import HEOMSolver

max_depth = 5 # maximum hierarchy depth to retain
options = {"nsteps": 15_000}

solver = HEOMSolver(H_sys, bath, max_depth=max_depth, options=options)
```

and to calculate the system evolution as a function of time:

```
tlist = [0, 10, 20] # times to evaluate the system state at
result = solver.run(rho0, tlist)
```

The `max_depth` parameter determines how many levels of the hierarchy to retain. As a first approximation hierarchy depth may be thought of as similar to the order of Feynman Diagrams (both classify terms by increasing number of interactions).

The `result` is a standard QuTiP results object with the attributes:

- `times`: the times at which the state was evaluated (i.e. `tlist`)
- `states`: the system states at each time
- `expect`: a list with the values of each `e_ops` at each time
- `e_data`: a dictionary with the values of each `e_op` at each time
- `ado_states`: see below (an instance of *HierarchyADOsState*)

If `ado_return=True` is passed to `.run(...)` the full set of auxilliary density operators (ADOs) that make up the hierarchy at each time will be returned as `.ado_states`. We will describe how to use these to determine other properties, such as system-bath currents, later in the fermionic guide (see *Determining currents*).

If one has a full set of ADOs from a previous call of `.run(...)` you may supply it as the initial state of the solver by calling `.run(result.ado_states[-1], tlist, ado_init=True)`.

As with other QuTiP solvers, if expectation operators or functions are supplied using `.run(..., e_ops=[...])` the expectation values are available in `result.expect` and `result.e_data`.

Below we run the solver again, but use `e_ops` to store the expectation values of the population of the system states and the coherence:

```
# Define the operators that measure the populations of the two
# system states:
P11p = basis(2,0) * basis(2,0).dag()
P22p = basis(2,1) * basis(2,1).dag()

# Define the operator that measures the 0, 1 element of density matrix
# (corresponding to coherence):
P12p = basis(2,0) * basis(2,1).dag()

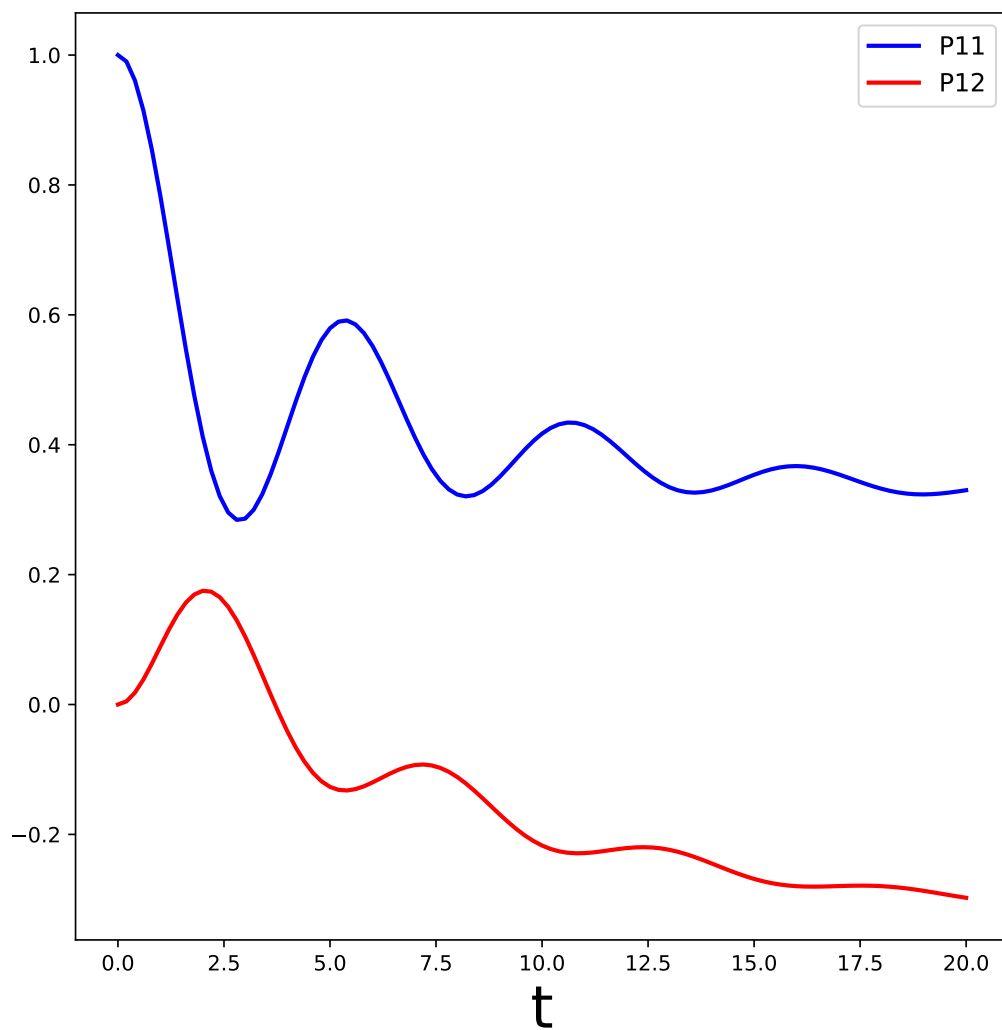
# Run the solver:
tlist = np.linspace(0, 20, 101)
result = solver.run(rho0, tlist, e_ops={"11": P11p, "22": P22p, "12": P12p})

# Plot the results:
fig, axes = plt.subplots(1, 1, sharex=True, figsize=(8,8))
axes.plot(result.times, result.e_data["11"], 'b', linewidth=2, label="P11")
axes.plot(result.times, result.e_data["12"], 'r', linewidth=2, label="P12")
```

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```
axes.set_xlabel(r't', fontsize=28)
axes.legend(loc=0, fontsize=12)
```



## Steady-state

Using the same solver, we can also determine the steady state of the combined system and bath using:

```
steady_state, steady_ados = solver.steady_state()
```

where `steady_state` is the steady state of the system and `steady_ados` if the steady state of the full hierarchy. The ADO states are described more fully in [Determining currents](#) and [HierarchyADOsState](#).



## Matsubara Terminator

When constructing the Drude-Lorentz bath we have truncated the expansion at  $N_k = 2$  terms and ignore the remaining terms.

However, since the coupling to these higher order terms is comparatively weak, we may consider the interaction with them to be Markovian, and construct an additional Lindbladian term that captures their interaction with the system and the lower order terms in the expansion.

This additional term is called the **terminator** because it terminates the expansion.

The `DrudeLorentzBath` and `DrudeLorentzPadeBath` both provide a means of calculating the terminator for a given expansion:

```
# Matsubara expansion:
bath = DrudeLorentzBath(Q, lam, gamma, T, Nk)

# Padé expansion:
bath = DrudeLorentzPadeBath(Q, lam, gamma, T, Nk)

# Add terminator to the system Liouvillian:
delta, terminator = bath.terminator()
HL = liouvillian(H_sys) + terminator

# Construct solver:
solver = HEOMSolver(HL, bath, max_depth=max_depth, options=options)
```

This captures the Markovian effect of the remaining terms in the expansion without having to fully model many more terms.

The value `delta` is an approximation to the strength of the effect of the remaining terms in the expansion (i.e. how strongly the terminator is coupled to the rest of the system).

## Matsubara expansion coefficients

So far we have relied on the built-in `DrudeLorentzBath` to construct the Drude-Lorentz bath expansion for us. Now we will calculate the coefficients ourselves and construct a `BosonicBath` directly. A similar procedure can be used to apply `HEOMSolver` to any bosonic bath for which we can calculate the expansion coefficients.

The real and imaginary parts of the correlation function,  $C(t)$ , for the bosonic bath is expanded in an exponential series:

$$C(t) = C_{real}(t) + iC_{imag}(t)$$

$$C_{real}(t) = \sum_{k=0}^{\infty} c_{k,real} e^{-\nu_{k,real} t}$$

$$C_{imag}(t) = \sum_{k=0}^{\infty} c_{k,imag} e^{-\nu_{k,imag} t}$$

In the specific case of Matsubara expansion for the Drude-Lorentz bath, the coefficients of this expansion are, for the real part,  $C_{real}(t)$ :

$$\nu_{k,real} = \begin{cases} \gamma & k = 0 \\ 2\pi k / \beta & k \geq 1 \end{cases}$$

$$c_{k,real} = \begin{cases} \lambda \gamma [\cot(\beta \gamma / 2) - i] & k = 0 \\ \frac{4\lambda \gamma \nu_k}{(\nu_k^2 - \gamma^2) \beta} & k \geq 1 \end{cases}$$

and the imaginary part,  $C_{imag}(t)$ :

$$\nu_{k,imag} = \begin{cases} \gamma & k = 0 \\ 0 & k \geq 1 \end{cases}$$

$$c_{k,imag} = \begin{cases} -\lambda\gamma & k = 0 \\ 0 & k \geq 1 \end{cases}$$

And now the same numbers calculated in Python:

```
# Convenience functions and parameters:

def cot(x):
    return 1. / np.tan(x)

beta = 1. / T

# Number of expansion terms to calculate:
Nk = 2

# C_real expansion terms:
ck_real = [lam * gamma / np.tan(gamma / (2 * T))]
ck_real.extend([
    (8 * lam * gamma * T * np.pi * k * T /
     ((2 * np.pi * k * T)**2 - gamma**2))
    for k in range(1, Nk + 1)
])
vk_real = [gamma]
vk_real.extend([2 * np.pi * k * T for k in range(1, Nk + 1)])

# C_imag expansion terms (this is the full expansion):
ck_imag = [lam * gamma * (-1.0)]
vk_imag = [gamma]
```

After all that, constructing the bath is very straight forward:

```
from qutip.solver.heom import BosonicBath

bath = BosonicBath(Q, ck_real, vk_real, ck_imag, vk_imag)
```

And we're done!

The *BosonicBath* can be used with the *HEOMSolver* in exactly the same way as the baths we constructed previously using the built-in Drude-Lorentz bath expansions.

## Multiple baths

The *HEOMSolver* supports having a system interact with multiple environments. All that is needed is to supply a list of baths instead of a single bath.

In the example below we calculate the evolution of a small system where each basis state of the system interacts with a separate bath. Such an arrangement can model, for example, the Fenna–Matthews–Olson (FMO) pigment-protein complex which plays an important role in photosynthesis ( for a full FMO example see the notebook <https://github.com/tehruhn/bofin/blob/main/examples/example-2-FMO-example.ipynb> ).

For each bath expansion, we also include the terminator in the system Liouvillian.

At the end, we plot the populations of the system states as a function of time, and show the long-time beating of quantum state coherence that occurs:

```

# The size of the system:
N_sys = 3

def proj(i, j):
    """ A helper function for creating an interaction operator. """
    return basis(N_sys, i) * basis(N_sys, j).dag()

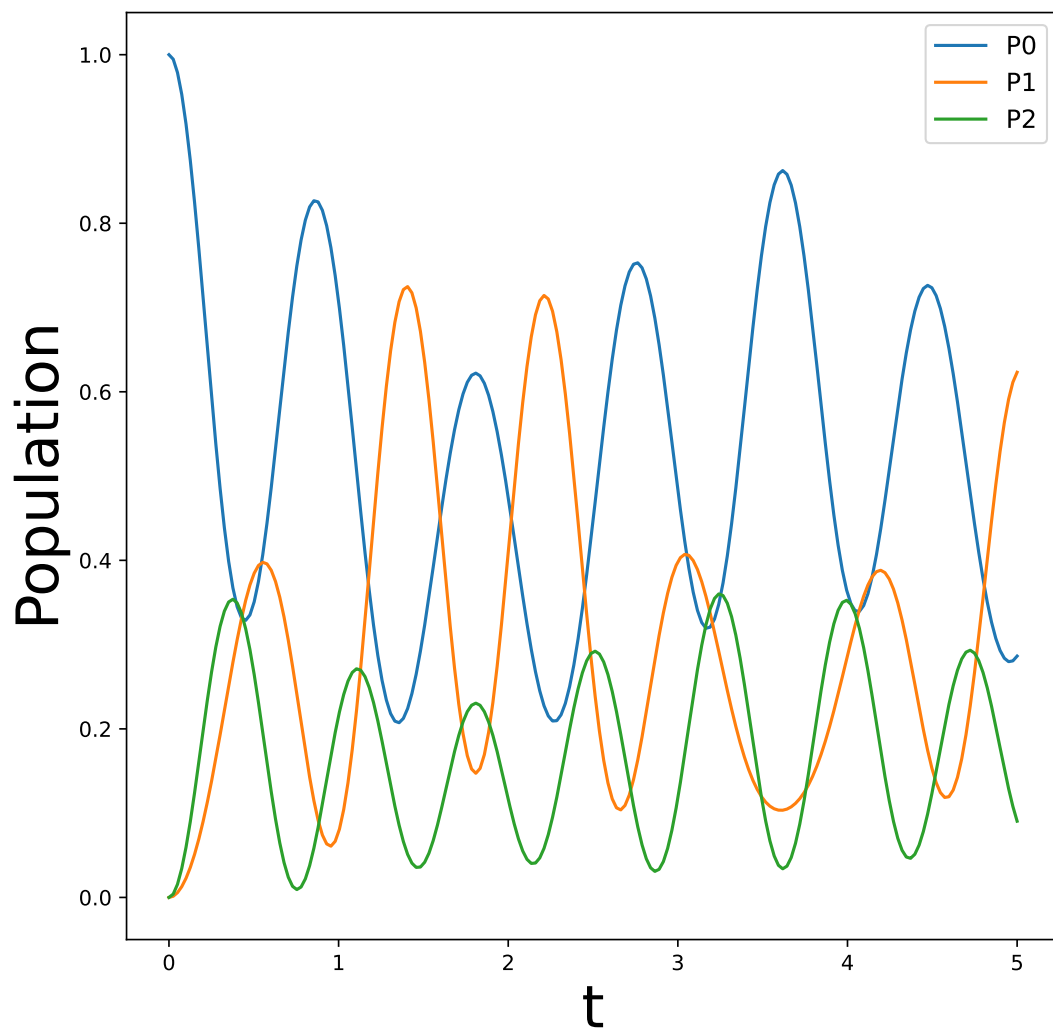
# Construct one bath for each system state:
baths = []
for i in range(N_sys):
    Q = proj(i, i)
    baths.append(DrudeLorentzBath(Q, lam, gamma, T, Nk))

# Construct the system Liouvillian from the system Hamiltonian and
# bath expansion terminators:
H_sys = sum((i + 0.5) * eps * proj(i, i) for i in range(N_sys))
H_sys += sum(
    (i + j + 0.5) * Del * proj(i, j)
    for i in range(N_sys) for j in range(N_sys)
    if i != j
)
HL = liouvillian(H_sys) + sum(bath.terminator()[1] for bath in baths)

# Construct the solver (pass a list of baths):
solver = HEOMSolver(HL, baths, max_depth=max_depth, options=options)

# Run the solver:
rho0 = basis(N_sys, 0) * basis(N_sys, 0).dag()
tlist = np.linspace(0, 5, 200)
e_ops = {
    f"P{i}": proj(i, i)
    for i in range(N_sys)
}
result = solver.run(rho0, tlist, e_ops=e_ops)

# Plot populations:
fig, axes = plt.subplots(1, 1, sharex=True, figsize=(8,8))
for label, values in result.e_data.items():
    axes.plot(result.times, values, label=label)
axes.set_xlabel(r't', fontsize=28)
axes.set_ylabel(r"Population", fontsize=28)
axes.legend(loc=0, fontsize=12)
    
```



### 3.7.3 Fermionic Environments

Here we model a single fermion coupled to two electronic leads or reservoirs (e.g., this can describe a single quantum dot, a molecular transistor, etc). The system hamiltonian,  $H_{sys}$ , and bath spectral density,  $J_D$ , are

$$H_{sys} = c^\dagger c$$

$$J_D = \frac{\Gamma W^2}{(w - \mu)^2 + W^2},$$

We will demonstrate how to describe the bath using two different expansions of the spectral density correlation function (Matsubara's expansion and a Pad  expansion), how to evolve the system in time, and how to calculate the steady state.

Since our fermion is coupled to two reservoirs, we will construct two baths – one for each reservoir or lead – and call them the left ( $L$ ) and right ( $R$ ) baths for convenience. Each bath will have a different chemical potential  $\mu$  which we will label  $\mu_L$  and  $\mu_R$ .

First we will do this using the built-in implementations of the bath expansions, `LorentzianBath` and `LorentzianPadeBath`.

Afterwards, we will show how to calculate the bath expansion coefficients and to use those coefficients to construct your own bath description so that you can implement your own fermionic baths.

Our implementation of fermionic baths primarily follows the definitions used by Christian Schinabeck in his dissertation ( <https://opus4.kobv.de/opus4-fau/files/10984/DissertationChristianSchinabeck.pdf> ) and related publications.

A notebook containing a complete example similar to this one implemented in BoFiN can be found in [example notebook 4b](#).

## Describing the system and bath

First, let us construct the system Hamiltonian,  $H_{sys}$ , and the initial system state,  $\rho_0$ :

```
from qutip import basis, destroy

# The system Hamiltonian:
e1 = 1. # site energy
H_sys = e1 * destroy(2).dag() * destroy(2)

# Initial state of the system:
rho0 = basis(2,0) * basis(2,0).dag()
```

Now let us describe the bath properties:

```
# Shared bath properties:
gamma = 0.01 # coupling strength
W = 1.0 # cut-off
T = 0.025851991 # temperature
beta = 1. / T

# Chemical potentials for the two baths:
mu_L = 1.
mu_R = -1.

# System-bath coupling operator:
Q = destroy(2)
```

where  $\Gamma$  (gamma),  $W$  and  $T$  are the parameters of an Lorentzian bath,  $\mu_L$  (mu\_L) and  $\mu_R$  (mu\_R) are the chemical potentials of the left and right baths, and  $Q$  is the coupling operator between the system and the baths.

We may pass these parameters to either LorentzianBath or LorentzianPadeBath to construct an expansion of the bath correlations:

```
from qutip.solver.heom import LorentzianBath
from qutip.solver.heom import LorentzianPadeBath

# Number of expansion terms to retain:
Nk = 2

# Matsubara expansion:
bath_L = LorentzianBath(Q, gamma, W, mu_L, T, Nk, tag="L")
bath_R = LorentzianBath(Q, gamma, W, mu_R, T, Nk, tag="R")

# Padé expansion:
bath_L = LorentzianPadeBath(Q, gamma, W, mu_L, T, Nk, tag="L")
bath_R = LorentzianPadeBath(Q, gamma, W, mu_R, T, Nk, tag="R")
```

Where  $N_k$  is the number of terms to retain within the expansion of the bath.

Note that we have labelled each bath with a tag (either “L” or “R”) so that we can identify the exponents from individual baths later when calculating the currents between the system and the bath.

## System and bath dynamics

Now we are ready to construct a solver:

```
from qutip.solver.heom import HEOMSolver

max_depth = 5 # maximum hierarchy depth to retain
options = {"nsteps": 15_000}
baths = [bath_L, bath_R]

solver = HEOMSolver(H_sys, baths, max_depth=max_depth, options=options)
```

and to calculate the system evolution as a function of time:

```
tlist = [0, 10, 20] # times to evaluate the system state at
result = solver.run(rho0, tlist)
```

As in the bosonic case, the `max_depth` parameter determines how many levels of the hierarchy to retain.

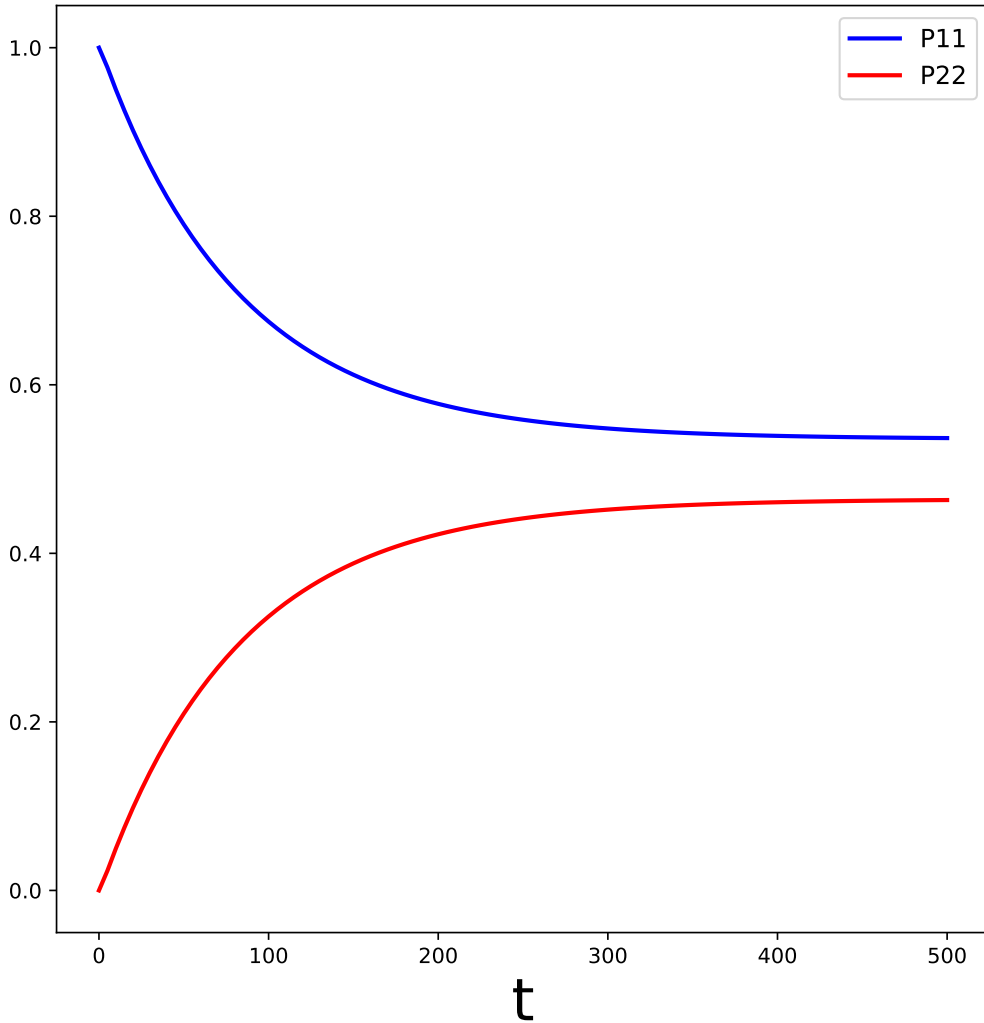
As in the bosonic case, we can specify `e_ops` in order to retrieve the expectation values of operators at each given time. See *System and bath dynamics* for a fuller description of the returned `result` object.

Below we run the solver again, but use `e_ops` to store the expectation values of the population of the system states:

```
# Define the operators that measure the populations of the two
# system states:
P11p = basis(2,0) * basis(2,0).dag()
P22p = basis(2,1) * basis(2,1).dag()

# Run the solver:
tlist = np.linspace(0, 500, 101)
result = solver.run(rho0, tlist, e_ops={"11": P11p, "22": P22p})

# Plot the results:
fig, axes = plt.subplots(1, 1, sharex=True, figsize=(8,8))
axes.plot(result.times, result.e_data["11"], 'b', linewidth=2, label="P11")
axes.plot(result.times, result.e_data["22"], 'r', linewidth=2, label="P22")
axes.set_xlabel(r't', fontsize=28)
axes.legend(loc=0, fontsize=12)
```



The plot above is not very exciting. What we would really like to see in this case are the currents between the system and the two baths. We will plot these in the next section using the auxiliary density operators (ADOs) returned by the solver.

### Determining currents

The currents between the system and a fermionic bath may be calculated from the first level auxiliary density operators (ADOs) associated with the exponents of that bath.

The contribution to the current into a given bath from each exponent in that bath is:

$$\text{Contribution from Exponent} = \pm i \text{Tr}(Q^\pm \cdot A)$$

where the  $\pm$  sign is the sign of the exponent (see the description later in *Padé expansion coefficients*) and  $Q^\pm$  is  $Q$  for + exponents and  $Q^\dagger$  for - exponents.

The first-level exponents for the left bath are retrieved by calling `.filter(tags=["L"])` on `ado_state` which is an instance of `HierarchyADOsState` and also provides access to the methods of `HierarchyADOs` which describes the structure of the hierarchy for a given problem.

Here the tag “L” matches the tag passed when constructing `bath_L` earlier in this example.

Similarly, we may calculate the current to the right bath from the exponents tagged with “R”.

```
def exp_current(aux, exp):
    """ Calculate the current for a single exponent. """
    sign = 1 if exp.type == exp.types["+"] else -1
    op = exp.Q if exp.type == exp.types["+"] else exp.Q.dag()
    return 1j * sign * (op * aux).tr()

def heom_current(tag, ado_state):
    """ Calculate the current between the system and the given bath. """
    level_1_ados = [
        (ado_state.extract(label), ado_state.exps(label)[0])
        for label in ado_state.filter(tags=[tag])
    ]
    return np.real(sum(exp_current(aux, exp) for aux, exp in level_1_ados))

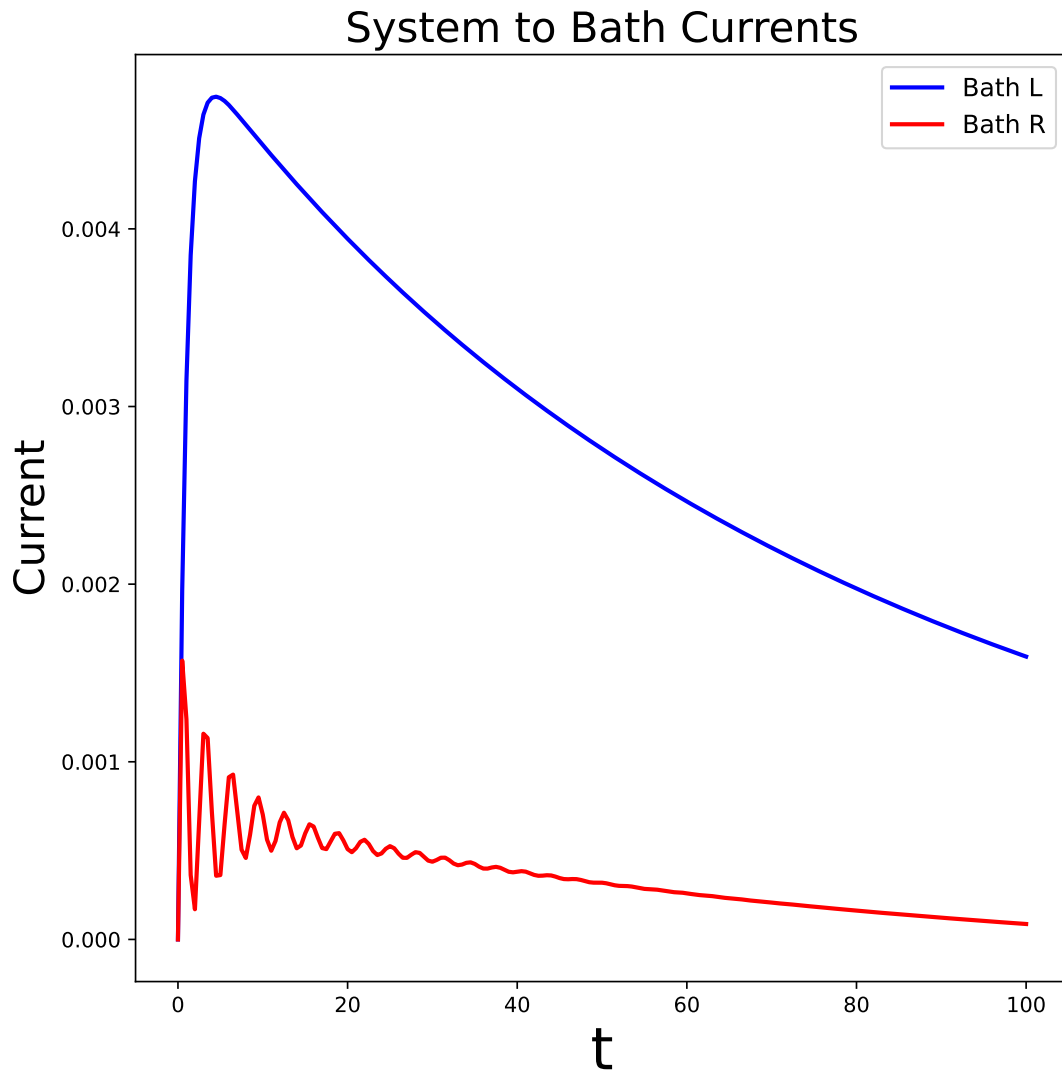
heom_left_current = lambda t, ado_state: heom_current("L", ado_state)
heom_right_current = lambda t, ado_state: heom_current("R", ado_state)
```

Once we have defined functions for retrieving the currents for the baths, we can pass them to `e_ops` and plot the results:

```
# Run the solver (returning ADO states):
tlist = np.linspace(0, 100, 201)
result = solver.run(rho0, tlist, e_ops={
    "left_currents": heom_left_current,
    "right_currents": heom_right_current,
})

# Plot the results:
fig, axes = plt.subplots(1, 1, sharex=True, figsize=(8,8))
axes.plot(
    result.times, result.e_data["left_currents"], 'b',
    linewidth=2, label=r"Bath L",
)
axes.plot(
    result.times, result.e_data["right_currents"], 'r',
    linewidth=2, label="Bath R",
)
axes.set_xlabel(r't', fontsize=28)
axes.set_ylabel(r'Current', fontsize=20)
axes.set_title(r'System to Bath Currents', fontsize=20)
axes.legend(loc=0, fontsize=12)
```





And now we have a more interesting plot that shows the currents to the left and right baths decaying towards their steady states!

In the next section, we will calculate the steady state currents directly.

### Steady state currents

Using the same solver, we can also determine the steady state of the combined system and bath using:

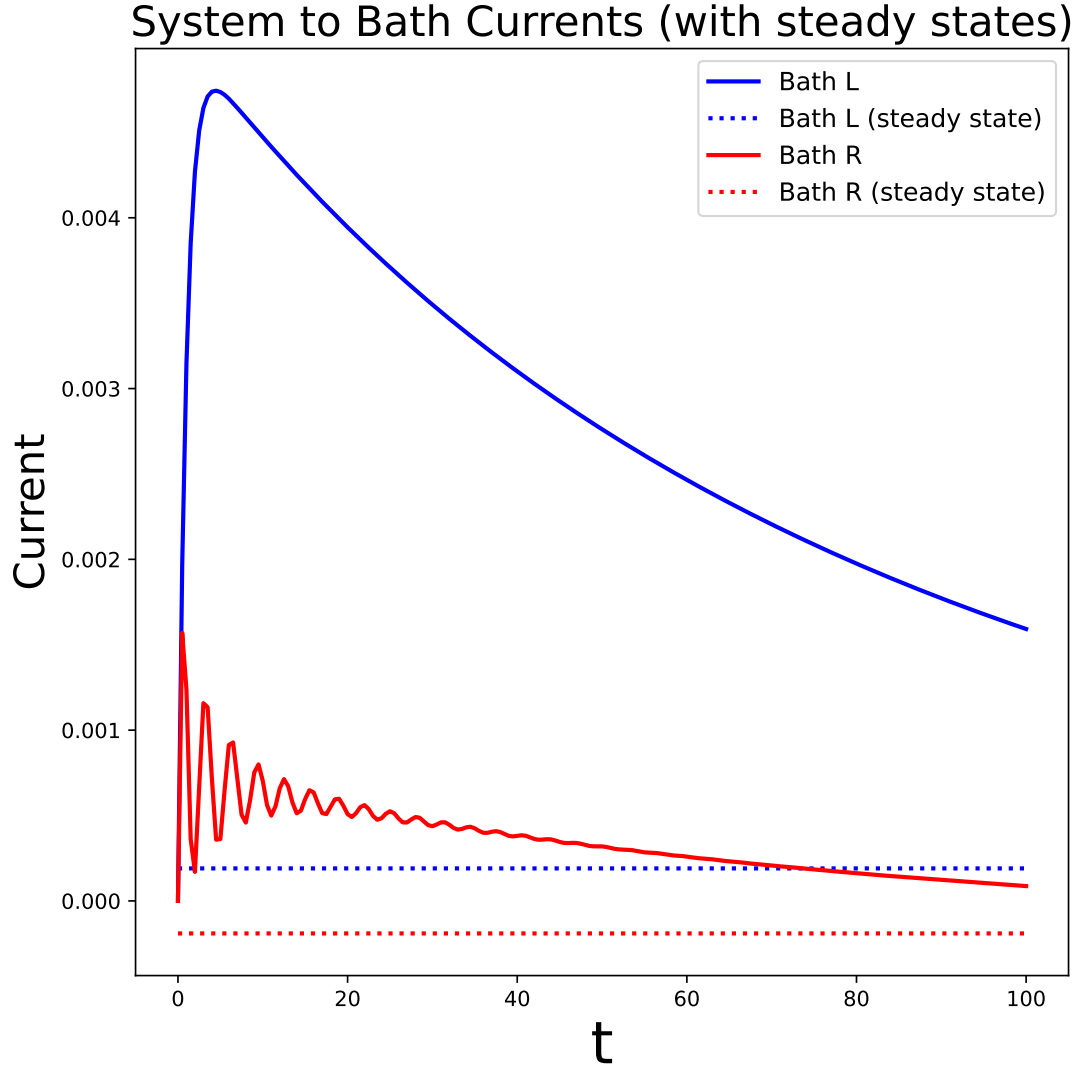
```
steady_state, steady_ados = solver.steady_state()
```

and calculate the steady state currents to the two baths from `steady_ados` using the same `heom_current` function we defined previously:

```
steady_state_current_left = heom_current("L", steady_ados)
steady_state_current_right = heom_current("R", steady_ados)
```

Now we can add the steady state currents to the previous plot:

```
# Plot the results and steady state currents:
fig, axes = plt.subplots(1, 1, sharex=True, figsize=(8,8))
axes.plot(
    result.times, result.e_data["left_currents"], 'b',
    linewidth=2, label=r"Bath L",
)
axes.plot(
    result.times, [steady_state_current_left] * len(result.times), 'b:',
    linewidth=2, label=r"Bath L (steady state)",
)
axes.plot(
    result.times, result.e_data["right_currents"], 'r',
    linewidth=2, label="Bath R",
)
axes.plot(
    result.times, [steady_state_current_right] * len(result.times), 'r:',
    linewidth=2, label=r"Bath R (steady state)",
)
axes.set_xlabel(r't', fontsize=28)
axes.set_ylabel(r'Current', fontsize=20)
axes.set_title(r'System to Bath Currents (with steady states)', fontsize=20)
axes.legend(loc=0, fontsize=12)
```



As you can see, there is still some way to go beyond  $t = 100$  before the steady state is reached!

### Padé expansion coefficients

We now look at how to calculate the correlation expansion coefficients for the Lorentzian spectral density ourselves. Once we have calculated the coefficients we can construct a *FermionicBath* directly from them. A similar procedure can be used to apply *HEOMSolver* to any fermionic bath for which we can calculate the expansion coefficients.

In the fermionic case we must discriminate between the order in which excitations are created within the bath, so we define two different correlation functions,  $C_+(t)$ , and  $C_-(t)$ :

$$C^\sigma(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega t} J(\omega) f_F[\sigma\beta(\omega - \mu)]$$

where  $\sigma$  is either + or - and,  $f_F$  is the Fermi distribution function, and  $J(\omega)$  is the Lorentzian spectral density we defined at the start.

The Fermi distribution function is:

$$f_F(x) = (\exp(x) + 1)^{-1}$$

As in the bosonic case we can approximate this integral with a Matsubara or Padé expansion. For the Lorentzian bath the Padé expansion converges much more quickly, so we will calculate the Padé expansion coefficients here.

The Padé decomposition approximates the Fermi distribution as:

$$f_F(x) \approx f_F^{\text{approx}}(x) = \frac{1}{2} - \sum_{l=0}^{Nk} \frac{2k_l x}{x^2 + \epsilon_l^2}$$

where  $k_l$  and  $\epsilon_l$  are coefficients defined in J. Chem Phys 133, “Efficient on the fly calculation of time correlation functions in computer simulations”, and  $Nk$  specifies the cut-off in the expansion.

Evaluating the integral for the correlation functions gives:

$$C^\sigma(t) \approx \sum_{l=0}^{Nk} \eta^{\sigma,l} e^{-\gamma_{\sigma,l} t}$$

where:

$$\eta_{\sigma,l} = \begin{cases} \frac{\Gamma W}{2} f_F^{\text{approx}}(i\beta W) & l = 0 \\ -i \cdot \frac{k_l}{\beta} \cdot \frac{\Gamma W^2}{-\frac{\epsilon_l^2}{\beta^2} + W^2} & l \neq 0 \end{cases}$$

$$\gamma_{\sigma,l} = \begin{cases} W - \sigma i\mu & l = 0 \\ \frac{\epsilon_l}{\beta} - \sigma i\mu & l \neq 0 \end{cases}$$

and  $\beta = \frac{1}{T}$ .

And now we calculate the same numbers in Python:

```
# Imports
from numpy.linalg import eigvalsh

# Convenience functions and parameters:
def deltafun(j, k):
    """ Kronecker delta function. """
    return 1.0 if j == k else 0.

def f_approx(x, Nk):
    """ Padé approximation to Fermi distribution. """
    f = 0.5
    for ll in range(1, Nk + 1):
        # kappa and epsilon are calculated further down
        f = f - 2 * kappa[ll] * x / (x**2 + epsilon[ll]**2)
    return f

def kappa_epsilon(Nk):
    """ Calculate kappa and epsilon coefficients. """

    alpha = np.zeros((2 * Nk, 2 * Nk))
    for j in range(2 * Nk):
        for k in range(2 * Nk):
            alpha[j][k] = (
                (deltafun(j, k + 1) + deltafun(j, k - 1))
                / np.sqrt((2 * (j + 1) - 1) * (2 * (k + 1) - 1))
            )

    eps = [-2. / val for val in eigvalsh(alpha)[:Nk]]

    alpha_p = np.zeros((2 * Nk - 1, 2 * Nk - 1))
    for j in range(2 * Nk - 1):
```

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```

    for k in range(2 * Nk - 1):
        alpha_p[j][k] = (
            (deltafun(j, k + 1) + deltafun(j, k - 1))
            / np.sqrt((2 * (j + 1) + 1) * (2 * (k + 1) + 1))
        )

    chi = [-2. / val for val in eigvalsh(alpha_p)[:Nk - 1]]

    eta_list = [
        0.5 * Nk * (2 * (Nk + 1) - 1) * (
            np.prod([chi[k]**2 - eps[j]**2 for k in range(Nk - 1)]) /
            np.prod([
                eps[k]**2 - eps[j]**2 + deltafun(j, k) for k in range(Nk)
            ])
        )
        for j in range(Nk)
    ]

    kappa = [0] + eta_list
    epsilon = [0] + eps

    return kappa, epsilon

kappa, epsilon = kappa_epsilon(Nk)

# Phew, we made it to function that calculates the coefficients for the
# correlation function expansions:

def C(sigma, mu, Nk):
    """ Calculate the expansion coefficients for C_\sigma. """
    beta = 1. / T
    ck = [0.5 * gamma * W * f_approx(1.0j * beta * W, Nk)]
    vk = [W - sigma * 1.0j * mu]
    for ll in range(1, Nk + 1):
        ck.append(
            -1.0j * (kappa[ll] / beta) * gamma * W**2
            / (-(epsilon[ll]**2 / beta**2) + W**2)
        )
        vk.append(epsilon[ll] / beta - sigma * 1.0j * mu)
    return ck, vk

ck_plus_L, vk_plus_L = C(1.0, mu_L, Nk) # C_+, left bath
ck_minus_L, vk_minus_L = C(-1.0, mu_L, Nk) # C_-, left bath

ck_plus_R, vk_plus_R = C(1.0, mu_R, Nk) # C_+, right bath
ck_minus_R, vk_minus_R = C(-1.0, mu_R, Nk) # C_-, right bath

```

Finally we are ready to construct the *FermionicBath*:

```

from qutip.solver.heom import FermionicBath

# Padé expansion:
bath_L = FermionicBath(Q, ck_plus_L, vk_plus_L, ck_minus_L, vk_minus_L)
bath_R = FermionicBath(Q, ck_plus_R, vk_plus_R, ck_minus_R, vk_minus_R)

```

And we're done!

The *FermionicBath* can be used with the *HEOMSolver* in exactly the same way as the baths we constructed previously using the built-in Lorentzian bath expansions.

### 3.7.4 Previous implementations

The current HEOM implementation in QuTiP is the latest in a succession of HEOM implementations by various contributors:

#### HSolverDL

The original HEOM solver was implemented by Neill Lambert, Anubhav Vardhan, and Alexander Pitchford. In QuTiP 4.7 it was still available as `qutip.solve.nonmarkov.dlheom_solver.HSolverDL` but the legacy implementation was removed in QuTiP 5.

It only directly provided support for the Drude-Lorentz bath although there was the possibility of sub-classing the solver to implement other baths.

A compatible interface using the current implementation is still available under the same name in `qutip.solver.heom.HSolverDL`.

#### BoFiN-HEOM

BoFiN-HEOM (the bosonic and fermionic HEOM solver) was a much more flexible re-write of the original QuTiP *HSolverDL* that added support for both bosonic and fermionic baths and for baths to be specified directly via their correlation function expansion coefficients. Its authors were Neill Lambert, Tarun Raheja, Shahnawaz Ahmed, and Alexander Pitchford.

BoFiN was written outside of QuTiP and is can still be found in its original repository at <https://github.com/tehruhn/bofin>.

The construction of the right-hand side matrix for BoFiN was slow, so BoFiN-fast, a hybrid C++ and Python implementation, was written that performed the right-hand side construction in C++. It was otherwise identical to the pure Python version. BoFiN-fast can be found at [https://github.com/tehruhn/bofin\\_fast](https://github.com/tehruhn/bofin_fast).

BoFiN also came with an extensive set of example notebooks that are available at <https://github.com/tehruhn/bofin/tree/main/examples>.

#### Current implementation

The current implementation is a rewrite of BoFiN in pure Python. It's right-hand side construction has similar speed to BoFiN-fast, but is written in pure Python. Built-in implementations of a variety of different baths are provided, and a single solver is used for both fermionic and bosonic baths. Multiple baths of either the same kind, or a mixture of fermionic and bosonic baths, may be specified in a single problem, and there is good support for working with the auxiliary density operator (ADO) state and extracting information from it.

The code was written by Neill Lambert and Simon Cross.

### 3.7.5 References

## 3.8 Solving for Steady-State Solutions

### 3.8.1 Introduction

For time-independent open quantum systems with decay rates larger than the corresponding excitation rates, the system will tend toward a steady state as  $t \rightarrow \infty$  that satisfies the equation

$$\frac{d\hat{\rho}_{ss}}{dt} = \mathcal{L}\hat{\rho}_{ss} = 0.$$

Although the requirement for time-independence seems quite restrictive, one can often employ a transformation to the interaction picture that yields a time-independent Hamiltonian. For many these systems, solving for the asymptotic density matrix  $\hat{\rho}_{ss}$  can be achieved using direct or iterative solution methods faster than using master equation or Monte Carlo simulations. Although the steady state equation has a simple mathematical form, the properties of the Liouvillian operator are such that the solutions to this equation are anything but straightforward to find.

### 3.8.2 Steady State solvers in QuTiP

In QuTiP, the steady-state solution for a system Hamiltonian or Liouvillian is given by `steadystate`. This function implements a number of different methods for finding the steady state, each with their own pros and cons, where the method used can be chosen using the `method` keyword argument.

Method	Keyword	Description
Direct (default)	'direct'	Direct solution solving $Ax = b$ .
Eigenvalue	'eigen'	Iteratively find the zero eigenvalue of $\mathcal{L}$ .
Inverse-Power	'power'	Solve using the inverse-power method.
SVD	'svd'	Steady-state solution via the <b>dense</b> SVD of the Liouvillian.

The function `steadystate` can take either a Hamiltonian and a list of collapse operators as input, generating internally the corresponding Liouvillian super operator in Lindblad form, or alternatively, a Liouvillian passed by the user.

Both the "direct" and "power" method need to solve a linear equation system. To do so, there are multiple solvers available: ``

Solver	Original function	Description
"solve"	<code>numpy.linalg.solve</code>	Dense solver from numpy.
"lstsq"	<code>numpy.linalg.lstsq</code>	Dense least-squares solver.
"spsolve"	<code>scipy.sparse.linalg.spsolve</code>	Sparse solver from scipy.
"gmres"	<code>scipy.sparse.linalg.gmres</code>	Generalized Minimal RESidual iterative solver.
"lgmres"	<code>scipy.sparse.linalg.lgmres</code>	LGMRES iterative solver.
"bicgstab"	<code>scipy.sparse.linalg.bicgstab</code>	BIConjugate Gradient STABILized iterative solver.
"mkl_spsolve"	<code>pardiso</code>	Intel Pardiso LU solver from MKL

QuTiP can take advantage of the Intel Pardiso LU solver in the Intel Math Kernel library that comes with the Anaconda (2.5+) and Intel Python distributions. This gives a substantial increase in performance compared with the standard SuperLU method used by SciPy. To verify that QuTiP can find the necessary libraries, one can check for `INTEL MKL Ext: True` in the QuTiP about box ([about](#)).

### 3.8.3 Using the Steadystate Solver

Solving for the steady state solution to the Lindblad master equation for a general system with `steadystate` can be accomplished using:

```
>>> rho_ss = steadystate(H, c_ops)
```

where `H` is a quantum object representing the system Hamiltonian, and `c_ops` is a list of quantum objects for the system collapse operators. The output, labelled as `rho_ss`, is the steady-state solution for the systems. If no other keywords are passed to the solver, the default 'direct' method is used with `numpy.linalg.solve`, generating a solution that is exact to machine precision at the expense of a large memory requirement. However Liouvillians are often quite sparse and using a sparse solver may be preferred:

```
rho_ss = steadystate(H, c_ops, method="power", solver="spsolve")
```

where `method='power'` indicates that we are using the inverse-power solution method, and `solver="spsolve"` indicate to use the sparse solver.

Sparse solvers may still use quite a large amount of memory when they factorize the matrix since the Liouvillian usually has a large bandwidth. To address this, `steadystate` allows one to use the bandwidth minimization algorithms listed in *Additional Solver Arguments*. For example:

```
rho_ss = steadystate(H, c_ops, solver="spsolve", use_rcm=True)
```

where `use_rcm=True` turns on a bandwidth minimization routine.

Although it is not obvious, the 'direct', 'eigen', and 'power' methods all use an LU decomposition internally and thus can have a large memory overhead. In contrast, iterative solvers such as the 'gmres', 'lgmres', and 'bicgstab' do not factor the matrix and thus take less memory than the LU methods and allow, in principle, for extremely large system sizes. The downside is that these methods can take much longer than the direct method as the condition number of the Liouvillian matrix is large, indicating that these iterative methods require a large number of iterations for convergence. To overcome this, one can use a preconditioner  $M$  that solves for an approximate inverse for the (modified) Liouvillian, thus better conditioning the problem, leading to faster convergence. The use of a preconditioner can actually make these iterative methods faster than the other solution methods. The problem with preconditioning is that it is only well defined for Hermitian matrices. Since the Liouvillian is non-Hermitian, the ability to find a good preconditioner is not guaranteed. And moreover, if a preconditioner is found, it is not guaranteed to have a good condition number. QuTiP can make use of an incomplete LU preconditioner when using the iterative 'gmres', 'lgmres', and 'bicgstab' solvers by setting `use_precond=True`. The preconditioner optionally makes use of a combination of symmetric and anti-symmetric matrix permutations that attempt to improve the preconditioning process. These features are discussed in the *Additional Solver Arguments* section. Even with these state-of-the-art permutations, the generation of a successful preconditioner for non-symmetric matrices is currently a trial-and-error process due to the lack of mathematical work done in this area. It is always recommended to begin with the direct solver with no additional arguments before selecting a different method.

Finding the steady-state solution is not limited to the Lindblad form of the master equation. Any time-independent Liouvillian constructed from a Hamiltonian and collapse operators can be used as an input:

```
>>> rho_ss = steadystate(L)
```

where `L` is the Liouvillian. All of the additional arguments can also be used in this case.



### 3.8.4 Additional Solver Arguments

The following additional solver arguments are available for the steady-state solver:

Key-word	Default	Description
weight	None	Set the weighting factor used in the 'direct' method.
use_precc	False	Generate a preconditioner when using the 'gmres' and 'lgmres' methods.
use_rcm	False	Use a Reverse Cuthill-Mckee reordering to minimize the bandwidth of the modified Liouvillian used in the LU decomposition.
use_wbm	False	Use a Weighted Bipartite Matching algorithm to attempt to make the modified Liouvillian more diagonally dominant, and thus for favorable for preconditioning.
power_tol	1e-12	Tolerance for the solution when using the 'power' method.
power_max	10	Maximum number of iterations of the power method.
power_ep	1e-15	Small weight used in the "power" method.
**kwargs	{}	Options to pass through the linalg solvers. See the corresponding documentation from scipy for a full list.

Further information can be found in the [steadystate](#) docstrings.

### 3.8.5 Example: Harmonic Oscillator in Thermal Bath

A simple example of a system that reaches a steady state is a harmonic oscillator coupled to a thermal environment. Below we consider a harmonic oscillator, initially in the  $|10\rangle$  number state, and weakly coupled to a thermal environment characterized by an average particle expectation value of  $\langle n \rangle = 2$ . We calculate the evolution via master equation and Monte Carlo methods, and see that they converge to the steady-state solution. Here we choose to perform only a few Monte Carlo trajectories so we can distinguish this evolution from the master-equation solution.

```
import numpy as np
import matplotlib.pyplot as plt

import qutip

# Define parameters
N = 20 # number of basis states to consider
a = qutip.destroy(N)
H = a.dag() * a
psi0 = qutip.basis(N, 10) # initial state
kappa = 0.1 # coupling to oscillator

# collapse operators
c_op_list = []
n_th_a = 2 # temperature with average of 2 excitations
rate = kappa * (1 + n_th_a)
if rate > 0.0:
    c_op_list.append(np.sqrt(rate) * a) # decay operators
rate = kappa * n_th_a
if rate > 0.0:
    c_op_list.append(np.sqrt(rate) * a.dag()) # excitation operators

# find steady-state solution
final_state = qutip.steadystate(H, c_op_list)
```

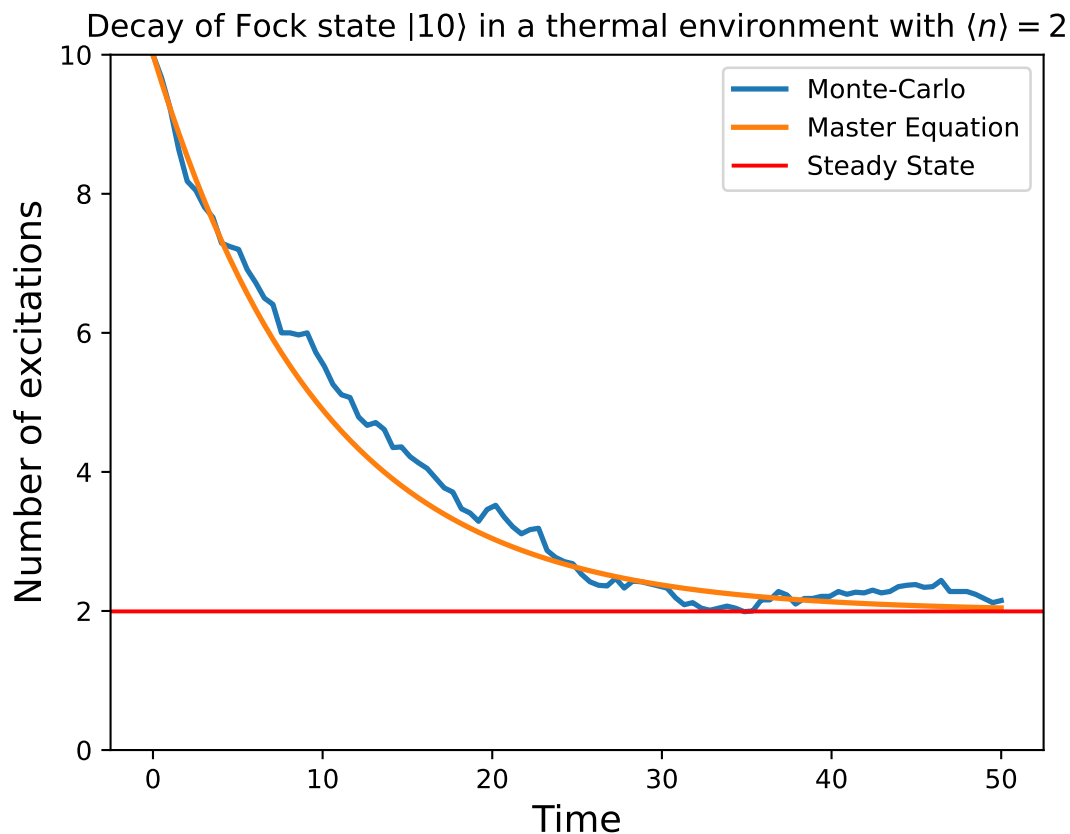
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```
# find expectation value for particle number in steady state
fexpt = qutip.expect(a.dag() * a, final_state)

tlist = np.linspace(0, 50, 100)
# monte-carlo
mcdata = qutip.mcsolve(H, psi0, tlist, c_op_list, [a.dag() * a], ntraj=100)
# master eq.
medata = qutip.mesolve(H, psi0, tlist, c_op_list, [a.dag() * a])

plt.plot(tlist, mcdata.expect[0], tlist, medata.expect[0], lw=2)
# plot steady-state expt. value as horizontal line (should be = 2)
plt.axhline(y=fexpt, color='r', lw=1.5)
plt.ylim([0, 10])
plt.xlabel('Time', fontsize=14)
plt.ylabel('Number of excitations', fontsize=14)
plt.legend(('Monte-Carlo', 'Master Equation', 'Steady State'))
plt.title(
    r'Decay of Fock state  $|\left|10\right\rangle$  in a thermal environment with  $\langle n \rangle = 2$ '
)
plt.show()
```



## 3.9 Permutational Invariance

### 3.9.1 Permutational Invariant Quantum Solver (PIQS)

The *Permutational Invariant Quantum Solver (PIQS)* is a QuTiP module that allows to study the dynamics of an open quantum system consisting of an ensemble of identical qubits that can dissipate through local and collective baths according to a Lindblad master equation.

The Liouvillian of an ensemble of  $N$  qubits, or two-level systems (TLSs),  $\mathcal{D}_{TLS}(\rho)$ , can be built using only polynomial – instead of exponential – resources. This has many applications for the study of realistic quantum optics models of many TLSs and in general as a tool in cavity QED.

Consider a system evolving according to the equation

$$\begin{aligned} \dot{\rho} = \mathcal{D}_{TLS}(\rho) = & -\frac{i}{\hbar}[H, \rho] + \frac{\gamma_{CE}}{2}\mathcal{L}_{J_-}[\rho] + \frac{\gamma_{CD}}{2}\mathcal{L}_{J_z}[\rho] + \frac{\gamma_{CP}}{2}\mathcal{L}_{J_+}[\rho] \\ & + \sum_{n=1}^N \left( \frac{\gamma_E}{2}\mathcal{L}_{J_{-,n}}[\rho] + \frac{\gamma_D}{2}\mathcal{L}_{J_{z,n}}[\rho] + \frac{\gamma_P}{2}\mathcal{L}_{J_{+,n}}[\rho] \right) \end{aligned}$$

where  $J_{\alpha,n} = \frac{1}{2}\sigma_{\alpha,n}$  are SU(2) Pauli spin operators, with  $\alpha = x, y, z$  and  $J_{\pm,n} = \sigma_{\pm,n}$ . The collective spin operators are  $J_{\alpha} = \sum_n J_{\alpha,n}$ . The Lindblad super-operators are  $\mathcal{L}_A = 2A\rho A^\dagger - A^\dagger A\rho - \rho A^\dagger A$ .

The inclusion of local processes in the dynamics lead to using a Liouvillian space of dimension  $4^N$ . By exploiting the permutational invariance of identical particles [2-8], the Liouvillian  $\mathcal{D}_{TLS}(\rho)$  can be built as a block-diagonal matrix in the basis of Dicke states  $|j, m\rangle$ .

The system under study is defined by creating an object of the *Dicke* class, e.g. simply named `system`, whose first attribute is

- `system.N`, the number of TLSs of the system  $N$ .

The rates for collective and local processes are simply defined as

- `collective_emission` defines  $\gamma_{CE}$ , collective (superradiant) emission
- `collective_dephasing` defines  $\gamma_{CD}$ , collective dephasing
- `collective_pumping` defines  $\gamma_{CP}$ , collective pumping.
- `emission` defines  $\gamma_E$ , incoherent emission (losses)
- `dephasing` defines  $\gamma_D$ , local dephasing
- `pumping` defines  $\gamma_P$ , incoherent pumping.

Then the `system.lindbladian()` creates the total TLS Lindbladian superoperator matrix. Similarly, `system.hamiltonian` defines the TLS hamiltonian of the system  $H_{TLS}$ .

The system's Liouvillian can be built using `system.liouvillian()`. The properties of a `Piqs` object can be visualized by simply calling `system`. We give two basic examples on the use of *PIQS*. In the first example the incoherent emission of  $N$  driven TLSs is considered.

```
from qutip import piqs
N = 10
system = piqs.Dicke(N, emission = 1, pumping = 2)
L = system.liouvillian()
steady = steadystate(L)
```

For more example of use, see the “Permutational Invariant Lindblad Dynamics” section in the tutorials section of the website, <https://qutip.org/tutorials.html>.

Table 2: Useful PIQS functions.

Operators	Command	Description
Collective spin algebra $J_x, J_y, J_z$	<code>jspin(N)</code>	The collective spin algebra $J_x, J_y, J_z$ for $N$ TLSs
Collective spin $J_x$	<code>jspin(N, "x")</code>	The collective spin operator $J_x$ . Requires $N$ number of TLSs
Collective spin $J_y$	<code>jspin(N, "y")</code>	The collective spin operator $J_y$ . Requires $N$ number of TLSs
Collective spin $J_z$	<code>jspin(N, "z")</code>	The collective spin operator $J_z$ . Requires $N$ number of TLSs
Collective spin $J_+$	<code>jspin(N, "+")</code>	The collective spin operator $J_+$ .
Collective spin $J_-$	<code>jspin(N, "-")</code>	The collective spin operator $J_-$ .
Collective spin $J_z$ in uncoupled basis	<code>jspin(N, "z", basis='uncoupled')</code>	The collective spin operator $J_z$ in the uncoupled basis of dimension $2^N$ .
Dicke state $ j, m\rangle$ density matrix	<code>dicke(N, j, m)</code>	The density matrix for the Dicke state given by $ j, m\rangle$
Excited-state density matrix in Dicke basis	<code>excited(N)</code>	The excited state in the Dicke basis
Excited-state density matrix in uncoupled basis	<code>excited(N, basis="uncoupled")</code>	The excited state in the uncoupled basis
Ground-state density matrix in Dicke basis	<code>ground(N)</code>	The ground state in the Dicke basis
GHZ-state density matrix in the Dicke basis	<code>ghz(N)</code>	The GHZ-state density matrix in the Dicke (default) basis for $N$ number of TLS
Collapse operators of the ensemble	<code>Dicke.c_ops()</code>	The collapse operators for the ensemble can be called by the <code>c_ops</code> method of the Dicke class.

Note that the mathematical object representing the density matrix of the full system that is manipulated (or obtained from *steadystate*) in the Dicke-basis formalism used here is a *representative of the density matrix*. This *representative object* is of linear size  $N^2$ , whereas the full density matrix is defined over a  $2^N$  Hilbert space. In order to calculate nonlinear functions of such density matrix, such as the Von Neumann entropy or the purity, it is necessary to take into account the degeneracy of each block of such block-diagonal density matrix. Note that as long as one calculates expected values of operators, being  $\text{Tr}[A \cdot \rho]$  a *linear* function of  $\rho$ , the *representative density matrix* give straightforwardly the correct result. When a *nonlinear* function of the density matrix needs to be calculated, one needs to weigh each degenerate block correctly; this is taken care by the `dicke_function_trace` in `piqs`, and the user can use it to define general nonlinear functions that can be described as the trace of a Taylor expandable function. Two nonlinear functions that use `dicke_function_trace` and are already implemented are `purity_dicke`, to calculate the purity of a density matrix in the Dicke basis, and `entropy_vn_dicke`, which can be used to calculate the Von Neumann entropy.

More functions relative to the `qutip.piqs` module can be found at [API documentation](#). Attributes to the `piqs.Dicke` and `piqs.Pim` class can also be found there.

## 3.10 Two-time correlation functions

With the QuTiP time-evolution functions (for example `mesolve` and `mcsolve`), a state vector or density matrix can be evolved from an initial state at  $t_0$  to an arbitrary time  $t$ ,  $\rho(t) = V(t, t_0) \{\rho(t_0)\}$ , where  $V(t, t_0)$  is the propagator defined by the equation of motion. The resulting density matrix can then be used to evaluate the expectation values of arbitrary combinations of *same-time* operators.

To calculate *two-time* correlation functions on the form  $\langle A(t + \tau)B(t) \rangle$ , we can use the quantum regression theorem (see, e.g., [Gar03]) to write

$$\langle A(t + \tau)B(t) \rangle = \text{Tr}[AV(t + \tau, t) \{B\rho(t)\}] = \text{Tr}[AV(t + \tau, t) \{BV(t, 0) \{\rho(0)\}\}]$$

We therefore first calculate  $\rho(t) = V(t, 0) \{\rho(0)\}$  using one of the QuTiP evolution solvers with  $\rho(0)$  as initial state, and then again use the same solver to calculate  $V(t + \tau, t) \{B\rho(t)\}$  using  $B\rho(t)$  as initial state.

Note that if the initial state is the steady state, then  $\rho(t) = V(t, 0) \{\rho_{ss}\} = \rho_{ss}$  and

$$\langle A(t + \tau)B(t) \rangle = \text{Tr} [AV(t + \tau, t) \{B\rho_{ss}\}] = \text{Tr} [AV(\tau, 0) \{B\rho_{ss}\}] = \langle A(\tau)B(0) \rangle,$$

which is independent of  $t$ , so that we only have one time coordinate  $\tau$ .

QuTiP provides a family of functions that assists in the process of calculating two-time correlation functions. The available functions and their usage is shown in the table below. Each of these functions can use one of the following evolution solvers: Master-equation, Exponential series and the Monte-Carlo. The choice of solver is defined by the optional argument `solver`.

QuTiP function	Correlation function
<code>qutip.correlation_2op_2t</code>	$\langle A(t + \tau)B(t) \rangle$ or $\langle A(t)B(t + \tau) \rangle$ .
<code>qutip.correlation_2op_1t</code>	$\langle A(\tau)B(0) \rangle$ or $\langle A(0)B(\tau) \rangle$ .
<code>qutip.correlation_3op_1t</code>	$\langle A(0)B(\tau)C(0) \rangle$ .
<code>qutip.correlation_3op_2t</code>	$\langle A(t)B(t + \tau)C(t) \rangle$ .
<code>qutip.correlation_3op</code>	$\langle A(t)B(t + \tau)C(t) \rangle$ .

The most common use-case is to calculate the two time correlation function  $\langle A(\tau)B(0) \rangle$ . `correlation_2op_1t` performs this task with sensible default values, but only allows using the `mesolve` solver. From QuTiP 5.0 we added `correlation_3op`. This function can also calculate correlation functions with two or three operators and with one or two times. Most importantly, this function accepts alternative solvers such as `brmesolve`.

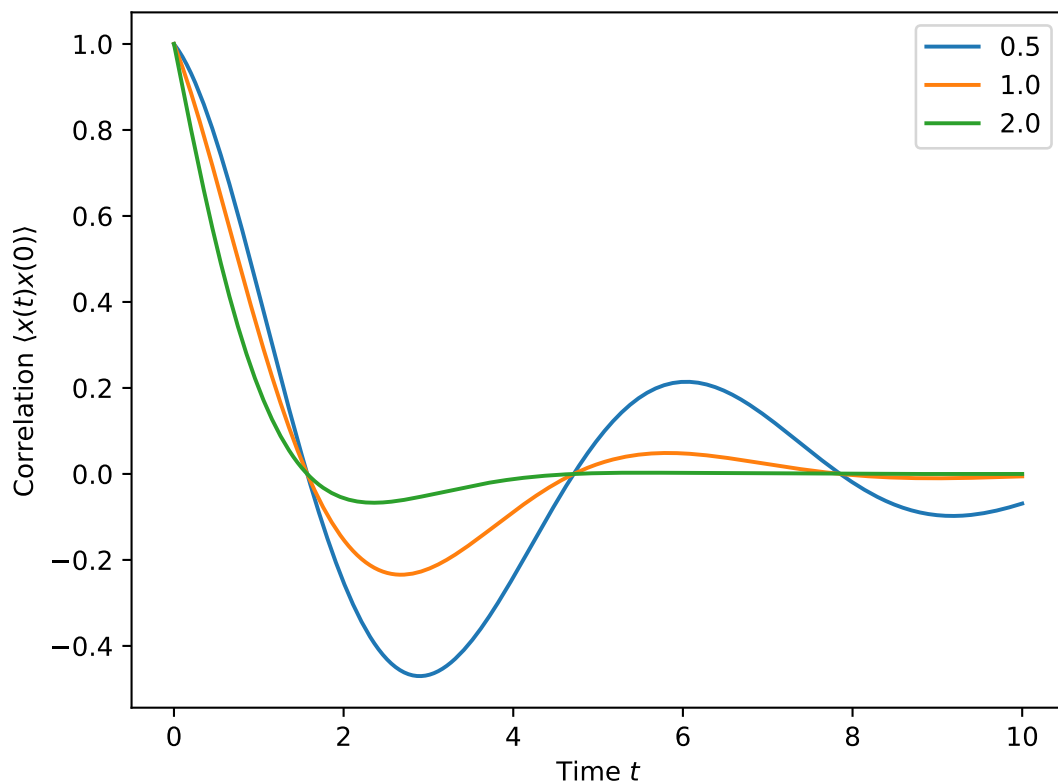
### 3.10.1 Steadystate correlation function

The following code demonstrates how to calculate the  $\langle x(t)x(0) \rangle$  correlation for a leaky cavity with three different relaxation rates.

```
times = np.linspace(0, 10.0, 200)
a = destroy(10)
x = a.dag() + a
H = a.dag() * a

corr1 = correlation_2op_1t(H, None, times, [np.sqrt(0.5) * a], x, x)
corr2 = correlation_2op_1t(H, None, times, [np.sqrt(1.0) * a], x, x)
corr3 = correlation_2op_1t(H, None, times, [np.sqrt(2.0) * a], x, x)

plt.figure()
plt.plot(times, np.real(corr1))
plt.plot(times, np.real(corr2))
plt.plot(times, np.real(corr3))
plt.legend(['0.5', '1.0', '2.0'])
plt.xlabel(r'Time $t$')
plt.ylabel(r'Correlation $\langle x(t)x(0) \rangle$')
plt.show()
```



### 3.10.2 Emission spectrum

Given a correlation function  $\langle A(\tau)B(0) \rangle$  we can define the corresponding power spectrum as

$$S(\omega) = \int_{-\infty}^{\infty} \langle A(\tau)B(0) \rangle e^{-i\omega\tau} d\tau.$$

In QuTiP, we can calculate  $S(\omega)$  using either `spectrum`, which first calculates the correlation function using one of the time-dependent solvers and then performs the Fourier transform semi-analytically, or we can use the function `spectrum_correlation_fft` to numerically calculate the Fourier transform of a given correlation data using FFT.

The following example demonstrates how these two functions can be used to obtain the emission power spectrum.

```
import numpy as np
from matplotlib import pyplot
import qutip

N = 4                                # number of cavity fock states
wc = wa = 1.0 * 2 * np.pi          # cavity and atom frequency
g = 0.1 * 2 * np.pi                 # coupling strength
kappa = 0.75                         # cavity dissipation rate
gamma = 0.25                         # atom dissipation rate

# Jaynes-Cummings Hamiltonian
a = qutip.tensor(qutip.destroy(N), qutip.qeye(2))
sm = qutip.tensor(qutip.qeye(N), qutip.destroy(2))
H = wc*a.dag()*a + wa*sm.dag()*sm + g*(a.dag()*sm + a*sm.dag())
```

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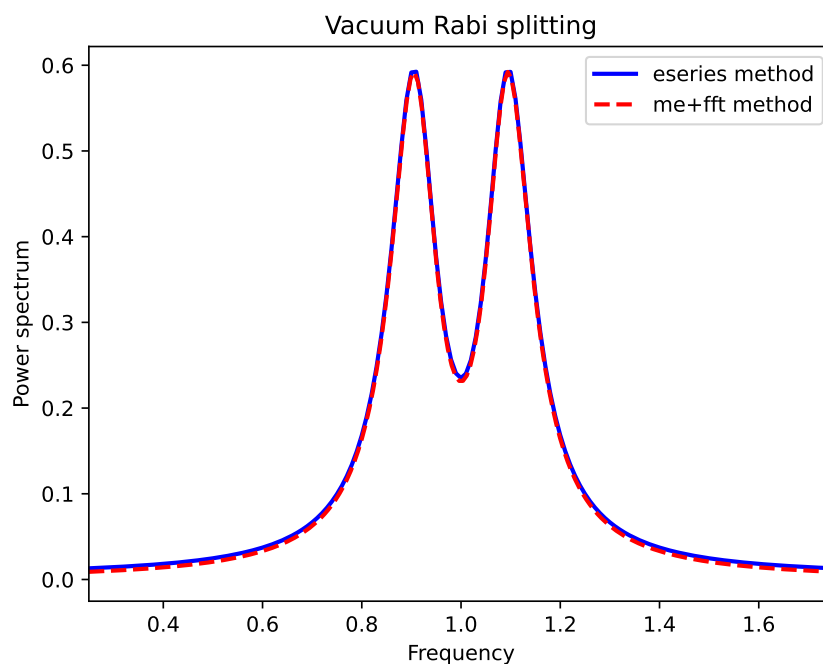
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```
# collapse operators
n_th = 0.25
c_ops = [
    np.sqrt(kappa * (1 + n_th)) * a,
    np.sqrt(kappa * n_th) * a.dag(),
    np.sqrt(gamma) * sm,
]

# calculate the correlation function using the mesolve solver, and then fft to
# obtain the spectrum. Here we need to make sure to evaluate the correlation
# function for a sufficient long time and sufficiently high sampling rate so
# that the discrete Fourier transform (FFT) captures all the features in the
# resulting spectrum.
tlist = np.linspace(0, 100, 5000)
corr = qutip.correlation_2op_1t(H, None, tlist, c_ops, a.dag(), a)
wlist1, spec1 = qutip.spectrum_correlation_fft(tlist, corr)

# calculate the power spectrum using spectrum, which internally uses essolve
# to solve for the dynamics (by default)
wlist2 = np.linspace(0.25, 1.75, 200) * 2 * np.pi
spec2 = qutip.spectrum(H, wlist2, c_ops, a.dag(), a)

# plot the spectra
fig, ax = pyplot.subplots(1, 1)
ax.plot(wlist1 / (2 * np.pi), spec1, 'b', lw=2, label='eseries method')
ax.plot(wlist2 / (2 * np.pi), spec2, 'r--', lw=2, label='me+fft method')
ax.legend()
ax.set_xlabel('Frequency')
ax.set_ylabel('Power spectrum')
ax.set_title('Vacuum Rabi splitting')
ax.set_xlim(wlist2[0]/(2*np.pi), wlist2[-1]/(2*np.pi))
plt.show()
```



### 3.10.3 Non-steadystate correlation function

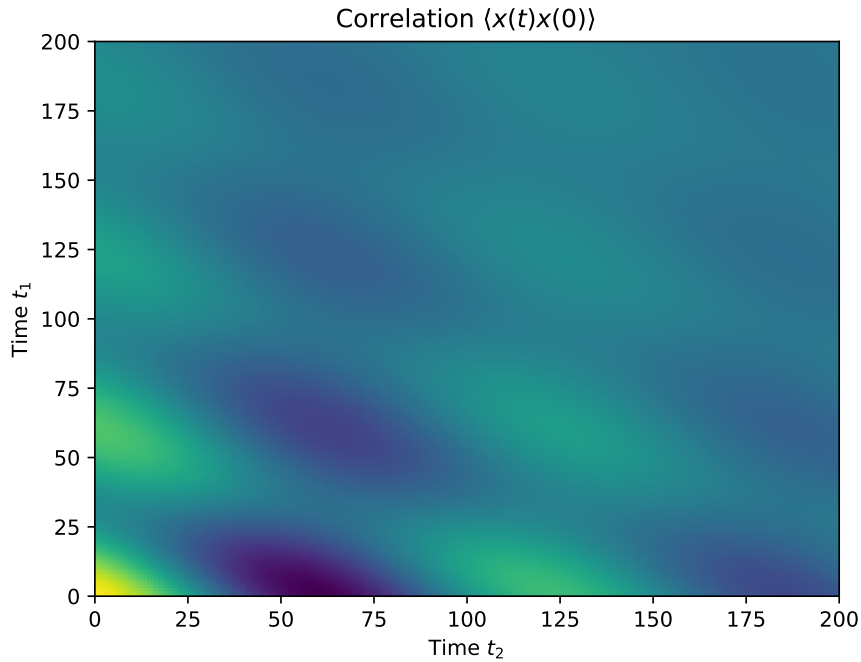
More generally, we can also calculate correlation functions of the kind  $\langle A(t_1 + t_2)B(t_1) \rangle$ , i.e., the correlation function of a system that is not in its steady state. In QuTiP, we can evaluate such correlation functions using the function `correlation_2op_2t`. The default behavior of this function is to return a matrix with the correlations as a function of the two time coordinates ( $t_1$  and  $t_2$ ).

```
import numpy as np
import matplotlib.pyplot as plt
import qutip

times = np.linspace(0, 10.0, 200)
a = qutip.destroy(10)
x = a.dag() + a
H = a.dag() * a
alpha = 2.5
rho0 = qutip.coherent_dm(10, alpha)
corr = qutip.correlation_2op_2t(H, rho0, times, times, [np.sqrt(0.25) * a], x, x)

plt.pcolor(np.real(corr))
plt.xlabel(r'Time $t_2$')
plt.ylabel(r'Time $t_1$')
plt.title(r'Correlation $\langle x(t)x(0) \rangle$')
plt.show()
```





However, in some cases we might be interested in the correlation functions on the form  $\langle A(t_1 + t_2)B(t_1) \rangle$ , but only as a function of time coordinate  $t_2$ . In this case we can also use the `correlation_2op_2t` function, if we pass the density matrix at time  $t_1$  as second argument, and `None` as third argument. The `correlation_2op_2t` function then returns a vector with the correlation values corresponding to the times in `taulist` (the fourth argument).

### Example: first-order optical coherence function

This example demonstrates how to calculate a correlation function on the form  $\langle A(\tau)B(0) \rangle$  for a non-steady initial state. Consider an oscillator that is interacting with a thermal environment. If the oscillator initially is in a coherent state, it will gradually decay to a thermal (incoherent) state. The amount of coherence can be quantified using the first-order optical coherence function  $g^{(1)}(\tau) = \frac{\langle a^\dagger(\tau)a(0) \rangle}{\sqrt{\langle a^\dagger(\tau)a(\tau) \rangle \langle a^\dagger(0)a(0) \rangle}}$ . For a coherent state  $|g^{(1)}(\tau)| = 1$ , and for a completely incoherent (thermal) state  $g^{(1)}(\tau) = 0$ . The following code calculates and plots  $g^{(1)}(\tau)$  as a function of  $\tau$ .

```
import numpy as np
import matplotlib.pyplot as plt
import qutip

N = 15
taus = np.linspace(0, 10.0, 200)
a = qutip.destroy(N)
H = 2 * np.pi * a.dag() * a

# collapse operator
G1 = 0.75
n_th = 2.00 # bath temperature in terms of excitation number
c_ops = [np.sqrt(G1 * (1 + n_th)) * a, np.sqrt(G1 * n_th) * a.dag()]

# start with a coherent state
rho0 = qutip.coherent_dm(N, 2.0)

# first calculate the occupation number as a function of time
```

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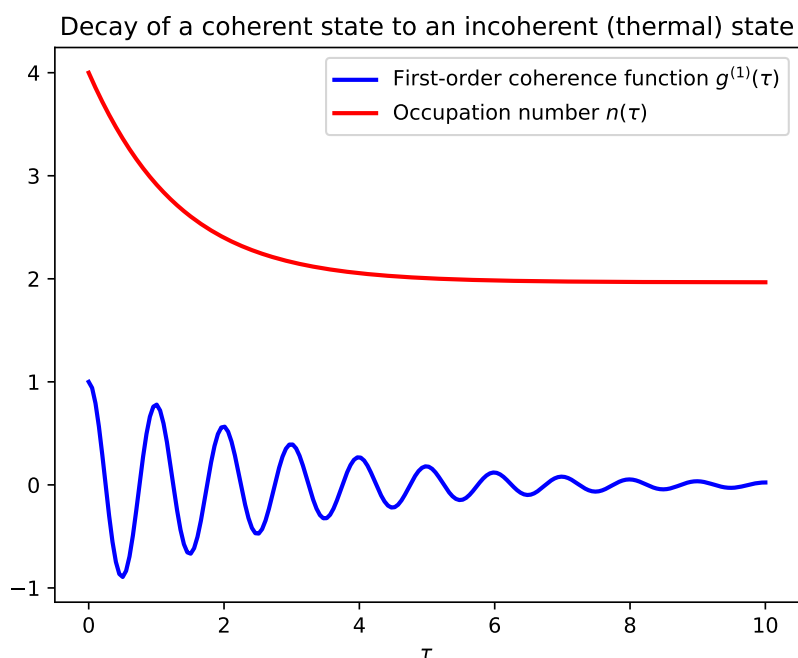
```

n = qutip.mesolve(H, rho0, taus, c_ops, [a.dag() * a]).expect[0]

# calculate the correlation function G1 and normalize with n to obtain g1
G1 = qutip.correlation_2op_1t(H, rho0, taus, c_ops, a.dag(), a)
g1 = np.array(G1) / np.sqrt(n[0] * np.array(n))

plt.plot(taus, np.real(g1), 'b', lw=2)
plt.plot(taus, n, 'r', lw=2)
plt.title('Decay of a coherent state to an incoherent (thermal) state')
plt.xlabel(r'$\tau$')
plt.legend([
    r'First-order coherence function $g^{(1)}(\tau)$',
    r'Occupation number $n(\tau)$',
])
plt.show()

```



For convenience, the steps for calculating the first-order coherence function have been collected in the function `coherence_function_g1`.

### Example: second-order optical coherence function

The second-order optical coherence function, with time-delay  $\tau$ , is defined as

$$g^{(2)}(\tau) = \frac{\langle a^\dagger(0)a^\dagger(\tau)a(\tau)a(0) \rangle}{\langle a^\dagger(0)a(0) \rangle^2}$$

For a coherent state  $g^{(2)}(\tau) = 1$ , for a thermal state  $g^{(2)}(\tau = 0) = 2$  and it decreases as a function of time (bunched photons, they tend to appear together), and for a Fock state with  $n$  photons  $g^{(2)}(\tau = 0) = n(n - 1)/n^2 < 1$  and it increases with time (anti-bunched photons, more likely to arrive separated in time).

To calculate this type of correlation function with QuTiP, we can use `correlation_3op_1t`, which computes a correlation function on the form  $\langle A(0)B(\tau)C(0) \rangle$  (three operators, one delay-time vector). We first have to

combine the central two operators into one single one as they are evaluated at the same time, e.g. here we do  $a^\dagger(\tau)a(\tau) = (a^\dagger a)(\tau)$ .

The following code calculates and plots  $g^{(2)}(\tau)$  as a function of  $\tau$  for a coherent, thermal and Fock state.

```
import numpy as np
import matplotlib.pyplot as plt
import qutip

N = 25
taus = np.linspace(0, 25.0, 200)
a = qutip.destroy(N)
H = 2 * np.pi * a.dag() * a

kappa = 0.25
n_th = 2.0 # bath temperature in terms of excitation number
c_ops = [np.sqrt(kappa * (1 + n_th)) * a, np.sqrt(kappa * n_th) * a.dag()]

states = [
    {'state': qutip.coherent_dm(N, np.sqrt(2)), 'label': "coherent state"},
    {'state': qutip.thermal_dm(N, 2), 'label': "thermal state"},
    {'state': qutip.fock_dm(N, 2), 'label': "Fock state"},
]

fig, ax = plt.subplots(1, 1)

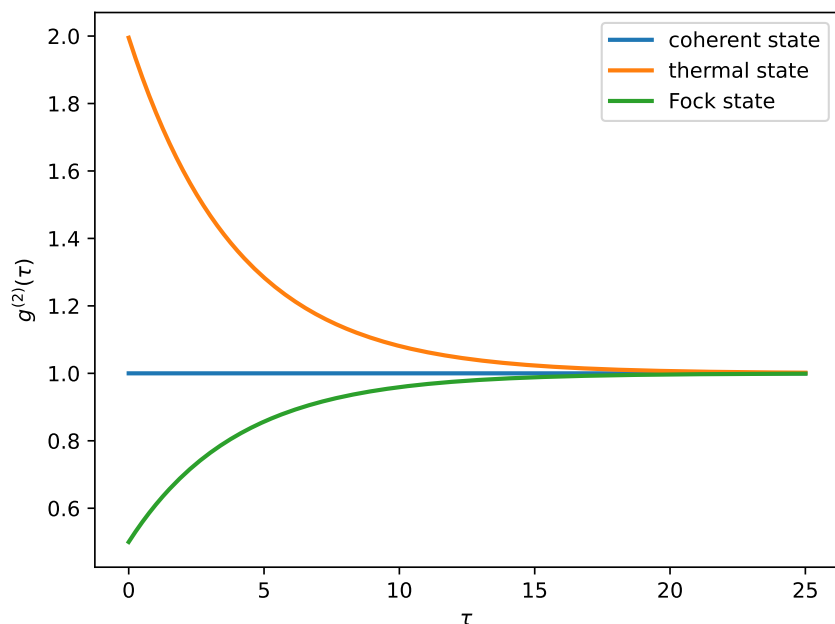
for state in states:
    rho0 = state['state']

    # first calculate the occupation number as a function of time
    n = qutip.mesolve(H, rho0, taus, c_ops, [a.dag() * a]).expect[0]

    # calculate the correlation function G2 and normalize with n(0)n(t) to
    # obtain g2
    G2 = qutip.correlation_3op_1t(H, rho0, taus, c_ops, a.dag(), a.dag()*a, a)
    g2 = np.array(G2) / (n[0] * np.array(n))

    ax.plot(taus, np.real(g2), label=state['label'], lw=2)

ax.legend(loc=0)
ax.set_xlabel(r'$\tau$')
ax.set_ylabel(r'$g^{(2)}(\tau)$')
plt.show()
```



For convenience, the steps for calculating the second-order coherence function have been collected in the function `coherence_function_g2`.

## 3.11 Plotting on the Bloch Sphere

### 3.11.1 Introduction

When studying the dynamics of a two-level system, it is often convenient to visualize the state of the system by plotting the state-vector or density matrix on the Bloch sphere. In QuTiP, there is a class to allow for easy creation and manipulation of data sets, both vectors and data points, on the Bloch sphere.

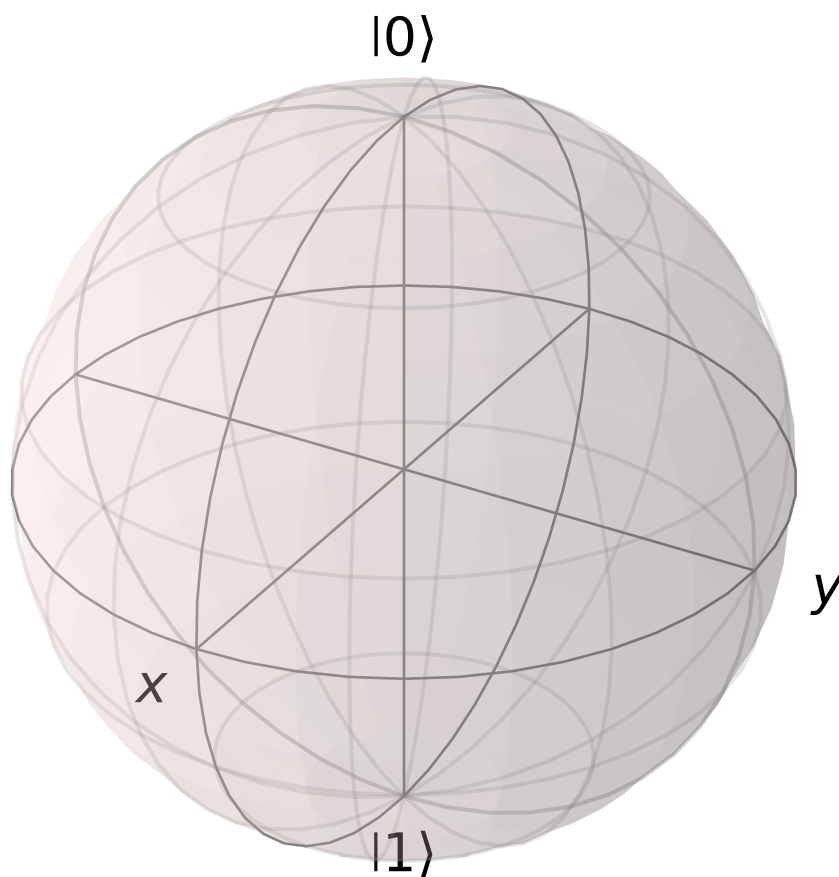
### 3.11.2 The Bloch Class

In QuTiP, creating a Bloch sphere is accomplished by calling either:

```
b = qutip.Bloch()
```

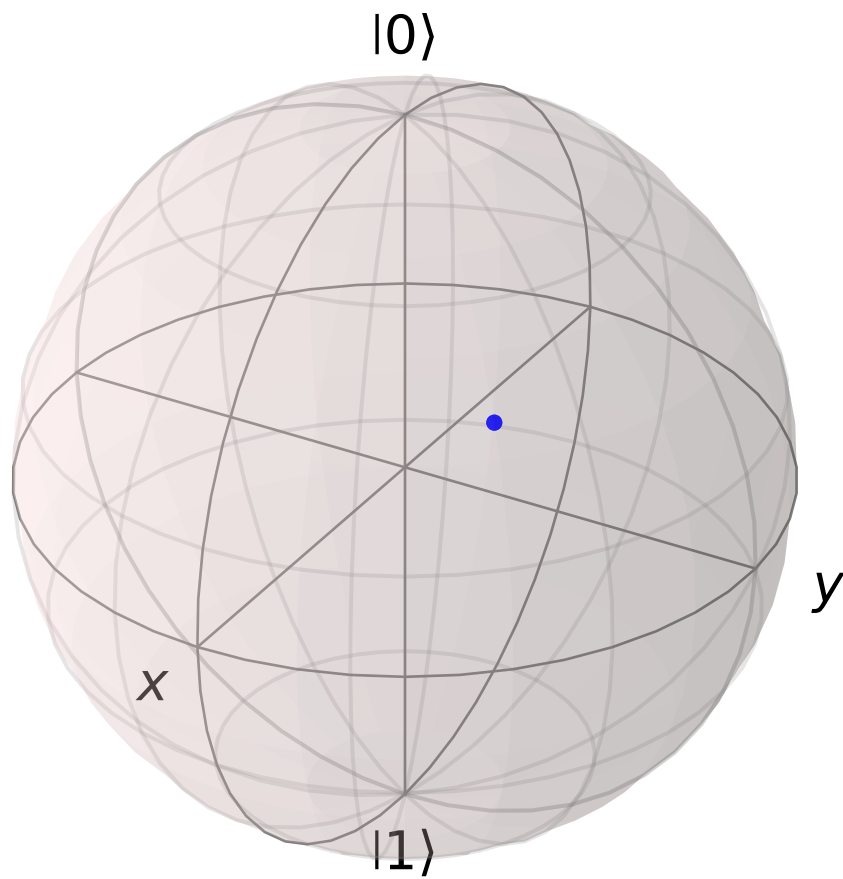
which will load an instance of the `Bloch` class. Before getting into the details of these objects, we can simply plot the blank Bloch sphere associated with these instances via:

```
b.make_sphere()
```



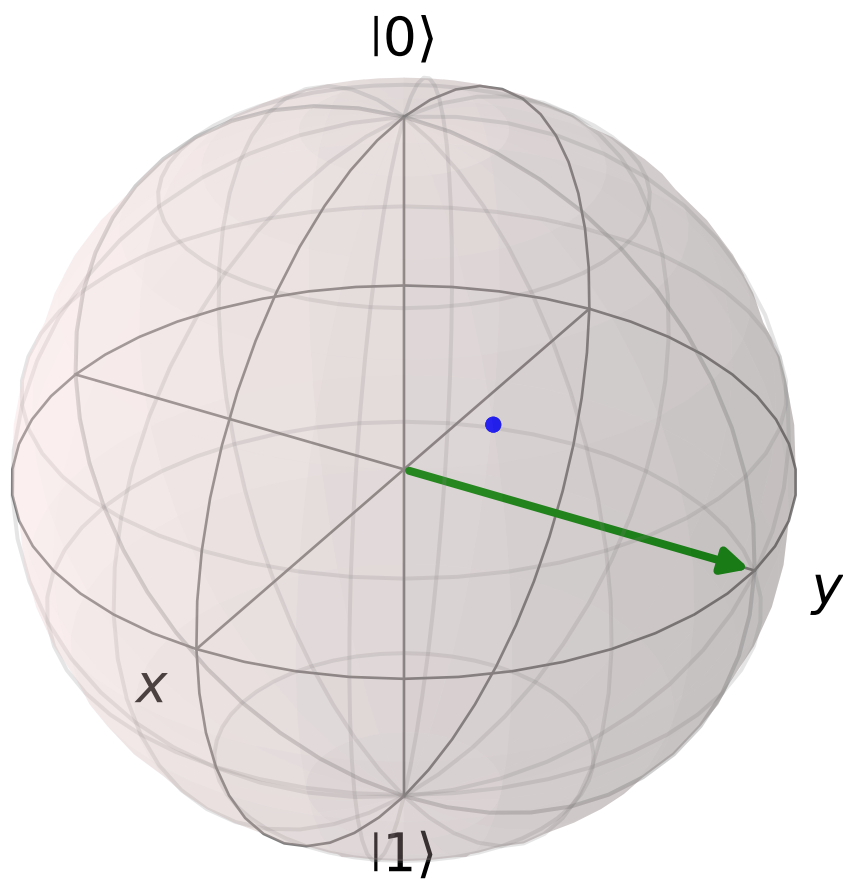
In addition to the `show` command, see the API documentation for [Bloch](#) for a full list of other available functions. As an example, we can add a single data point:

```
pnt = [1/np.sqrt(3), 1/np.sqrt(3), 1/np.sqrt(3)]  
b.add_points(pnt)  
b.render()
```



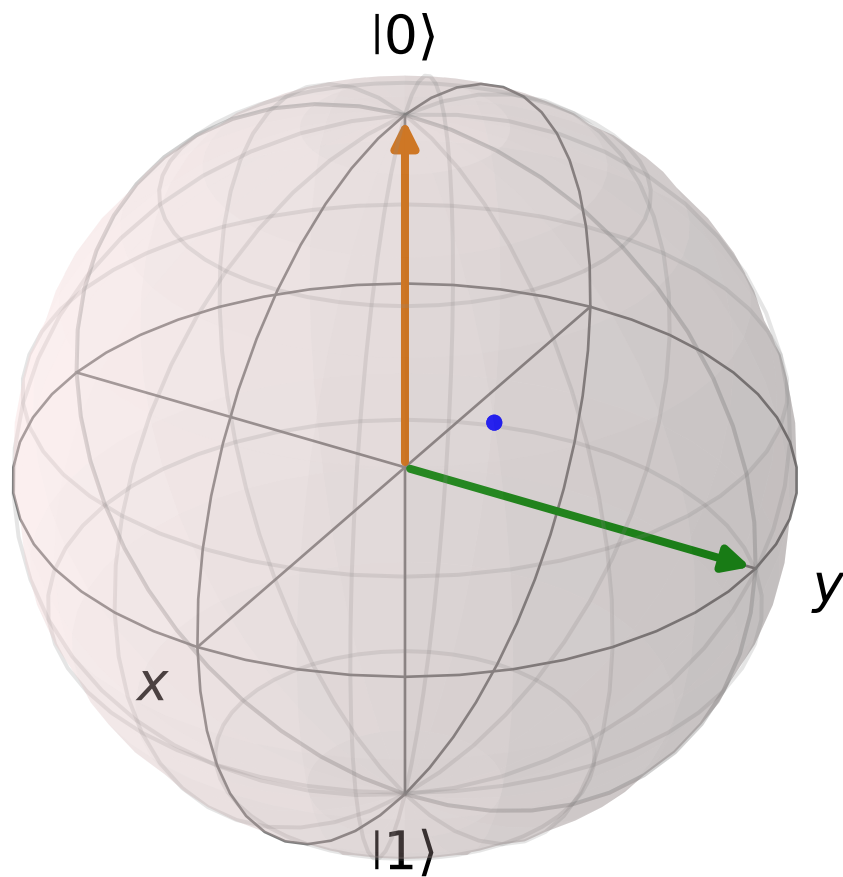
and then a single vector:

```
b.fig.clf()
vec = [0, 1, 0]
b.add_vectors(vec)
b.render()
```



and then add another vector corresponding to the  $|\text{up}\rangle$  state:

```
up = qutip.basis(2, 0)
b.add_states(up)
b.render()
```

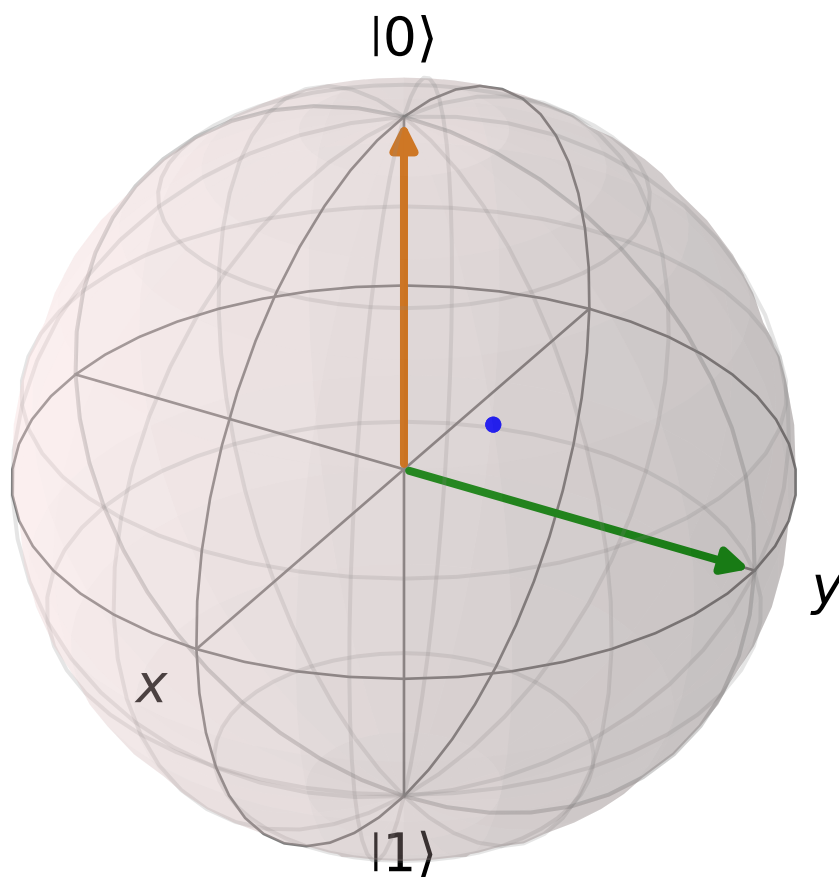


Notice that when we add more than a single vector (or data point), a different color will automatically be applied to the later data set (mod 4). In total, the code for constructing our Bloch sphere with one vector, one state, and a single data point is:

```
b = qutip.Bloch()

pnt = [1./np.sqrt(3), 1./np.sqrt(3), 1./np.sqrt(3)]
b.add_points(pnt)
vec = [0, 1, 0]
b.add_vectors(vec)
up = qutip.basis(2, 0)
b.add_states(up)
b.render()
```

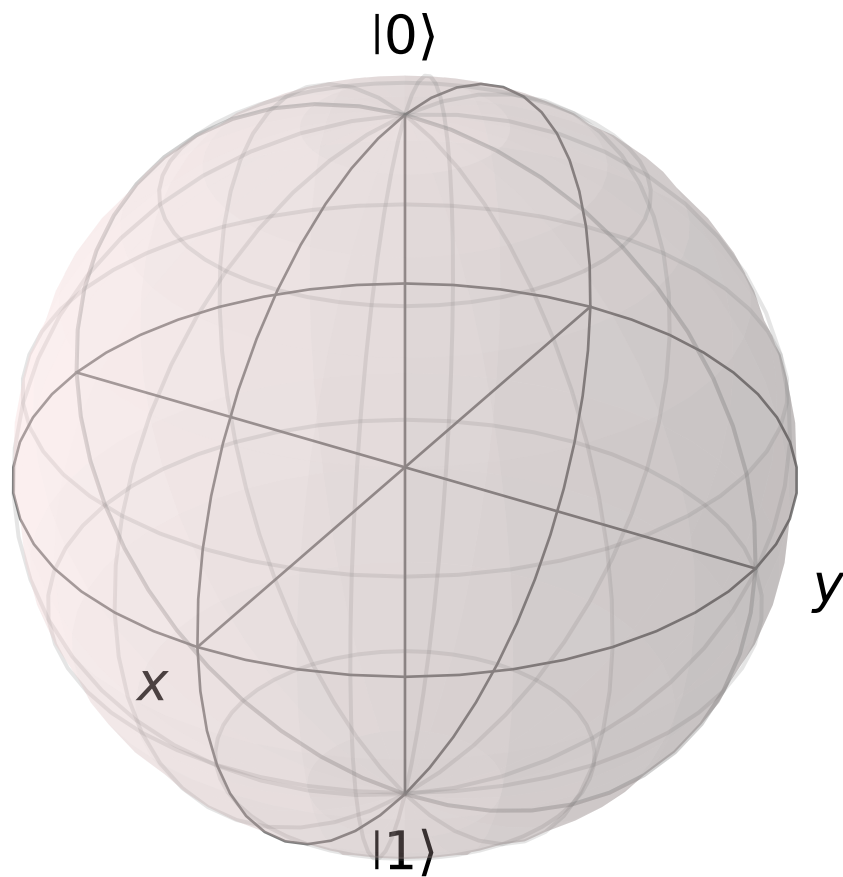




where we have removed the extra `show()` commands.

We can also plot multiple points, vectors, and states at the same time by passing list or arrays instead of individual elements. Before giving an example, we can use the `clear()` command to remove the current data from our Bloch sphere instead of creating a new instance:

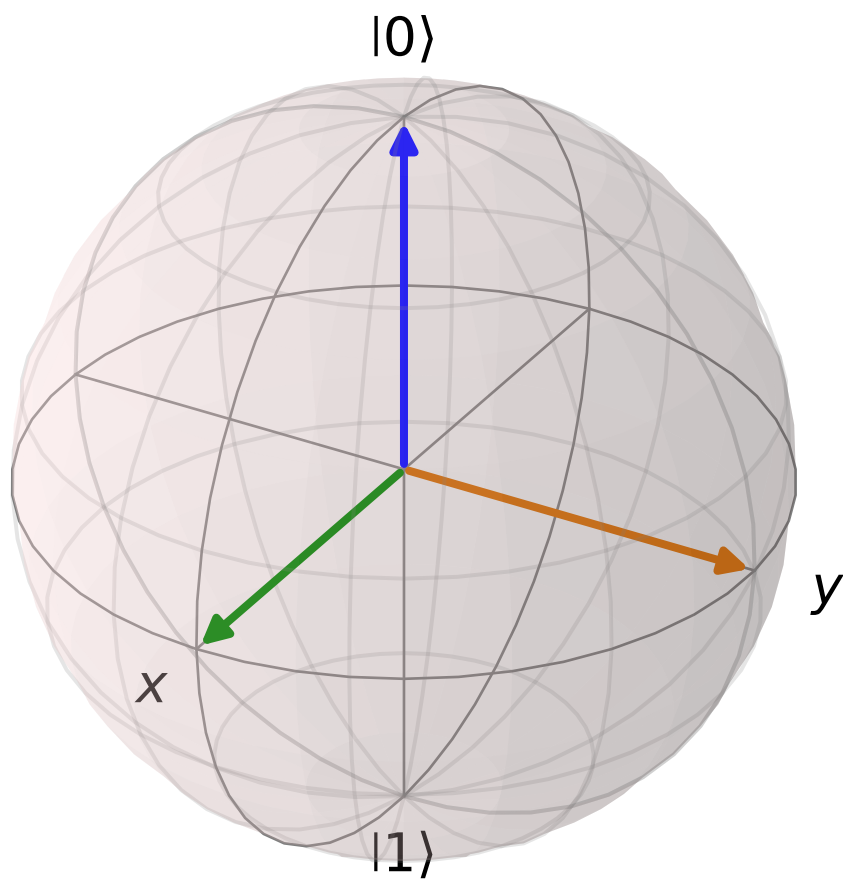
```
b.clear()
b.render()
```



Now on the same Bloch sphere, we can plot the three states associated with the x, y, and z directions:

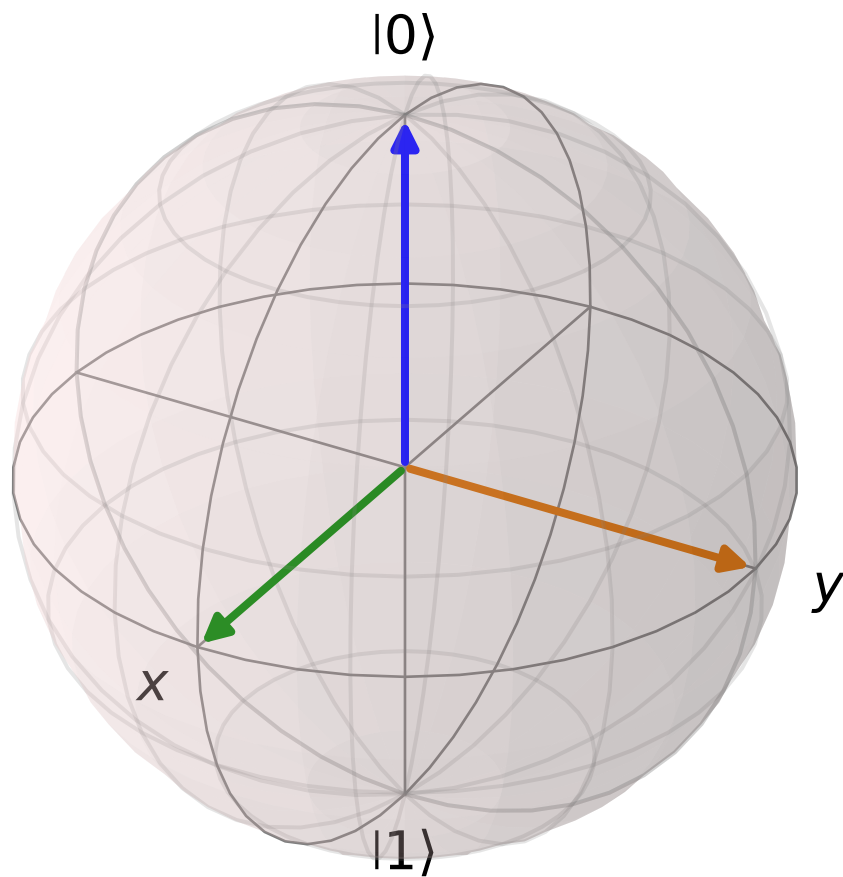
```
x = (qutip.basis(2, 0) + (1+0j)*qutip.basis(2, 1)).unit()
y = (qutip.basis(2, 0) + (0+1j)*qutip.basis(2, 1)).unit()
z = (qutip.basis(2, 0) + (0+0j)*qutip.basis(2, 1)).unit()

b.add_states([x, y, z])
b.render()
```



a similar method works for adding vectors:

```
b.clear()
vec = [[1, 0, 0], [0, 1, 0], [0, 0, 1]]
b.add_vectors(vec)
b.render()
```

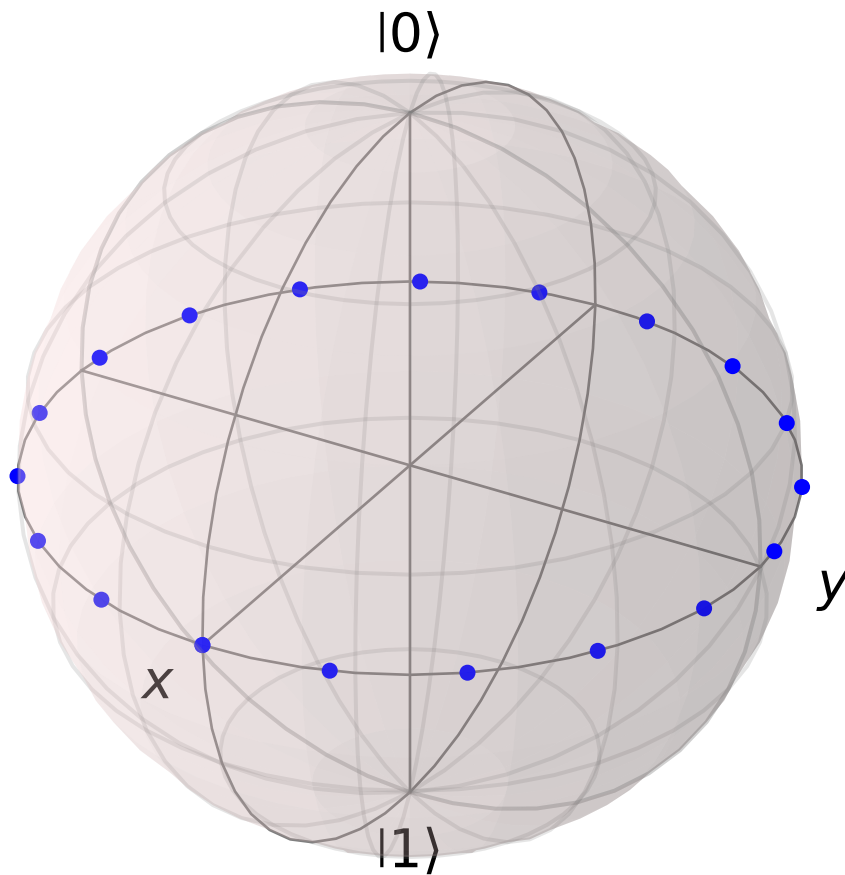


Adding multiple points to the Bloch sphere works slightly differently than adding multiple states or vectors. For example, let's add a set of 20 points around the equator (after calling `clear()`):

```
b.clear()

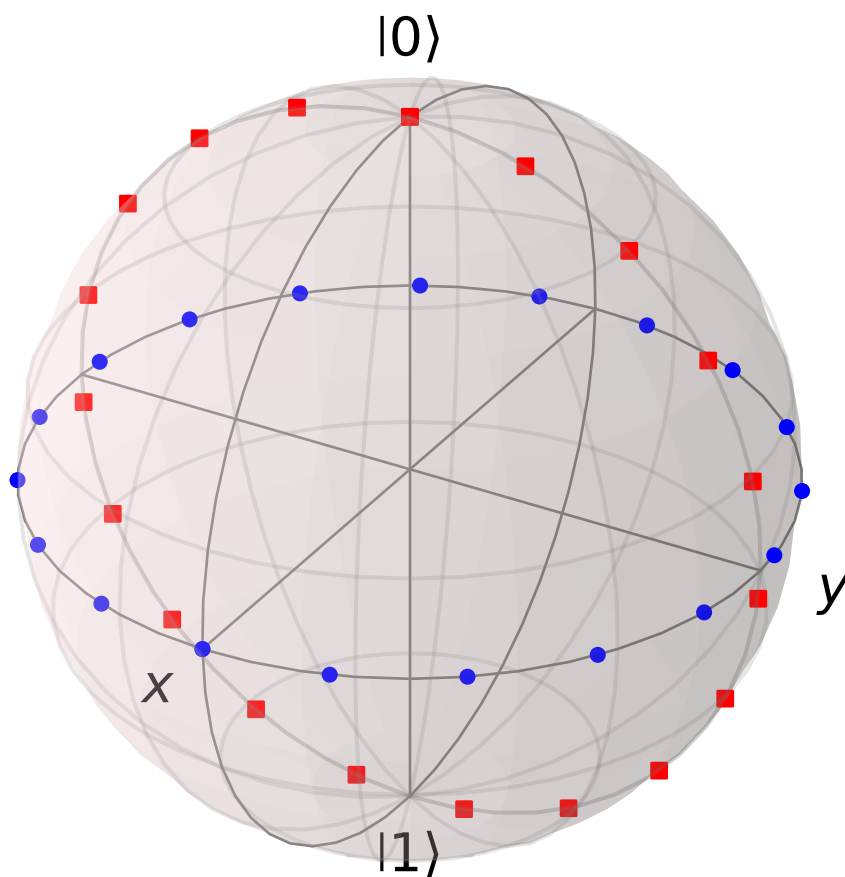
th = np.linspace(0, 2*np.pi, 20)
xp = np.cos(th)
yp = np.sin(th)
zp = np.zeros(20)

pnts = [xp, yp, zp]
b.add_points(pnts)
b.render()
```



Notice that, in contrast to states or vectors, each point remains the same color as the initial point. This is because adding multiple data points using the `add_points` function is interpreted, by default, to correspond to a single data point (single qubit state) plotted at different times. This is very useful when visualizing the dynamics of a qubit. An example of this is given in the example . If we want to plot additional qubit states we can call additional `add_points` functions:

```
xz = np.zeros(20)
yz = np.sin(th)
zz = np.cos(th)
b.add_points([xz, yz, zz])
b.render()
```

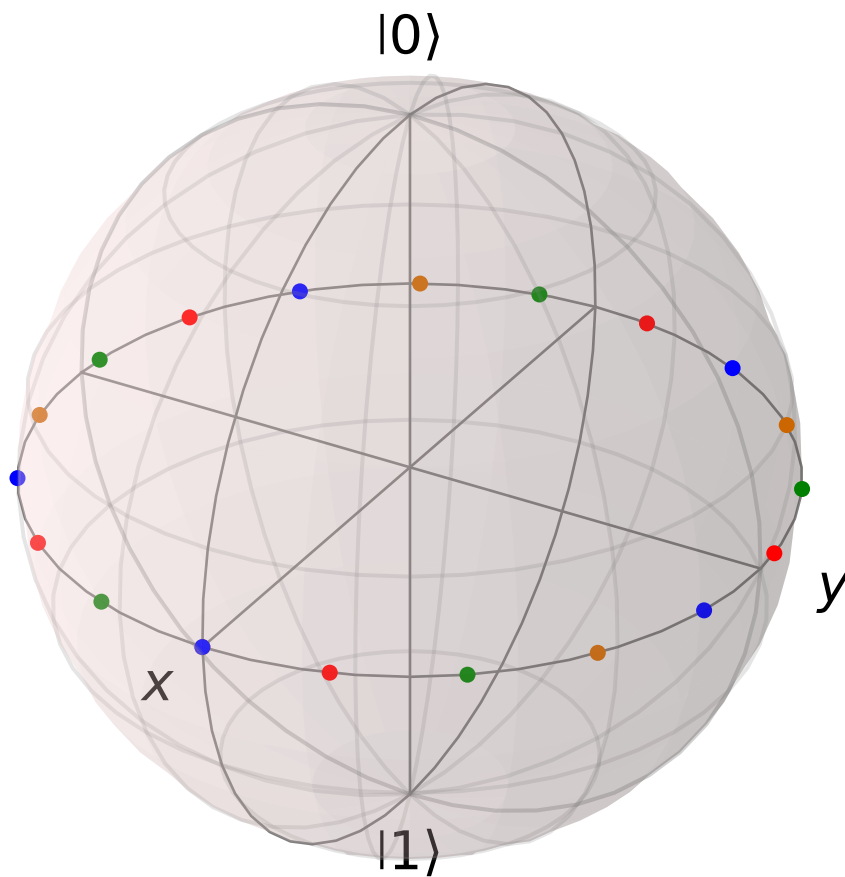


The color and shape of the data points is varied automatically by the Bloch class. Notice how the color and point markers change for each set of data. Again, we have had to call `add_points` twice because adding more than one set of multiple data points is *not* supported by the `add_points` function.

What if we want to vary the color of our points. We can tell the `qutip.bloch.Bloch` class to vary the color of each point according to the colors listed in the `b.point_color` list (see [Configuring the Bloch sphere](#) below). Again after `clear()`:

```
b.clear()

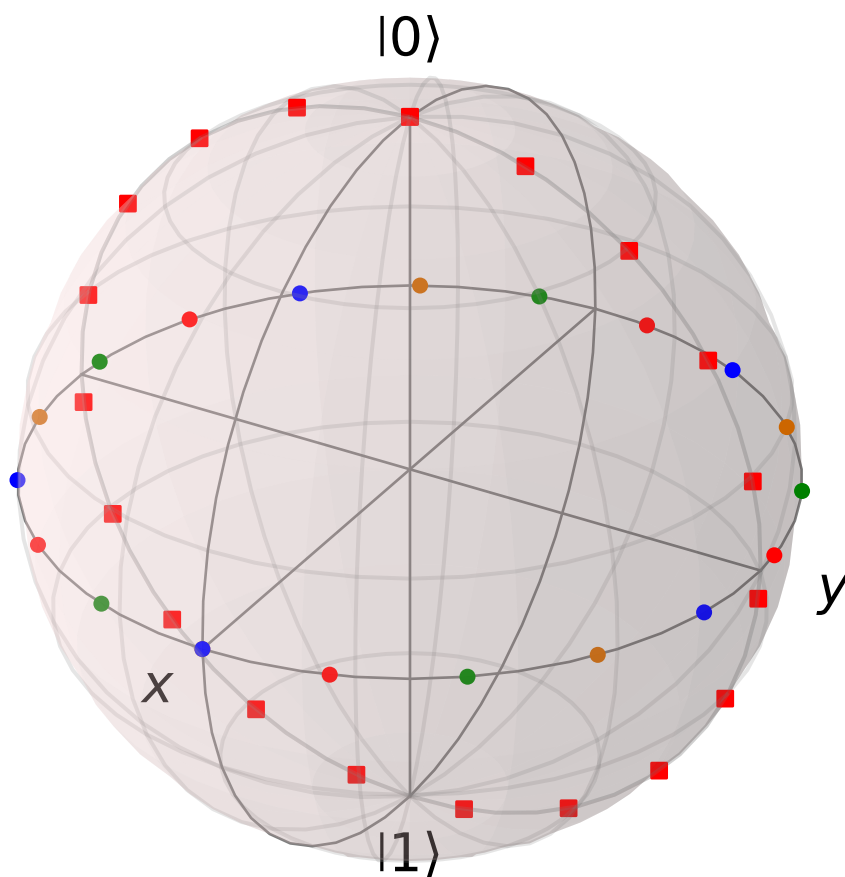
xp = np.cos(th)
yp = np.sin(th)
zp = np.zeros(20)
pnts = [xp, yp, zp]
b.add_points(pnts, 'm') # <-- add a 'm' string to signify 'multi' colored points
b.render()
```



Now, the data points cycle through a variety of predefined colors. Now lets add another set of points, but this time we want the set to be a single color, representing say a qubit going from the  $|up\rangle$  state to the  $|down\rangle$  state in the y-z plane:

```
xz = np.zeros(20)
yz = np.sin(th)
zz = np.cos(th)

b.add_points([xz, yz, zz]) # no 'm'
b.render()
```



A more slick way of using this ‘multi’ color feature is also given in the example, where we set the color of the markers as a function of time.

### 3.11.3 Configuring the Bloch sphere

#### Bloch Class Options

At the end of the last section we saw that the colors and marker shapes of the data plotted on the Bloch sphere are automatically varied according to the number of points and vectors added. But what if you want a different choice of color, or you want your sphere to be purple with different axes labels? Well then you are in luck as the Bloch class has 22 attributes which one can control. Assuming `b=Bloch()`:



Attribute	Function	Default Setting
b.axes	Matplotlib axes instance for animations. Set by axes keyword arg.	None
b.fig	User supplied Matplotlib Figure instance. Set by fig keyword arg.	None
b.font_color	Color of fonts	'black'
b.font_size	Size of fonts	20
b.frame_alpha	Transparency of wireframe	0.1
b.frame_color	Color of wireframe	'gray'
b.frame_width	Width of wireframe	1
b.point_color	List of colors for Bloch point markers to cycle through	['b', 'r', 'g', '#CC6600']
b.point_marker	List of point marker shapes to cycle through	['o', 's', 'd', '^']
b.point_size	List of point marker sizes (not all markers look the same size when plotted)	[55, 62, 65, 75]
b.sphere_alpha	Transparency of Bloch sphere	0.2
b.sphere_color	Color of Bloch sphere	'#FFDDDD'
b.size	Sets size of figure window	[7, 7] (700x700 pixels)
b.vector_color	List of colors for Bloch vectors to cycle through	['g', '#CC6600', 'b', 'r']
b.vector_width	Width of Bloch vectors	4
b.view	Azimuthal and Elevation viewing angles	[-60, 30]
b.xlabel	Labels for x-axis	['\$x\$', ''] +x and -x (labels use LaTeX)
b.xlpos	Position of x-axis labels	[1.1, -1.1]
b.ylabel	Labels for y-axis	['\$y\$', ''] +y and -y (labels use LaTeX)
b.ylpos	Position of y-axis labels	[1.2, -1.2]
b.zlabel	Labels for z-axis	['\$\left 0\right\rangle\$', '\$\left 1\right\rangle\$'] +z and -z (labels use LaTeX)
b.zlpos	Position of z-axis labels	[1.2, -1.2]

These properties can also be accessed via the print command:

```
>>> b = qutip.Bloch()

>>> print(b)
Bloch data:
-----
Number of points: 0
Number of vectors: 0

Bloch sphere properties:
-----
font_color:      black
font_size:       20
frame_alpha:     0.2
frame_color:     gray
frame_width:     1
point_color:     ['b', 'r', 'g', '#CC6600']
point_marker:    ['o', 's', 'd', '^']
point_size:      [25, 32, 35, 45]
sphere_alpha:    0.2
sphere_color:    #FFDDDD
figsize:         [5, 5]
vector_color:    ['g', '#CC6600', 'b', 'r']
vector_width:    3
vector_style:    -|>
vector_mutation: 20
```

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```
view:          [-60, 30]
xlabel:        ['$x$', '']
xlpos:         [1.2, -1.2]
ylabel:        ['$y$', '']
ylpos:         [1.2, -1.2]
zlabel:        ['$\\left|0\\right>$', '$\\left|1\\right>']
zlpos:         [1.2, -1.2]
```

### 3.11.4 Animating with the Bloch sphere

The Bloch class was designed from the outset to generate animations. To animate a set of vectors or data points the basic idea is: plot the data at time  $t_1$ , save the sphere, clear the sphere, plot data at  $t_2, \dots$ . The Bloch sphere will automatically number the output file based on how many times the object has been saved (this is stored in `b.savenum`). The easiest way to animate data on the Bloch sphere is to use the `save()` method and generate a series of images to convert into an animation. However, as of Matplotlib version 1.1, creating animations is built-in. We will demonstrate both methods by looking at the decay of a qubit on the bloch sphere.

#### Example: Qubit Decay

The code for calculating the expectation values for the Pauli spin operators of a qubit decay is given below. This code is common to both animation examples.

```
import numpy as np
import qutip

def qubit_integrate(w, theta, gamma1, gamma2, psi0, tlist):
    # operators and the hamiltonian
    sx = qutip.sigmax()
    sy = qutip.sigmay()
    sz = qutip.sigmaz()
    sm = qutip.sigmam()
    H = w * (np.cos(theta) * sz + np.sin(theta) * sx)
    # collapse operators
    c_op_list = []
    n_th = 0.5 # temperature
    rate = gamma1 * (n_th + 1)
    if rate > 0.0: c_op_list.append(np.sqrt(rate) * sm)
    rate = gamma1 * n_th
    if rate > 0.0: c_op_list.append(np.sqrt(rate) * sm.dag())
    rate = gamma2
    if rate > 0.0: c_op_list.append(np.sqrt(rate) * sz)
    # evolve and calculate expectation values
    output = qutip.mesolve(H, psi0, tlist, c_op_list, [sx, sy, sz])
    return output.expect[0], output.expect[1], output.expect[2]

## calculate the dynamics
w      = 1.0 * 2 * np.pi # qubit angular frequency
theta  = 0.2 * np.pi    # qubit angle from sigma_z axis (toward sigma_x axis)
gamma1  = 0.5             # qubit relaxation rate
gamma2  = 0.2             # qubit dephasing rate
# initial state
a = 1.0
psi0 = (a*qutip.basis(2, 0) + (1-a)*qutip.basis(2, 1))/np.sqrt(a**2 + (1-a)**2)
tlist = np.linspace(0, 4, 250)
```

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```
#expectation values for plotting
sx, sy, sz = qubit_integrate(w, theta, gamma1, gamma2, psi0, tlist)
```

## Generating Images for Animation

An example of generating images for generating an animation outside of Python is given below:

```
import numpy as np
b = qutip.Bloch()
b.vector_color = ['r']
b.view = [-40, 30]
for i in range(len(sx)):
    b.clear()
    b.add_vectors([np.sin(theta), 0, np.cos(theta)])
    b.add_points([sx[i+1], sy[i+1], sz[i+1]])
    b.save(dirc='temp') # saving images to temp directory in current working_
→directory
```

Generating an animation using FFmpeg (for example) is fairly simple:

```
ffmpeg -i temp/bloch_%01d.png bloch.mp4
```

## Directly Generating an Animation

**Important:** Generating animations directly from Matplotlib requires installing either MEncoder or FFmpeg. While either choice works on linux, it is best to choose FFmpeg when running on the Mac. If using macports just do: `sudo port install ffmpeg`.

The code to directly generate an mp4 movie of the Qubit decay is as follows

```
from matplotlib import pyplot, animation
from mpl_toolkits.mplot3d import Axes3D

fig = pyplot.figure()
ax = Axes3D(fig, azimuth=-40, elev=30)
sphere = qutip.Bloch(axes=ax)

def animate(i):
    sphere.clear()
    sphere.add_vectors([np.sin(theta), 0, np.cos(theta)])
    sphere.add_points([sx[i+1], sy[i+1], sz[i+1]])
    sphere.make_sphere()
    return ax

def init():
    sphere.vector_color = ['r']
    return ax

ani = animation.FuncAnimation(fig, animate, np.arange(len(sx)),
                             init_func=init, blit=False, repeat=False)
ani.save('bloch_sphere.mp4', fps=20)
```

The resulting movie may be viewed here: [bloch\\_decay.mp4](#)

## 3.12 Visualization of quantum states and processes

Visualization is often an important complement to a simulation of a quantum mechanical system. The first method of visualization that come to mind might be to plot the expectation values of a few selected operators. But on top of that, it can often be instructive to visualize for example the state vectors or density matrices that describe the state of the system, or how the state is transformed as a function of time (see process tomography below). In this section we demonstrate how QuTiP and matplotlib can be used to perform a few types of visualizations that often can provide additional understanding of quantum system.

### 3.12.1 Fock-basis probability distribution

In quantum mechanics probability distributions plays an important role, and as in statistics, the expectation values computed from a probability distribution does not reveal the full story. For example, consider an quantum harmonic oscillator mode with Hamiltonian  $H = \hbar\omega a^\dagger a$ , which is in a state described by its density matrix  $\rho$ , and which on average is occupied by two photons,  $\text{Tr}[\rho a^\dagger a] = 2$ . Given this information we cannot say whether the oscillator is in a Fock state, a thermal state, a coherent state, etc. By visualizing the photon distribution in the Fock state basis important clues about the underlying state can be obtained.

One convenient way to visualize a probability distribution is to use histograms. Consider the following histogram visualization of the number-basis probability distribution, which can be obtained from the diagonal of the density matrix, for a few possible oscillator states with on average occupation of two photons.

First we generate the density matrices for the coherent, thermal and fock states.

```
N = 20

rho_coherent = coherent_dm(N, np.sqrt(2))

rho_thermal = thermal_dm(N, 2)

rho_fock = fock_dm(N, 2)
```

Next, we plot histograms of the diagonals of the density matrices:

```
fig, axes = plt.subplots(1, 3, figsize=(12,3))

bar0 = axes[0].bar(np.arange(0, N)-.5, rho_coherent.diag())

lbl0 = axes[0].set_title("Coherent state")

lim0 = axes[0].set_xlim([-0.5, N])

bar1 = axes[1].bar(np.arange(0, N)-.5, rho_thermal.diag())

lbl1 = axes[1].set_title("Thermal state")

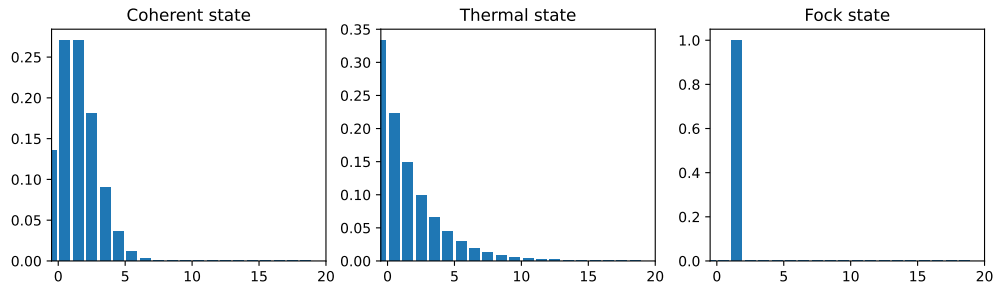
lim1 = axes[1].set_xlim([-0.5, N])

bar2 = axes[2].bar(np.arange(0, N)-.5, rho_fock.diag())

lbl2 = axes[2].set_title("Fock state")

lim2 = axes[2].set_xlim([-0.5, N])

plt.show()
```



All these states correspond to an average of two photons, but by visualizing the photon distribution in Fock basis the differences between these states are easily appreciated.

One frequently need to visualize the Fock-distribution in the way described above, so QuTiP provides a convenience function for doing this, see [qutip.visualization.plot\\_fock\\_distribution](#), and the following example:

```
fig, axes = plt.subplots(1, 3, figsize=(12,3))

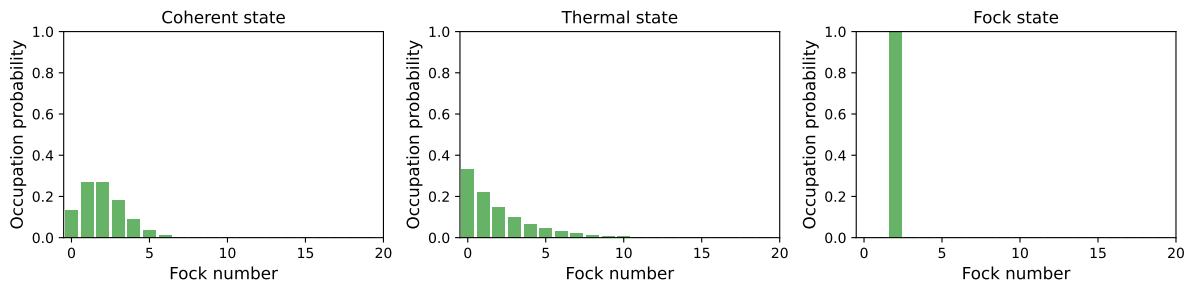
fig, axes[0] = plot_fock_distribution(rho_coherent, fig=fig, ax=axes[0]);
axes[0].set_title('Coherent state')

fig, axes[1] = plot_fock_distribution(rho_thermal, fig=fig, ax=axes[1]);
axes[1].set_title('Thermal state')

fig, axes[2] = plot_fock_distribution(rho_fock, fig=fig, ax=axes[2]);
axes[2].set_title('Fock state')

fig.tight_layout()

plt.show()
```



### 3.12.2 Quasi-probability distributions

The probability distribution in the number (Fock) basis only describes the occupation probabilities for a discrete set of states. A more complete phase-space probability-distribution-like function for harmonic modes are the Wigner and Husimi Q-functions, which are full descriptions of the quantum state (equivalent to the density matrix). These are called quasi-distribution functions because unlike real probability distribution functions they can for example be negative. In addition to being more complete descriptions of a state (compared to only the occupation probabilities plotted above), these distributions are also great for demonstrating if a quantum state is quantum mechanical, since for example a negative Wigner function is a definite indicator that a state is distinctly nonclassical.

## Wigner function

In QuTiP, the Wigner function for a harmonic mode can be calculated with the function `qutip.wigner.wigner`. It takes a ket or a density matrix as input, together with arrays that define the ranges of the phase-space coordinates (in the x-y plane). In the following example the Wigner functions are calculated and plotted for the same three states as in the previous section.

```
xvec = np.linspace(-5,5,200)

W_coherent = wigner(rho_coherent, xvec, xvec)

W_thermal = wigner(rho_thermal, xvec, xvec)

W_fock = wigner(rho_fock, xvec, xvec)

# plot the results

fig, axes = plt.subplots(1, 3, figsize=(12,3))

cont0 = axes[0].contourf(xvec, xvec, W_coherent, 100)

lbl0 = axes[0].set_title("Coherent state")

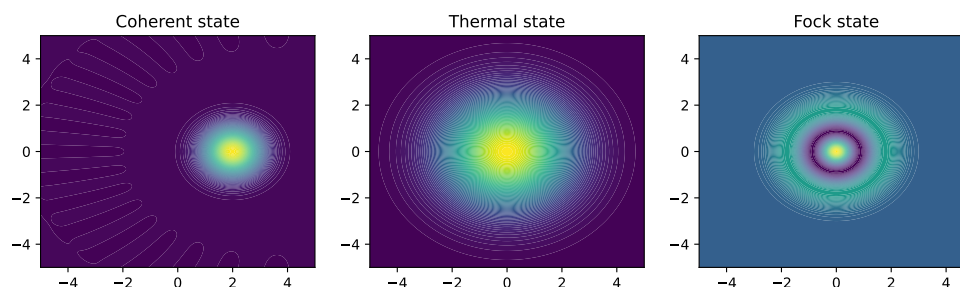
cont1 = axes[1].contourf(xvec, xvec, W_thermal, 100)

lbl1 = axes[1].set_title("Thermal state")

cont0 = axes[2].contourf(xvec, xvec, W_fock, 100)

lbl2 = axes[2].set_title("Fock state")

plt.show()
```



## Custom Color Maps

The main objective when plotting a Wigner function is to demonstrate that the underlying state is nonclassical, as indicated by negative values in the Wigner function. Therefore, making these negative values stand out in a figure is helpful for both analysis and publication purposes. Unfortunately, all of the color schemes used in Matplotlib (or any other plotting software) are linear colormaps where small negative values tend to be near the same color as the zero values, and are thus hidden. To fix this dilemma, QuTiP includes a nonlinear colormap function `qutip.matplotlib_utilities.wigner_cmap` that colors all negative values differently than positive or zero values. Below is a demonstration of how to use this function in your Wigner figures:

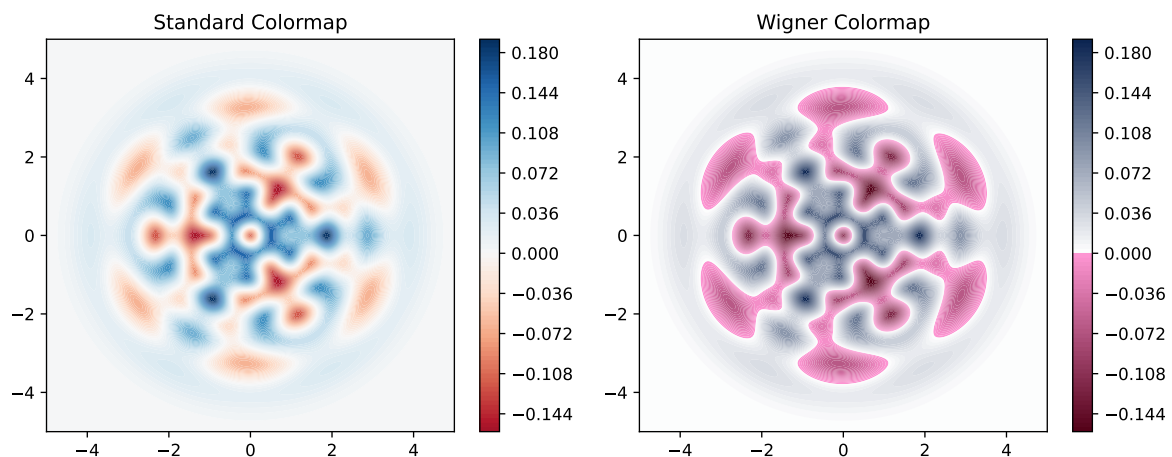
```
import matplotlib as mpl

from matplotlib import cm
```

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```
psi = (basis(10, 0) + basis(10, 3) + basis(10, 9)).unit()
xvec = np.linspace(-5, 5, 500)
W = wigner(psi, xvec, xvec)
wmap = wigner_cmap(W) # Generate Wigner colormap
nrm = mpl.colors.Normalize(-W.max(), W.max())
fig, axes = plt.subplots(1, 2, figsize=(10, 4))
plt1 = axes[0].contourf(xvec, xvec, W, 100, cmap=cm.RdBu, norm=nrm)
axes[0].set_title("Standard Colormap");
cb1 = fig.colorbar(plt1, ax=axes[0])
plt2 = axes[1].contourf(xvec, xvec, W, 100, cmap=wmap) # Apply Wigner colormap
axes[1].set_title("Wigner Colormap");
cb2 = fig.colorbar(plt2, ax=axes[1])
fig.tight_layout()
plt.show()
```



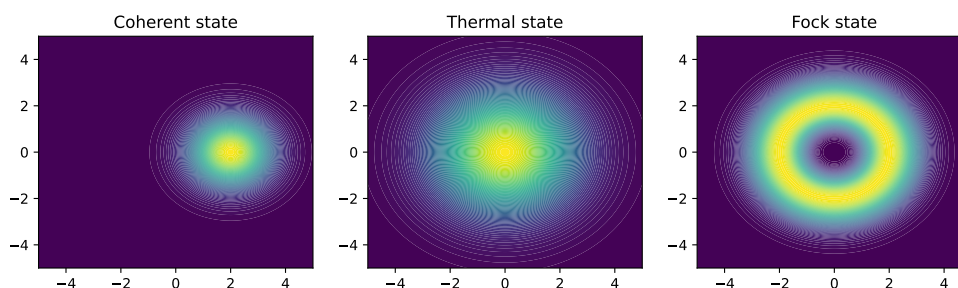
## Husimi Q-function

The Husimi Q function is, like the Wigner function, a quasiprobability distribution for harmonic modes. It is defined as

$$Q(\alpha) = \frac{1}{\pi} \langle \alpha | \rho | \alpha \rangle$$

where  $|\alpha\rangle$  is a coherent state and  $\alpha = x + iy$ . In QuTiP, the Husimi Q function can be computed given a state ket or density matrix using the function `qfunc`, as demonstrated below.

```
Q_coherent = qfunc(rho_coherent, xvec, xvec)
Q_thermal = qfunc(rho_thermal, xvec, xvec)
Q_fock = qfunc(rho_fock, xvec, xvec)
fig, axes = plt.subplots(1, 3, figsize=(12,3))
cont0 = axes[0].contourf(xvec, xvec, Q_coherent, 100)
lbl0 = axes[0].set_title("Coherent state")
cont1 = axes[1].contourf(xvec, xvec, Q_thermal, 100)
lbl1 = axes[1].set_title("Thermal state")
cont0 = axes[2].contourf(xvec, xvec, Q_fock, 100)
lbl2 = axes[2].set_title("Fock state")
plt.show()
```



If you need to calculate the Q function for many states with the same phase-space coordinates, it is more efficient to use the `QFunc` class. This stores various intermediary results to achieve an order-of-magnitude improvement compared to calling `qfunc` in a loop.

```
xs = np.linspace(-1, 1, 101)
qfunc_calculator = qutip.QFunc(xs, xs)
q_state1 = qfunc_calculator(qutip.rand_dm(5))
q_state2 = qfunc_calculator(qutip.rand_ket(100))
```

### 3.12.3 Visualizing operators

Sometimes, it may also be useful to directly visualizing the underlying matrix representation of an operator. The density matrix, for example, is an operator whose elements can give insights about the state it represents, but one might also be interesting in plotting the matrix of an Hamiltonian to inspect the structure and relative importance of various elements.

QuTiP offers a few functions for quickly visualizing matrix data in the form of histograms, `qutip.visualization.matrix_histogram` and as Hinton diagram of weighted squares, `qutip.visualization.hinton`. These functions takes a `Qobj` as first argument, and optional arguments to, for example, set the axis labels and figure title (see the function's documentation for details).

For example, to illustrate the use of `qutip.visualization.matrix_histogram`, let's visualize of the Jaynes-Cummings Hamiltonian:



```

N = 5

a = tensor(destroy(N), qeye(2))
b = tensor(qeye(N), destroy(2))
sx = tensor(qeye(N), sigmax())

H = a.dag() * a + sx - 0.5 * (a * b.dag() + a.dag() * b)

# visualize H

lbls_list = [[str(d) for d in range(N)], ["u", "d"]]

xlabels = []

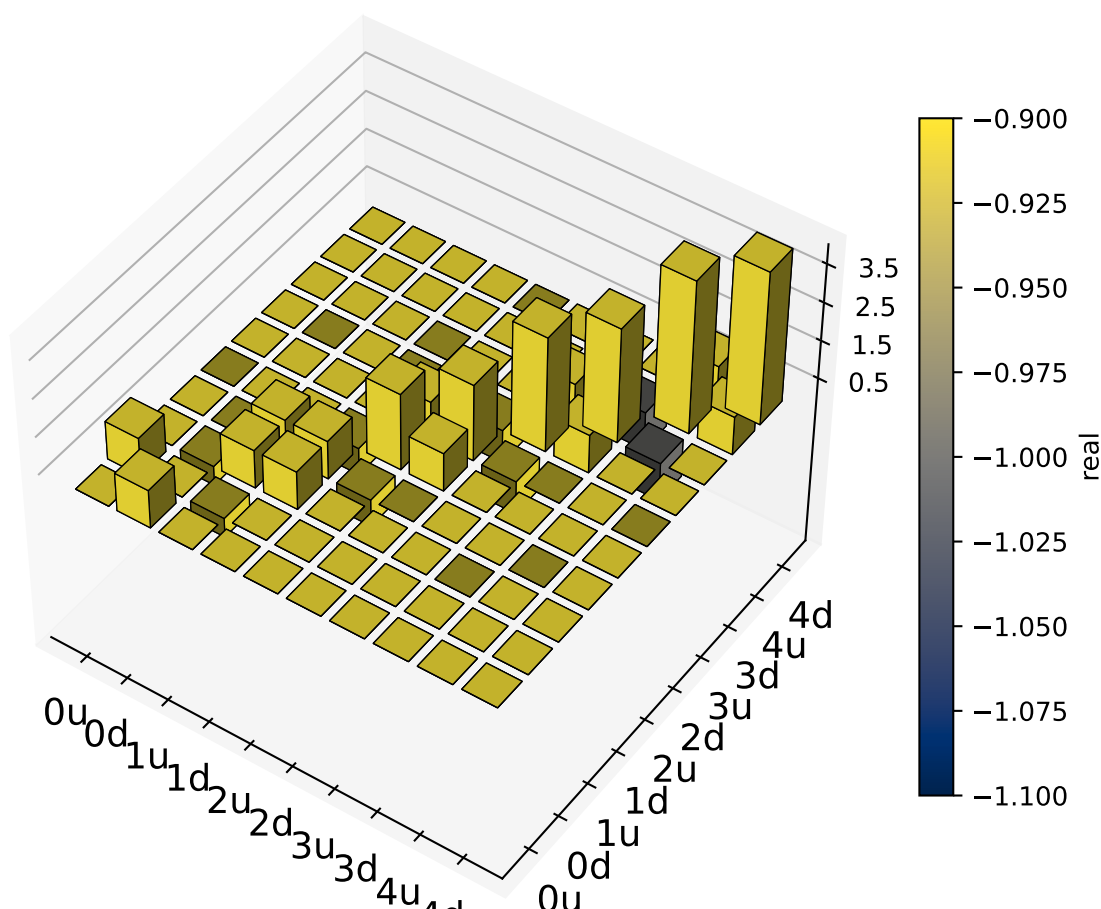
for inds in tomography._index_permutations([len(lbls) for lbls in lbls_list]):
    xlabels.append(''.join([lbls_list[k][inds[k]] for k in range(len(lbls_list))]))

fig, ax = matrix_histogram(H, xlabels, xlabels, limits=[-4,4])

ax.view_init(azim=-55, elev=45)

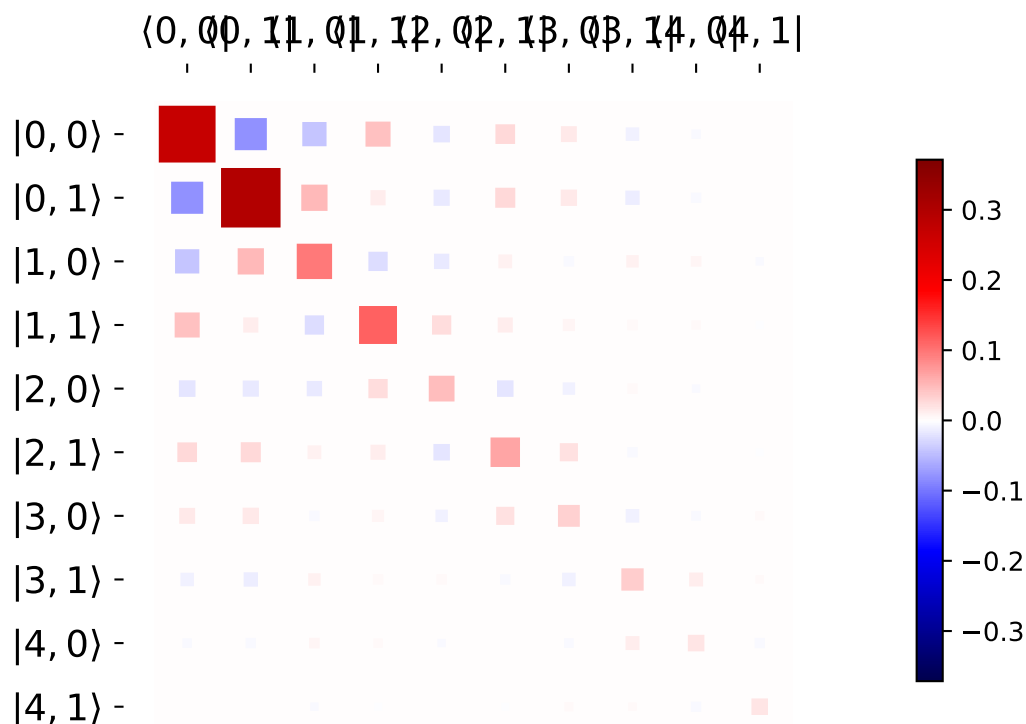
plt.show()

```



Similarly, we can use the function `qutip.visualization.hinton`, which is used below to visualize the corresponding steadystate density matrix:

```
rho_ss = steadystate(H, [np.sqrt(0.1) * a, np.sqrt(0.4) * b.dag()])
hinton(rho_ss)
plt.show()
```



### 3.12.4 Quantum process tomography

Quantum process tomography (QPT) is a useful technique for characterizing experimental implementations of quantum gates involving a small number of qubits. It can also be a useful theoretical tool that can give insight in how a process transforms states, and it can be used for example to study how noise or other imperfections deteriorate a gate. Whereas a fidelity or distance measure can give a single number that indicates how far from ideal a gate is, a quantum process tomography analysis can give detailed information about exactly what kind of errors various imperfections introduce.

The idea is to construct a transformation matrix for a quantum process (for example a quantum gate) that describes how the density matrix of a system is transformed by the process. We can then decompose the transformation in some operator basis that represent well-defined and easily interpreted transformations of the input states.

To see how this works (see e.g. [Moh08] for more details), consider a process that is described by quantum map  $\epsilon(\rho_{\text{in}}) = \rho_{\text{out}}$ , which can be written

$$\epsilon(\rho_{\text{in}}) = \rho_{\text{out}} = \sum_i^{N^2} A_i \rho_{\text{in}} A_i^\dagger, \quad (3.39)$$

where  $N$  is the number of states of the system (that is,  $\rho$  is represented by an  $[N \times N]$  matrix). Given an orthogonal

operator basis of our choice  $\{B_i\}_i^{N^2}$ , which satisfies  $\text{Tr}[B_i^\dagger B_j] = N\delta_{ij}$ , we can write the map as

$$\epsilon(\rho_{\text{in}}) = \rho_{\text{out}} = \sum_{mn} \chi_{mn} B_m \rho_{\text{in}} B_n^\dagger. \quad (3.40)$$

where  $\chi_{mn} = \sum_{ij} b_{im} b_{jn}^*$  and  $A_i = \sum_m b_{im} B_m$ . Here, matrix  $\chi$  is the transformation matrix we are after, since it describes how much  $B_m \rho_{\text{in}} B_n^\dagger$  contributes to  $\rho_{\text{out}}$ .

In a numerical simulation of a quantum process we usually do not have access to the quantum map in the form Eq. (3.39). Instead, what we usually can do is to calculate the propagator  $U$  for the density matrix in superoperator form, using for example the QuTiP function `qutip.propagator.propagator`. We can then write

$$\epsilon(\tilde{\rho}_{\text{in}}) = U \tilde{\rho}_{\text{in}} = \tilde{\rho}_{\text{out}}$$

where  $\tilde{\rho}$  is the vector representation of the density matrix  $\rho$ . If we write Eq. (3.40) in superoperator form as well we obtain

$$\tilde{\rho}_{\text{out}} = \sum_{mn} \chi_{mn} \tilde{B}_m \tilde{B}_n^\dagger \tilde{\rho}_{\text{in}} = U \tilde{\rho}_{\text{in}}.$$

so we can identify

$$U = \sum_{mn} \chi_{mn} \tilde{B}_m \tilde{B}_n^\dagger.$$

Now this is a linear equation systems for the  $N^2 \times N^2$  elements in  $\chi$ . We can solve it by writing  $\chi$  and the superoperator propagator as  $[N^4]$  vectors, and likewise write the superoperator product  $\tilde{B}_m \tilde{B}_n^\dagger$  as a  $[N^4 \times N^4]$  matrix  $M$ :

$$U_I = \sum_J M_{IJ} \chi_J$$

with the solution

$$\chi = M^{-1} U.$$

Note that to obtain  $\chi$  with this method we have to construct a matrix  $M$  with a size that is the square of the size of the superoperator for the system. Obviously, this scales very badly with increasing system size, but this method can still be a very useful for small systems (such as system comprised of a small number of coupled qubits).

### Implementation in QuTiP

In QuTiP, the procedure described above is implemented in the function `qutip.tomography.qpt`, which returns the  $\chi$  matrix given a density matrix propagator. To illustrate how to use this function, let's consider the SWAP gate for two qubits. In QuTiP the function `swap` generates the unitary transformation for the state kets:

```
from qutip.core.gates import swap

U_psi = swap()
```

To be able to use this unitary transformation matrix as input to the function `qutip.tomography.qpt`, we first need to convert it to a transformation matrix for the corresponding density matrix:

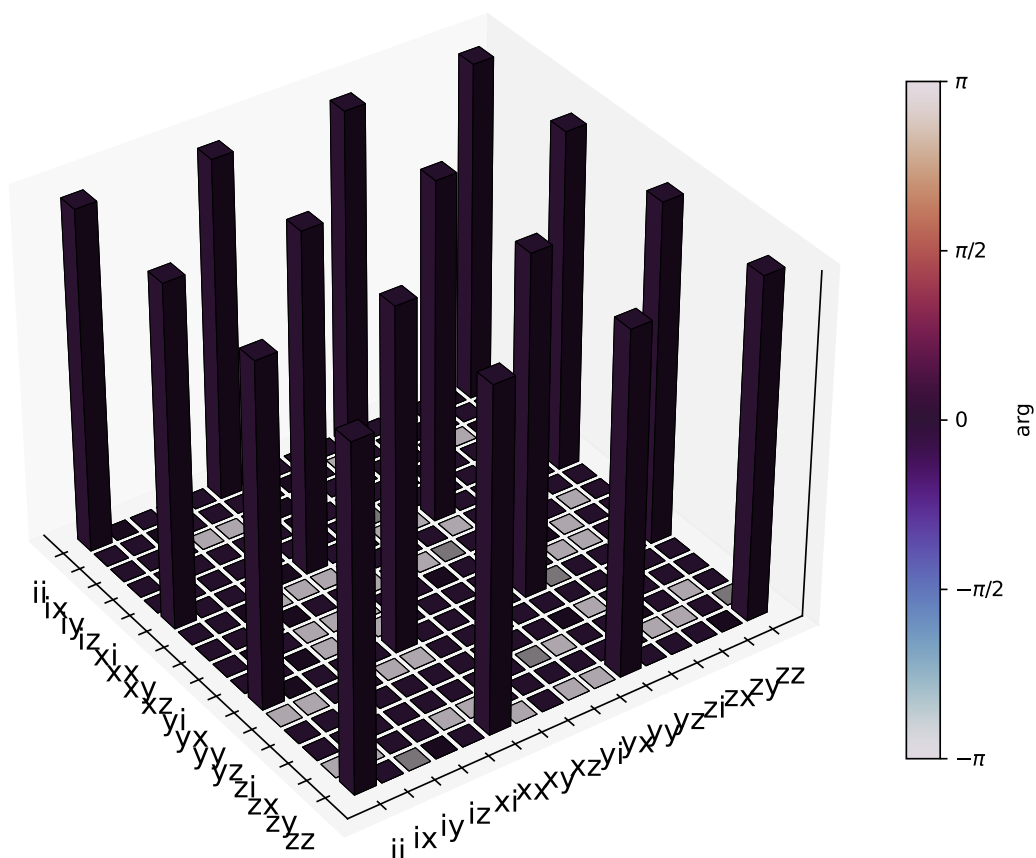
```
U_rho = spre(U_psi) * spost(U_psi.dag())
```

Next, we construct a list of operators that define the basis  $\{B_i\}$  in the form of a list of operators for each composite system. At the same time, we also construct a list of corresponding labels that will be used when plotting the  $\chi$  matrix.

```
op_basis = [[qeye(2), sigmax(), sigmay(), sigmaz()]] * 2
op_label = [["i", "x", "y", "z"]] * 2
```

We are now ready to compute  $\chi$  using `qutip.tomography.qpt`, and to plot it using `qutip.tomography.qpt_plot_combined`.

```
chi = qpt(U_rho, op_basis)
fig = qpt_plot_combined(chi, op_label, r'SWAP')
plt.show()
```



For a slightly more advanced example, where the density matrix propagator is calculated from the dynamics of a system defined by its Hamiltonian and collapse operators using the function `propagator`, see notebook “Time-dependent master equation: Landau-Zener transitions” on the tutorials section on the QuTiP web site.

## 3.13 Saving QuTiP Objects and Data Sets

With time-consuming calculations it is often necessary to store the results to files on disk, so it can be post-processed and archived. In QuTiP there are two facilities for storing data: Quantum objects can be stored to files and later read back as python pickles, and numerical data (vectors and matrices) can be exported as plain text files in for example CSV (comma-separated values), TSV (tab-separated values), etc. The former method is preferred when further calculations will be performed with the data, and the latter when the calculations are completed and data is to be imported into a post-processing tool (e.g. for generating figures).

### 3.13.1 Storing and loading QuTiP objects

To store and load arbitrary QuTiP related objects (*Qobj*, *Result*, etc.) there are two functions: `qutip.fileio.qsave` and `qutip.fileio.qload`. The function `qutip.fileio.qsave` takes an arbitrary object as first parameter and an optional filename as second parameter (default filename is `qutip_data.qu`). The filename extension is always `.qu`. The function `qutip.fileio.qload` takes a mandatory filename as first argument and loads and returns the objects in the file.

To illustrate how these functions can be used, consider a simple calculation of the steadystate of the harmonic oscillator

```
>>> a = destroy(10); H = a.dag() * a
>>> c_ops = [np.sqrt(0.5) * a, np.sqrt(0.25) * a.dag()]
>>> rho_ss = steadystate(H, c_ops)
```

The steadystate density matrix `rho_ss` is an instance of *Qobj*. It can be stored to a file `steadystate.qu` using

```
>>> qsave(rho_ss, 'steadystate')
>>> !ls *.qu
density_matrix_vs_time.qu  steadystate.qu
```

and it can later be loaded again, and used in further calculations

```
>>> rho_ss_loaded = qload('steadystate')
Loaded Qobj object:
Quantum object: dims = [[10], [10]], shape = (10, 10), type = oper, isHerm = True
>>> a = destroy(10)
>>> np.testing.assert_almost_equal(expect(a.dag() * a, rho_ss_loaded), 0.
↪9902248289345061)
```

The nice thing about the `qutip.fileio.qsave` and `qutip.fileio.qload` functions is that almost any object can be stored and load again later on. We can for example store a list of density matrices as returned by *mesolve*

```
>>> a = destroy(10); H = a.dag() * a ; c_ops = [np.sqrt(0.5) * a, np.sqrt(0.25) * a.
↪dag()]
>>> psi0 = rand_ket(10)
>>> times = np.linspace(0, 10, 10)
>>> dm_list = mesolve(H, psi0, times, c_ops, [])
>>> qsave(dm_list, 'density_matrix_vs_time')
```

And it can then be loaded and used again, for example in an other program

```
>>> dm_list_loaded = qload('density_matrix_vs_time')
Loaded Result object:
Result object with mesolve data.
-----
states = True
num_collapse = 0
```

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```
>>> a = destroy(10)
>>> expect(a.dag() * a, dm_list_loaded.states)
array([4.63317086, 3.59150315, 2.90590183, 2.41306641, 2.05120716,
       1.78312503, 1.58357995, 1.4346382 , 1.32327398, 1.23991233])
```

### 3.13.2 Storing and loading datasets

The `qutip.fileio.qsave` and `qutip.fileio.qload` are great, but the file format used is only understood by QuTiP (python) programs. When data must be exported to other programs the preferred method is to store the data in the commonly used plain-text file formats. With the QuTiP functions `qutip.fileio.file_data_store` and `qutip.fileio.file_data_read` we can store and load **numpy** arrays and matrices to files on disk using a delimiter-separated value format (for example comma-separated values CSV). Almost any program can handle this file format.

The `qutip.fileio.file_data_store` takes two mandatory and three optional arguments:

```
>>> file_data_store(filename, data, numtype="complex", numformat="decimal", sep=",")
```

where *filename* is the name of the file, *data* is the data to be written to the file (must be a *numpy* array), *numtype* (optional) is a flag indicating numerical type that can take values *complex* or *real*, *numformat* (optional) specifies the numerical format that can take the values *exp* for the format *1.0e1* and *decimal* for the format *10.0*, and *sep* (optional) is an arbitrary single-character field separator (usually a tab, space, comma, semicolon, etc.).

A common use for the `qutip.fileio.file_data_store` function is to store the expectation values of a set of operators for a sequence of times, e.g., as returned by the `mesolve` function, which is what the following example does

```
>>> a = destroy(10); H = a.dag() * a ; c_ops = [np.sqrt(0.5) * a, np.sqrt(0.25) * a.
↳ dag()]
>>> psi0 = rand_ket(10)
>>> times = np.linspace(0, 100, 100)
>>> medata = mesolve(H, psi0, times, c_ops, [a.dag() * a, a + a.dag(), -1j * (a - a.
↳ dag())])
>>> np.shape(medata.expect)
(3, 100)
>>> times.shape
(100,)
>>> output_data = np.vstack((times, medata.expect)) # join time and expt data
>>> file_data_store('expect.dat', output_data.T) # Note the .T for transpose!
>>> with open("expect.dat", "r") as f:
...     print('\n'.join(f.readlines()[:10]))
# Generated by QuTiP: 100x4 complex matrix in decimal format [' ',' ' separated values].
0.0000000000+0.0000000000j,3.2109553666+0.0000000000j,0.3689771549+0.0000000000j,0.
↳ 0185002867+0.0000000000j
1.0101010101+0.0000000000j,2.6754598872+0.0000000000j,0.1298251132+0.0000000000j,-0.
↳ 3303672956+0.0000000000j
2.0202020202+0.0000000000j,2.2743186810+0.0000000000j,-0.2106241300+0.0000000000j,-0.
↳ 2623894277+0.0000000000j
3.0303030303+0.0000000000j,1.9726633457+0.0000000000j,-0.3037311621+0.0000000000j,0.
↳ 0397330921+0.0000000000j
4.0404040404+0.0000000000j,1.7435892209+0.0000000000j,-0.1126550232+0.0000000000j,0.
↳ 2497182058+0.0000000000j
5.0505050505+0.0000000000j,1.5687324121+0.0000000000j,0.1351622725+0.0000000000j,0.
↳ 2018398581+0.0000000000j
6.0606060606+0.0000000000j,1.4348632045+0.0000000000j,0.2143080535+0.0000000000j,-0.
↳ 0067820038+0.0000000000j
```

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```
7.0707070707+0.0000000000j,1.3321818015+0.0000000000j,0.0950352763+0.0000000000j,-0.
↪1630920429+0.0000000000j
8.0808080808+0.0000000000j,1.2533244850+0.0000000000j,-0.0771210981+0.0000000000j,-0.
↪1468923919+0.0000000000j
```

In this case we didn't really need to store both the real and imaginary parts, so instead we could use the `numtype="real"` option

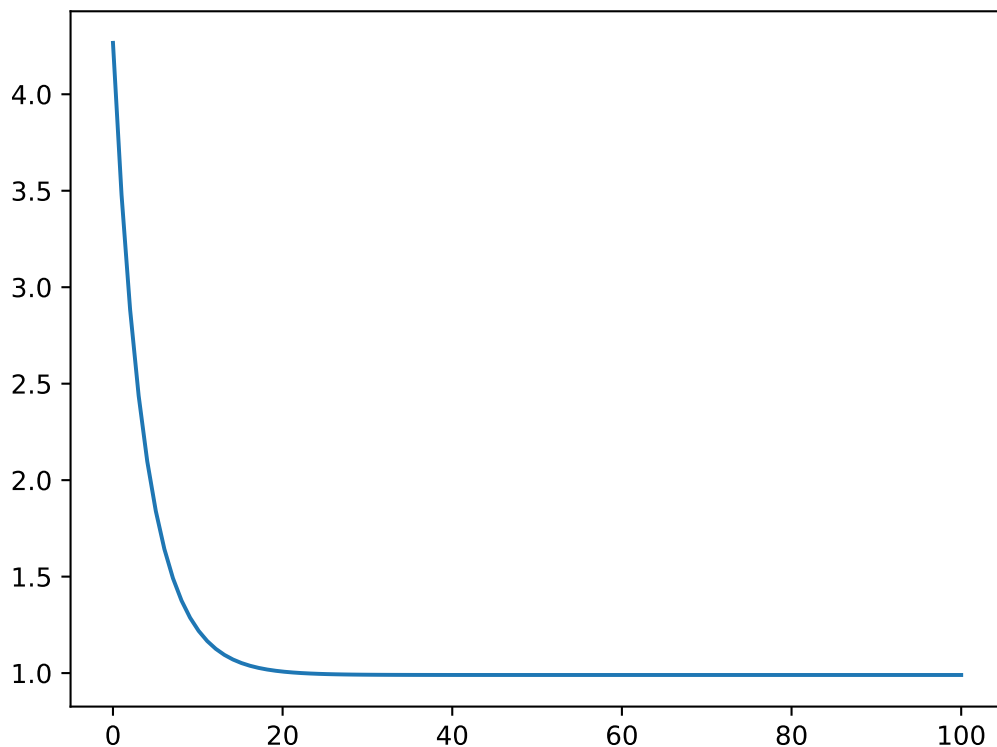
```
>>> file_data_store('expect.dat', output_data.T, numtype="real")
>>> with open("expect.dat", "r") as f:
...     print('\n'.join(f.readlines()[:5]))
# Generated by QuTiP: 100x4 real matrix in decimal format [' ',' ' separated values].
0.0000000000,3.2109553666,0.3689771549,0.0185002867
1.0101010101,2.6754598872,0.1298251132,-0.3303672956
2.0202020202,2.2743186810,-0.2106241300,-0.2623894277
3.0303030303,1.9726633457,-0.3037311621,0.0397330921
```

and if we prefer scientific notation we can request that using the `numformat="exp"` option

```
>>> file_data_store('expect.dat', output_data.T, numtype="real", numformat="exp")
```

Loading data previously stored using `qutip.fileio.file_data_store` (or some other software) is a even easier. Regardless of which delimiter was used, if data was stored as complex or real numbers, if it is in decimal or exponential form, the data can be loaded using the `qutip.fileio.file_data_read`, which only takes the filename as mandatory argument.

```
input_data = file_data_read('expect.dat')
plt.plot(input_data[:,0], input_data[:,1]); # plot the data
```



(If a particularly obscure choice of delimitator was used it might be necessary to use the optional second argument, for example `sep="_"` if `_` is the delimitator).

## 3.14 Generating Random Quantum States & Operators

QuTiP includes a collection of random state, unitary and channel generators for simulations, Monte Carlo evaluation, theorem evaluation, and code testing. Each of these objects can be sampled from one of several different distributions.

For example, a random Hermitian operator can be sampled by calling `rand_herm` function:

```
>>> rand_herm(5)
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[-0.25091976+0.j          0.          +0.j          0.          +0.j
 -0.21793701+0.47037633j -0.23212846-0.61607187j]
 [ 0.          +0.j          -0.88383278+0.j          0.836086   -0.23956218j
 -0.09464275+0.45370863j -0.15243356+0.65392096j]
 [ 0.          +0.j          0.836086   +0.23956218j  0.66488528+0.j
 -0.26290446+0.64984451j -0.52603038-0.07991553j]
 [-0.21793701-0.47037633j -0.09464275-0.45370863j -0.26290446-0.64984451j
 -0.13610996+0.j          -0.34240902-0.2879303j ]
 [-0.23212846+0.61607187j -0.15243356-0.65392096j -0.52603038+0.07991553j
 -0.34240902+0.2879303j  0.          +0.j          ]]
```

Random Variable Type	Sampling Functions	Dimensions
State vector (ket)	<code>rand_ket</code>	$N \times 1$
Hermitian operator (oper)	<code>rand_herm</code>	$N \times N$
Density operator (oper)	<code>rand_dm</code>	$N \times N$
Unitary operator (oper)	<code>rand_unitary</code>	$N \times N$
stochastic matrix (oper)	<code>rand_stochastic</code>	$N \times N$
CPTP channel (super)	<code>rand_super</code> , <code>rand_super_bcsz</code>	$(N \times N) \times (N \times N)$
CPTP map (list of oper)	<code>rand_kraus_map</code>	$N \times N$ ( $N^2$ operators)

In all cases, these functions can be called with a single parameter *dimensions* that can be the size of the relevant Hilbert space or the dimensions of a random state, unitary or channel.

```
>>> rand_super_bcsz(7).dims
[[[7], [7]], [[7], [7]]]
>>> rand_super_bcsz([[2, 3], [2, 3]]).dims
[[[2, 3], [2, 3]], [[2, 3], [2, 3]]]
```

Several of the random *Qobj* function in QuTiP support additional parameters as well, namely *density* and *distribution*. `rand_dm`, `rand_herm`, `rand_unitary` and `rand_ket` can be created using multiple method controlled by *distribution*. The `rand_ket`, `rand_herm` and `rand_unitary` functions can return quantum objects such that a fraction of the elements are identically equal to zero. The ratio of nonzero elements is passed as the *density*



keyword argument. By contrast, `rand_super_bcsz` take as an argument the rank of the generated object, such that passing `rank=1` returns a random pure state or unitary channel, respectively. Passing `rank=None` specifies that the generated object should be full-rank for the given dimension. `rand_dm` can support `density` or `rank` depending on the chosen distribution.

For example,

```
>>> rand_dm(5, density=0.5, distribution="herm")
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[ 0.298+0.j , 0. +0.j , -0.095+0.1j , 0. +0.j , -0.105+0.122j],
 [ 0. +0.j , 0.088+0.j , 0. +0.j , -0.018-0.001j, 0. +0.j ],
 [-0.095-0.1j , 0. +0.j , 0.328+0.j , 0. +0.j , -0.077-0.033j],
 [ 0. +0.j , -0.018+0.001j, 0. +0.j , 0.084+0.j , 0. +0.j ],
 [-0.105-0.122j, 0. +0.j , -0.077+0.033j, 0. +0.j , 0.201+0.j ]]

>>> rand_dm_ginibre(5, rank=2)
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[ 0.307+0.j , -0.258+0.039j, -0.039+0.184j, 0.041-0.054j, 0.016+0.045j],
 [-0.258-0.039j, 0.239+0.j , 0.075-0.15j , -0.053+0.008j, -0.057-0.078j],
 [-0.039-0.184j, 0.075+0.15j , 0.136+0.j , -0.05 -0.052j, -0.028-0.058j],
 [ 0.041+0.054j, -0.053-0.008j, -0.05 +0.052j, 0.083+0.j , 0.101-0.056j],
 [ 0.016-0.045j, -0.057+0.078j, -0.028+0.058j, 0.101+0.056j, 0.236+0.j ]]
```

See the API documentation: [Quantum Objects](#) for details.

**Warning:** When using the `density` keyword argument, setting the density too low may result in not enough diagonal elements to satisfy trace constraints.

### 3.14.1 Random objects with a given eigen spectrum

It is also possible to generate random Hamiltonian (`rand_herm`) and density matrices (`rand_dm`) with a given eigen spectrum. This is done by passing an array to `eigenvalues` argument to either function and choosing the “eigen” distribution. For example,

```
>>> eigs = np.arange(5)

>>> H = rand_herm(5, density=0.5, eigenvalues=eigs, distribution="eigen")

>>> H
Quantum object: dims = [[5], [5]], shape = (5, 5), type = oper, isherm = True
Qobj data =
[[ 0.5 +0.j , 0.228+0.27j, 0. +0.j , 0. +0.j , -0.228-0.27j],
 [ 0.228-0.27j, 1.75 +0.j , 0.456+0.54j, 0. +0.j , 1.25 +0.j ],
 [ 0. +0.j , 0.456-0.54j, 3. +0.j , 0. +0.j , 0.456-0.54j],
 [ 0. +0.j , 0. +0.j , 0. +0.j , 3. +0.j , 0. +0.j ],
 [-0.228+0.27j, 1.25 +0.j , 0.456+0.54j, 0. +0.j , 1.75 +0.j ]]

>>> H.eigenenergies()
array([7.70647994e-17, 1.00000000e+00, 2.00000000e+00, 3.00000000e+00,
       4.00000000e+00])
```

In order to generate a random object with a given spectrum QuTiP applies a series of random complex Jacobi rotations. This technique requires many steps to build the desired quantum object, and is thus suitable only for objects with Hilbert dimensionality  $\lesssim 1000$ .

### 3.14.2 Composite random objects

In many cases, one is interested in generating random quantum objects that correspond to composite systems generated using the `tensor` function. Specifying the tensor structure of a quantum object is done passing a list for the first argument. The resulting quantum objects size will be the product of the elements in the list and the resulting *Qobj* dimensions will be `[dims, dims]`:

```
>>> rand_unitary([2, 2], density=0.5)
Quantum object: dims = [[2, 2], [2, 2]], shape = (4, 4), type = oper, isherm = True
Qobj data =
[[ 0.887+0.061j,  0.    +0.j    ,  0.    +0.j    , -0.191-0.416j],
 [ 0.    +0.j    ,  0.604+0.116j, -0.32 -0.721j,  0.    +0.j    ],
 [ 0.    +0.j    ,  0.768+0.178j,  0.227+0.572j,  0.    +0.j    ],
 [ 0.412-0.2j   ,  0.    +0.j    ,  0.    +0.j    ,  0.724+0.516j]]
```

### 3.14.3 Controlling the random number generator

Qutip uses numpy random number generator to create random quantum objects. To control the random number, a seed as an *int* or *numpy.random.SeedSequence* or a *numpy.random.Generator* can be passed to the *seed* keyword argument:

```
>>> rng = np.random.default_rng(12345)
>>> rand_ket(2, seed=rng)
Quantum object: dims=[[2], [1]], shape=(2, 1), type='ket'
Qobj data =
[[-0.697+0.618j],
 [-0.326-0.163j]]
```

### 3.14.4 Internal matrix format

The internal storage type of the generated random quantum objects can be set with the *dtype* keyword.

```
>>> rand_ket(2, dtype="dense").data
Dense(shape=(2, 1), fortran=True)

>>> rand_ket(2, dtype="CSR").data
CSR(shape=(2, 1), nnz=2)
```

## 3.15 Modifying Internal QuTiP Settings

### 3.15.1 User Accessible Parameters

In this section we show how to modify a few of the internal parameters used by QuTiP. The settings that can be modified are given in the following table:

Setting	Description	Options
<code>auto_tidyup</code>	Automatically tidyup sparse quantum objects.	True / False
<code>auto_tidyup_atol</code>	Tolerance used by tidyup. (sparse only)	float { 1e-14 }
<code>atol</code>	General absolute tolerance.	float { 1e-12 }
<code>rtol</code>	General relative tolerance.	float { 1e-12 }
<code>function_coefficient_style</code>	Signature expected by function coefficients.	{ "auto", "pythonic", "dict" }

### 3.15.2 Example: Changing Settings

The two most important settings are `auto_tidyup` and `auto_tidyup_atol` as they control whether the small elements of a quantum object should be removed, and what number should be considered as the cut-off tolerance. Modifying these, or any other parameters, is quite simple:

```
>>> qutip.settings.core["auto_tidyup"] = False
```

The settings can also be changed for a code block:

```
>>> with qutip.CoreOptions(atol=1e-5):
>>>     assert qutip.qeye(2) * 1e-9 == qutip.qzero(2)
```

## 3.16 Measurement of Quantum Objects

**Note:** New in QuTiP 4.6

### 3.16.1 Introduction

Measurement is a fundamental part of the standard formulation of quantum mechanics and is the process by which classical readings are obtained from a quantum object. Although the interpretation of the procedure is at times contentious, the procedure itself is mathematically straightforward and is described in many good introductory texts.

Here we will show you how to perform simple measurement operations on QuTiP objects. The same functions `measure` and `measurement_statistics` can be used to handle both observable-style measurements and projective style measurements.

### 3.16.2 Performing a basic measurement (Observable)

First we need to select some states to measure. For now, let us create an *up* state and a *down* state:

```
up = basis(2, 0)

down = basis(2, 1)
```

which represent spin-1/2 particles with their spin pointing either up or down along the z-axis.

We choose what to measure (in this case) by selecting a **measurement operator**. For example, we could select `sigmaz` which measures the z-component of the spin of a spin-1/2 particle, or `sigmax` which measures the x-component:

```
spin_z = sigmaz()

spin_x = sigmax()
```

How do we know what these operators measure? The answer lies in the measurement procedure itself:

- A quantum measurement transforms the state being measured by projecting it into one of the eigenvectors of the measurement operator.
- Which eigenvector to project onto is chosen probabilistically according to the square of the amplitude of the state in the direction of the eigenvector.
- The value returned by the measurement is the eigenvalue corresponding to the chosen eigenvector.

---

**Note:** How to interpret this “random choosing” is the famous “quantum measurement problem”.

---

The eigenvectors of *spin\_z* are the states with their spin pointing either up or down, so it measures the component of the spin along the z-axis.

The eigenvectors of *spin\_x* are the states with their spin pointing either left or right, so it measures the component of the spin along the x-axis.

When we measure our *up* and *down* states using the operator *spin\_z*, we always obtain:

```
from qutip.measurement import measure, measurement_statistics

measure(up, spin_z) == (1.0, up)

measure(down, spin_z) == (-1.0, down)
```

because *up* is the eigenvector of *spin\_z* with eigenvalue *1.0* and *down* is the eigenvector with eigenvalue *-1.0*. The minus signs are just an arbitrary global phase – *up* and *-up* represent the same quantum state.

Neither eigenvector has any component in the direction of the other (they are orthogonal), so *measure(spin\_z, up)* returns the state *up* 100% percent of the time and *measure(spin\_z, down)* returns the state *down* 100% of the time.

Note how *measure* returns a pair of values. The first is the measured value, i.e. an eigenvalue of the operator (e.g. *1.0*), and the second is the state of the quantum system after the measurement, i.e. an eigenvector of the operator (e.g. *up*).

Now let us consider what happens if we measure the x-component of the spin of *up*:

```
measure(up, spin_x)
```

The *up* state is not an eigenvector of *spin\_x*. *spin\_x* has two eigenvectors which we will call *left* and *right*. The *up* state has equal components in the direction of these two vectors, so measurement will select each of them 50% of the time.

These *left* and *right* states are:

```
left = (up - down).unit()

right = (up + down).unit()
```

When *left* is chosen, the result of the measurement will be *(-1.0, -left)*.

When *right* is chosen, the result of measurement will be *(1.0, right)*.

---

**Note:** When *measure* is invoked with the second argument being an observable, it acts as an alias to *measure\_observable*.

---

### 3.16.3 Performing a basic measurement (Projective)

We can also choose what to measure by specifying a *list of projection operators*. For example, we could select the projection operators  $|0\rangle\langle 0|$  and  $|1\rangle\langle 1|$  which measure the state in the  $|0\rangle, |1\rangle$  basis. Note that these projection operators are simply the projectors determined by the eigenstates of the `sigmaz` operator.

```
Z0, Z1 = ket2dm(basis(2, 0)), ket2dm(basis(2, 1))
```

The probabilities and respective output state are calculated for each projection operator.

```
measure(up, [Z0, Z1]) == (0, up)

measure(down, [Z0, Z1]) == (1, down)
```

In this case, the projection operators are conveniently eigenstates corresponding to subspaces of dimension 1. However, this might not be the case, in which case it is not possible to have unique eigenvalues for each eigenstate. Suppose we want to measure only the first qubit in a two-qubit system. Consider the two qubit state  $|0+\rangle$

```
state_0 = basis(2, 0)

state_plus = (basis(2, 0) + basis(2, 1)).unit()

state_0plus = tensor(state_0, state_plus)
```

Now, suppose we want to measure only the first qubit in the computational basis. We can do that by measuring with the projection operators  $|0\rangle\langle 0| \otimes I$  and  $|1\rangle\langle 1| \otimes I$ .

```
PZ1 = [tensor(Z0, identity(2)), tensor(Z1, identity(2))]

PZ2 = [tensor(identity(2), Z0), tensor(identity(2), Z1)]
```

Now, as in the previous example, we can measure by supplying a list of projection operators and the state.

```
measure(state_0plus, PZ1) == (0, state_0plus)
```

The output of the measurement is the index of the measurement outcome as well as the output state on the full Hilbert space of the input state. It is crucial to note that we do not discard the measured qubit after measurement (as opposed to when measuring on quantum hardware).

---

**Note:** When `measure` is invoked with the second argument being a list of projectors, it acts as an alias to `measure_povm`.

---

The `measure` function can perform measurements on density matrices too. You can read about these and other details at [measure\\_povm](#) and [measure\\_observable](#).

Now you know how to measure quantum states in QuTiP!

### 3.16.4 Obtaining measurement statistics(Observable)

You’ve just learned how to perform measurements in QuTiP, but you’ve also learned that measurements are probabilistic. What if instead of just making a single measurement, we want to determine the probability distribution of a large number of measurements?

One way would be to repeat the measurement many times – and this is what happens in many quantum experiments. In QuTiP one could simulate this using:

```
results = {1.0: 0, -1.0: 0} # 1 and -1 are the possible outcomes
for _ in range(1000):
    value, new_state = measure(up, spin_x)
    results[round(value)] += 1
print(results)
```

Output:

```
{1.0: 497, -1.0: 503}
```

which measures the x-component of the spin of the *up* state 1000 times and stores the results in a dictionary. Afterwards we expect to have seen the result *1.0* (i.e. left) roughly 500 times and the result *-1.0* (i.e. right) roughly 500 times, but, of course, the number of each will vary slightly each time we run it.

But what if we want to know the distribution of results precisely? In a physical system, we would have to perform the measurement many many times, but in QuTiP we can peak at the state itself and determine the probability distribution of the outcomes exactly in a single line:

```
>>> eigenvalues, eigenstates, probabilities = measurement_statistics(up, spin_x)

>>> eigenvalues
array([-1., 1.])

>>> eigenstates
array([Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[ 0.70710678]
 [-0.70710678]],
      Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[0.70710678]
 [0.70710678]]], dtype=object)

>>> probabilities
[0.5000000000000001, 0.4999999999999999]
```

The `measurement_statistics` function then returns three values when called with a single observable:

- *eigenvalues* is an array of eigenvalues of the measurement operator, i.e. a list of the possible measurement results. In our example the value is `array([-1., 1.])`.
- *eigenstates* is an array of the eigenstates of the measurement operator, i.e. a list of the possible final states after the measurement is complete. Each element of the array is a *Qobj*.
- *probabilities* is a list of the probabilities of each measurement result. In our example the value is `[0.5, 0.5]` since the *up* state has equal probability of being measured to be in the left (*-1.0*) or right (*1.0*) eigenstates.

All three lists are in the same order – i.e. the first eigenvalue is `eigenvalues[0]`, its corresponding eigenstate is `eigenstates[0]`, and its probability is `probabilities[0]`, and so on.

**Note:** When `measurement_statistics` is invoked with the second argument being an observable, it acts as an

alias to [measurement\\_statistics\\_observable](#).

### 3.16.5 Obtaining measurement statistics(Projective)

Similarly, when we want to obtain measurement statistics for projection operators, we can use the [measurement\\_statistics](#) function with the second argument being a list of projectors. Consider again, the state  $|0+\rangle$ . Suppose, now we want to obtain the measurement outcomes for the second qubit. We must use the projectors specified earlier by *PZ2* which allow us to measure only on the second qubit. Since the second qubit has the state  $|+\rangle$ , we get the following result.

```
collapsed_states, probabilities = measurement_statistics(state_0plus, PZ2)

print(collapsed_states)
```

Output:

```
[Quantum object: dims = [[2, 2], [1, 1]], shape = (4, 1), type = ket
Qobj data =
[[1.]
 [0.]
 [0.]
 [0.]], Quantum object: dims = [[2, 2], [1, 1]], shape = (4, 1), type = ket
Qobj data =
[[0.]
 [1.]
 [0.]
 [0.]]]
```

```
print(probabilities)
```

Output:

```
[0.4999999999999999, 0.4999999999999999]
```

The function [measurement\\_statistics](#) then returns two values:

- *collapsed\_states* is an array of the possible final states after the measurement is complete. Each element of the array is a *Qobj*.
- *probabilities* is a list of the probabilities of each measurement outcome.

Note that the collapsed\_states are exactly  $|00\rangle$  and  $|01\rangle$  with equal probability, as expected. The two lists are in the same order.

---

**Note:** When [measurement\\_statistics](#) is invoked with the second argument being a list of projectors, it acts as an alias to [measurement\\_statistics\\_povm](#).

---

The [measurement\\_statistics](#) function can provide statistics for measurements of density matrices too. You can read about these and other details at [measurement\\_statistics\\_observable](#) and [measurement\\_statistics\\_povm](#).

Furthermore, the [measure\\_povm](#) and [measurement\\_statistics\\_povm](#) functions can handle POVM measurements which are more general than projective measurements.

## 3.17 Quantum Optimal Control

### 3.17.1 Introduction

In quantum control we look to prepare some specific state, effect some state-to-state transfer, or effect some transformation (or gate) on a quantum system. For a given quantum system there will always be factors that effect the dynamics that are outside of our control. As examples, the interactions between elements of the system or a magnetic field required to trap the system. However, there may be methods of affecting the dynamics in a controlled way, such as the time varying amplitude of the electric component of an interacting laser field. And so this leads to some questions; given a specific quantum system with known time-independent dynamics generator (referred to as the *drift* dynamics generators) and set of externally controllable fields for which the interaction can be described by *control* dynamics generators:

1. What states or transformations can we achieve (if any)?
2. What is the shape of the control pulse required to achieve this?

These questions are addressed as *controllability* and *quantum optimal control* [dAless08]. The answer to question of *controllability* is determined by the commutability of the dynamics generators and is formalised as the *Lie Algebra Rank Criterion* and is discussed in detail in [dAless08]. The solutions to the second question can be determined through optimal control algorithms, or control pulse optimisation.

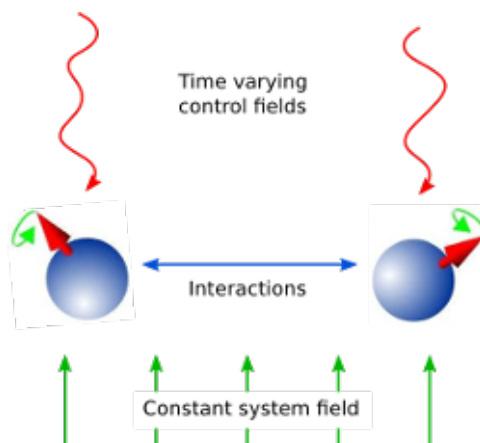


Fig. 3: Schematic showing the principle of quantum control.

Quantum Control has many applications including NMR, *quantum metrology*, *control of chemical reactions*, and *quantum information processing*.

To explain the physics behind these algorithms we will first consider only finite-dimensional, closed quantum systems.

### 3.17.2 Closed Quantum Systems

In closed quantum systems the states can be represented by kets, and the transformations on these states are unitary operators. The dynamics generators are Hamiltonians. The combined Hamiltonian for the system is given by

$$H(t) = H_0 + \sum_{j=1} u_j(t) H_j$$

where  $H_0$  is the drift Hamiltonian and the  $H_j$  are the control Hamiltonians. The  $u_j$  are time varying amplitude functions for the specific control.

The dynamics of the system are governed by *Schrödinger's equation*.

$$\frac{d}{dt} |\psi\rangle = -iH(t) |\psi\rangle$$



Note we use units where  $\hbar = 1$  throughout. The solutions to Schrödinger's equation are of the form:

$$|\psi(t)\rangle = U(t) |\psi_0\rangle$$

where  $\psi_0$  is the state of the system at  $t = 0$  and  $U(t)$  is a unitary operator on the Hilbert space containing the states.  $U(t)$  is a solution to the *Schrödinger operator equation*

$$\frac{d}{dt}U = -iH(t)U, \quad U(0) = \mathbb{I}$$

We can use optimal control algorithms to determine a set of  $u_j$  that will drive our system from  $|\psi_0\rangle$  to  $|\psi_1\rangle$ , this is state-to-state transfer, or drive the system from some arbitrary state to a given state  $|\psi_1\rangle$ , which is state preparation, or effect some unitary transformation  $U_{target}$ , called gate synthesis. The latter of these is most important in quantum computation.

### 3.17.3 The GRAPE algorithm

The **GR**radient **A**scent **P**ulse **E**ngineering was first proposed in [NKanej]. Solutions to Schrödinger's equation for a time-dependent Hamiltonian are not generally possible to obtain analytically. Therefore, a piecewise constant approximation to the pulse amplitudes is made. Time allowed for the system to evolve  $T$  is split into  $M$  timeslots (typically these are of equal duration), during which the control amplitude is assumed to remain constant. The combined Hamiltonian can then be approximated as:

$$H(t) \approx H(t_k) = H_0 + \sum_{j=1}^N u_{jk} H_j$$

where  $k$  is a timeslot index,  $j$  is the control index, and  $N$  is the number of controls. Hence  $t_k$  is the evolution time at the start of the timeslot, and  $u_{jk}$  is the amplitude of control  $j$  throughout timeslot  $k$ . The time evolution operator, or propagator, within the timeslot can then be calculated as:

$$X_k := e^{-iH(t_k)\Delta t_k}$$

where  $\Delta t_k$  is the duration of the timeslot. The evolution up to (and including) any timeslot  $k$  (including the full evolution  $k = M$ ) can be calculated as

$$X(t_k) := X_k X_{k-1} \cdots X_1 X_0$$

If the objective is state-to-state transfer then  $X_0 = |\psi_0\rangle$  and the target  $X_{target} = |\psi_1\rangle$ , for gate synthesis  $X_0 = U(0) = \mathbb{I}$  and the target  $X_{target} = U_{target}$ .

A *figure of merit* or *fidelity* is some measure of how close the evolution is to the target, based on the control amplitudes in the timeslots. The typical figure of merit for unitary systems is the normalised overlap of the evolution and the target.

$$f_{PSU} = \frac{1}{d} |\text{tr}\{X_{target}^\dagger X(T)\}|$$

where  $d$  is the system dimension. In this figure of merit the absolute value is taken to ignore any differences in global phase, and  $0 \leq f \leq 1$ . Typically the fidelity error (or *infidelity*) is more useful, in this case defined as  $\varepsilon = 1 - f_{PSU}$ . There are many other possible objectives, and hence figures of merit.

As there are now  $N \times M$  variables (the  $u_{jk}$ ) and one parameter to minimise  $\varepsilon$ , then the problem becomes a finite multi-variable optimisation problem, for which there are many established methods, often referred to as 'hill-climbing' methods. The simplest of these to understand is that of steepest ascent (or descent). The gradient of the fidelity with respect to all the variables is calculated (or approximated) and a step is made in the variable space in the direction of steepest ascent (or descent). This method is a first order gradient method. In two dimensions this describes a method of climbing a hill by heading in the direction where the ground rises fastest. This analogy also clearly illustrates one of the main challenges in multi-variable optimisation, which is that all methods have a tendency to get stuck in local maxima. It is hard to determine whether one has found a global maximum or not - a local peak is likely not to be the highest mountain in the region. In quantum optimal control we can typically define an infidelity that has a lower bound of zero. We can then look to minimise the infidelity (from here on we will

only consider optimising for infidelity minima). This means that we can terminate any pulse optimisation when the infidelity reaches zero (to a sufficient precision). This is however only possible for fully controllable systems; otherwise it is hard (if not impossible) to know that the minimum possible infidelity has been achieved. In the hill walking analogy the step size is roughly fixed to a stride, however, in computations the step size must be chosen. Clearly there is a trade-off here between the number of steps (or iterations) required to reach the minima and the possibility that we might step over a minima. In practice it is difficult to determine an efficient and effective step size.

The second order differentials of the infidelity with respect to the variables can be used to approximate the local landscape to a parabola. This way a step (or jump) can be made to where the minima would be if it were parabolic. This typically vastly reduces the number of iterations, and removes the need to guess a step size. The method where all the second differentials are calculated explicitly is called the *Newton-Raphson* method. However, calculating the second-order differentials (the Hessian matrix) can be computationally expensive, and so there are a class of methods known as *quasi-Newton* that approximate the Hessian based on successive iterations. The most popular of these (in quantum optimal control) is the Broyden–Fletcher–Goldfarb–Shanno algorithm (BFGS). The default method in the QuTiP Qtrl GRAPE implementation is the L-BFGS-B method in Scipy, which is a wrapper to the implementation described in [Byrd95]. This limited memory and bounded method does not need to store the entire Hessian, which reduces the computer memory required, and allows bounds to be set for variable values, which considering these are field amplitudes is often physical.

The pulse optimisation is typically far more efficient if the gradients can be calculated exactly, rather than approximated. For simple fidelity measures such as  $f_{PSU}$  this is possible. Firstly the propagator gradient for each timeslot with respect to the control amplitudes is calculated. For closed systems, with unitary dynamics, a method using the eigendecomposition is used, which is efficient as it is also used in the propagator calculation (to exponentiate the combined Hamiltonian). More generally (for example open systems and symplectic dynamics) the Frechet derivative (or augmented matrix) method is used, which is described in [Flo12]. For other optimisation goals it may not be possible to calculate analytic gradients. In these cases it is necessary to approximate the gradients, but this can be very expensive, and can lead to other algorithms out-performing GRAPE.

### 3.17.4 The CRAB Algorithm

It has been shown [Lloyd14], the dimension of a quantum optimal control problem is a polynomial function of the dimension of the manifold of the time-polynomial reachable states, when allowing for a finite control precision and evolution time. You can think of this as the information content of the pulse (as being the only effective input) being very limited e.g. the pulse is compressible to a few bytes without losing the target.

This is where the **Chopped RAndom Basis** (CRAB) algorithm [Doria11], [Caneva11] comes into play: Since the pulse complexity is usually very low, it is sufficient to transform the optimal control problem to a few parameter search by introducing a physically motivated function basis that builds up the pulse. Compared to the number of time slices needed to accurately simulate quantum dynamics (often equals basis dimension for Gradient based algorithms), this number is lower by orders of magnitude, allowing CRAB to efficiently optimize smooth pulses with realistic experimental constraints. It is important to point out, that CRAB does not make any suggestion on the basis function to be used. The basis must be chosen carefully considered, taking into account a priori knowledge of the system (such as symmetries, magnitudes of scales,...) and solution (e.g. sign, smoothness, bang-bang behavior, singularities, maximum excursion or rate of change,...). By doing so, this algorithm allows for native integration of experimental constraints such as maximum frequencies allowed, maximum amplitude, smooth ramping up and down of the pulse and many more. Moreover initial guesses, if they are available, can (however not have to) be included to speed up convergence.

As mentioned in the GRAPE paragraph, for CRAB local minima arising from algorithmic design can occur, too. However, for CRAB a ‘dressed’ version has recently been introduced [Rach15] that allows to escape local minima.

For some control objectives and/or dynamical quantum descriptions, it is either not possible to derive the gradient for the cost functional with respect to each time slice or it is computationally expensive to do so. The same can apply for the necessary (reverse) propagation of the co-state. All this trouble does not occur within CRAB as those elements are not in use here. CRAB, instead, takes the time evolution as a black-box where the pulse goes as an input and the cost (e.g. infidelity) value will be returned as an output. This concept, on top, allows for direct integration in a closed loop experimental environment where both the preliminarily open loop optimization, as well as the final adoption, and integration to the lab (to account for modeling errors, experimental systematic noise,...) can be done all in one, using this algorithm.

### 3.17.5 Optimal Quantum Control in QuTiP

The Quantum Control part of qutip has been moved to its own project.

The previously available implementation is now located in the [qutip-qtrl](#) module. If the `qutip-qtrl` package is installed, it can also be imported under the name `qutip.control` to ease porting code developed for QuTiP 4 to QuTiP 5.

A newer interface with upgraded capacities is being developed in [qutip-qoc](#).

Please give these modules a try.



## Chapter 4

# Gallery

This is the gallery for QuTiP examples, you can click on the image to see the source code.



# Chapter 5

## API documentation

This chapter contains automatically generated API documentation, including a complete list of QuTiP's public classes and functions.

### 5.1 Classes

#### 5.1.1 Qobj

**class Qobj**(*arg=None, dims=None, copy=True, superrep=None, isherm=None, isunitary=None*)

A class for representing quantum objects, such as quantum operators and states.

The Qobj class is the QuTiP representation of quantum operators and state vectors. This class also implements math operations  $+$ ,  $-$ ,  $*$  between Qobj instances (and  $/$  by a C-number), as well as a collection of common operator/state operations. The Qobj constructor optionally takes a dimension list and/or shape list as arguments.

#### Parameters

**inpt: array\_like, data object or :obj:`Qobj`**

Data for vector/matrix representation of the quantum object.

**dims: list**

Dimensions of object used for tensor products.

**shape: list**

Shape of underlying data structure (matrix shape).

**copy: bool**

Flag specifying whether Qobj should get a copy of the input data, or use the original.

#### Attributes

**data**

[object] The data object storing the vector / matrix representation of the *Qobj*.

**dtype**

[type] The data-layer type used for storing the data. The possible types are described in [Qobj.to](#).

**dims**

[list] List of dimensions keeping track of the tensor structure.

**shape**

[list] Return the shape of the Qobj data.

**type**

[str] Type of quantum object: 'bra', 'ket', 'oper', 'operator-ket', 'operator-bra', or 'super'.

**superrep**

[str] Representation used if *type* is 'super'. One of 'super' (Liouville form), 'choi' (Choi matrix with tr = dimension), or 'chi' (chi-matrix representation).

**isherm**

[bool] Indicates if quantum object represents Hermitian operator.

**isunitary**

[bool] Indicates if quantum object represents unitary operator.

**iscp**

[bool] Indicates if the quantum object represents a map, and if that map is completely positive (CP).

**ishp**

[bool] Indicates if the quantum object represents a map, and if that map is hermicity preserving (HP).

**istp**

[bool] Indicates if the quantum object represents a map, and if that map is trace preserving (TP).

**iscptp**

[bool] Indicates if the quantum object represents a map that is completely positive and trace preserving (CPTP).

**isket**

[bool] Indicates if the Qobj represents a ket state.

**isbra**

[bool] Indicates if the Qobj represents a bra state.

**isoper**

[bool] Indicates if the Qobj represents an operator.

**issuper**

[bool] Indicates if the Qobj represents a superoperator.

**isoperket**

[bool] Indicates if the Qobj represents a operator-ket state.

**isoperbra**

[bool] Indicates if the Qobj represents a operator-bra state.

## Methods

<b>copy()</b>	Create copy of Qobj
<b>conj()</b>	Conjugate of quantum object.
<b>contract()</b>	Contract subspaces of the tensor structure which
<b>cosm()</b>	Cosine of quantum object.
<b>dag()</b>	Adjoint (dagger) of quantum object.
<b>data_as(format, copy)</b>	Vector / matrix representation of quantum object
<b>diag()</b>	Diagonal elements of quantum object.
<b>dnorm()</b>	Diamond norm of quantum operator.
<b>dual_chan()</b>	Dual channel of quantum object representing a C
<b>eigenenergies(sparse=False, sort='low', eigvals=0, tol=0, maxiter=100000)</b>	Returns eigenenergies (eigenvalues) of a quantum
<b>eigenstates(sparse=False, sort='low', eigvals=0, tol=0, maxiter=100000)</b>	Returns eigenenergies and eigenstates of quantum
<b>expm()</b>	Matrix exponential of quantum object.
<b>full(order='C')</b>	Returns dense array of quantum object <i>data</i> attrib
<b>groundstate(sparse=False, tol=0, maxiter=100000)</b>	Returns eigenvalue and eigenket for the groundst
<b>inv()</b>	Return a Qobj corresponding to the matrix invers



Table 1 – continued from previous page

<b>logm()</b>	Matrix logarithm of quantum operator.
<b>matrix_element(bra, ket)</b>	Returns the matrix element of operator between $bra$ and $ket$ .
<b>norm(norm='tr', sparse=False, tol=0, maxiter=100000)</b>	Returns norm of a ket or an operator.
<b>overlap(other)</b>	Overlap between two state vectors or two operators.
<b>permute(order)</b>	Returns composite qobj with indices reordered.
<b>proj()</b>	Computes the projector for a ket or bra vector.
<b>ptrace(sel)</b>	Returns quantum object for selected dimensions.
<b>purity()</b>	Calculates the purity of a quantum object.
<b>sinm()</b>	Sine of quantum object.
<b>sqrtm()</b>	Matrix square root of quantum object.
<b>tidyup(atol=1e-12)</b>	Removes small elements from quantum object.
<b>tr()</b>	Trace of quantum object.
<b>trans()</b>	Transpose of quantum object.
<b>transform(inpt, inverse=False)</b>	Performs a basis transformation defined by $inpt$ matrix.
<b>trunc_neg(method='clip')</b>	Removes negative eigenvalues and returns a new quantum object.
<b>unit(norm='tr', sparse=False, tol=0, maxiter=100000)</b>	Returns normalized quantum object.

**\_\_call\_\_(other)**

Acts this Qobj on another Qobj either by left-multiplication, or by vectorization and devectorization, as appropriate.

**check\_herm()**

Check if the quantum object is hermitian.

**Returns**

**isherm**

[bool] Returns the new value of isherm property.

**conj()**

Get the element-wise conjugation of the quantum object.

**contract(inplace=False)**

Contract subspaces of the tensor structure which are 1D. Not defined on superoperators. If all dimensions are scalar, a Qobj of dimension  $[[1], [1]]$  is returned, i.e. `_multiple_` scalar dimensions are contracted, but one is left.

**Parameters**

**inplace: bool, optional**

If True, modify the dimensions in place. If False, return a copied object.

**Returns**

**out: Qobj**

Quantum object with dimensions contracted. Will be `self` if `inplace` is True.

**copy()**

Create identical copy

**cosm()**

Cosine of a quantum operator.

Operator must be square.

**Returns**

**oper**

[Qobj] Matrix cosine of operator.

**Raises**

### **TypeError**

Quantum object is not square.

### **Notes**

Uses the `Q.expm()` method.

### **dag()**

Get the Hermitian adjoint of the quantum object.

**data\_as**(*format=None, copy=True*)

Matrix from quantum object.

### **Parameters**

#### **format**

[str, default: None] Type of the output, “ndarray” for Dense, “csr\_matrix” for CSR. A `ValueError` will be raised if the format is not supported.

#### **copy**

[bool {False, True}] Whether to return a copy

### **Returns**

#### **data**

[numpy.ndarray, scipy.sparse.matrix\_csr, etc.] Matrix in the type of the underlying libraries.

### **diag()**

Diagonal elements of quantum object.

### **Returns**

#### **diags**

[array] Returns array of `real` values if operators is Hermitian, otherwise `complex` values are returned.

**dnorm**(*B=None*)

Calculates the diamond norm, or the diamond distance to another operator.

### **Parameters**

#### **B**

[*Qobj* or None] If B is not None, the diamond distance  $d(A, B) = \text{dnorm}(A - B)$  between this operator and B is returned instead of the diamond norm.

### **Returns**

#### **d**

[float] Either the diamond norm of this operator, or the diamond distance from this operator to B.

### **dual\_chan()**

Dual channel of quantum object representing a completely positive map.

**eigenenergies**(*sparse=False, sort='low', eigvals=0, tol=0, maxiter=100000*)

Eigenenergies of a quantum object.

Eigenenergies (eigenvalues) are defined for operators or superoperators only.

### **Parameters**

#### **sparse**

[bool] Use sparse Eigensolver

#### **sort**

[str] Sort eigenvalues ‘low’ to high, or ‘high’ to low.

**eigvals**

[int] Number of requested eigenvalues. Default is all eigenvalues.

**tol**

[float] Tolerance used by sparse Eigensolver (0=machine precision). The sparse solver may not converge if the tolerance is set too low.

**maxiter**

[int] Maximum number of iterations performed by sparse solver (if used).

**Returns**

**eigvals**

[array] Array of eigenvalues for operator.

**Notes**

The sparse eigensolver is much slower than the dense version. Use sparse only if memory requirements demand it.

**eigenstates**(*sparse=False, sort='low', eigvals=0, tol=0, maxiter=100000, phase\_fix=None*)

Eigenstates and eigenenergies.

Eigenstates and eigenenergies are defined for operators and superoperators only.

**Parameters**

**sparse**

[bool] Use sparse Eigensolver

**sort**

[str] Sort eigenvalues (and vectors) 'low' to high, or 'high' to low.

**eigvals**

[int] Number of requested eigenvalues. Default is all eigenvalues.

**tol**

[float] Tolerance used by sparse Eigensolver (0 = machine precision). The sparse solver may not converge if the tolerance is set too low.

**maxiter**

[int] Maximum number of iterations performed by sparse solver (if used).

**phase\_fix**

[int, None] If not None, set the phase of each kets so that ket[phase\_fix,0] is real positive.

**Returns**

**eigvals**

[array] Array of eigenvalues for operator.

**eigvecs**

[array] Array of quantum operators representing the operator eigenkets. Order of eigenkets is determined by order of eigenvalues.

## Notes

The sparse eigensolver is much slower than the dense version. Use sparse only if memory requirements demand it.

**expm**(*dtype*=<class 'qutip.core.data.dense.Dense'>)

Matrix exponential of quantum operator.

Input operator must be square.

### Parameters

#### **dtype**

[type] The data-layer type that should be output. As the matrix exponential is almost dense, this defaults to outputting dense matrices.

### Returns

#### **oper**

[*Qobj*] Exponentiated quantum operator.

### Raises

#### **TypeError**

Quantum operator is not square.

**full**(*order*='C', *squeeze*=False)

Dense array from quantum object.

### Parameters

#### **order**

[str {'C', 'F'}] Return array in C (default) or Fortran ordering.

#### **squeeze**

[bool {False, True}] Squeeze output array.

### Returns

#### **data**

[array] Array of complex data from quantum objects *data* attribute.

**groundstate**(*sparse*=False, *tol*=0, *maxiter*=100000, *safe*=True)

Ground state Eigenvalue and Eigenvector.

Defined for quantum operators or superoperators only.

### Parameters

#### **sparse**

[bool] Use sparse Eigensolver

#### **tol**

[float] Tolerance used by sparse Eigensolver (0 = machine precision). The sparse solver may not converge if the tolerance is set too low.

#### **maxiter**

[int] Maximum number of iterations performed by sparse solver (if used).

#### **safe**

[bool (default=True)] Check for degenerate ground state

### Returns

#### **eigval**

[float] Eigenvalue for the ground state of quantum operator.

#### **eigvec**

[*Qobj*] Eigenket for the ground state of quantum operator.

## Notes

The sparse eigensolver is much slower than the dense version. Use sparse only if memory requirements demand it.

**inv**(*sparse=False*)

Matrix inverse of a quantum operator

Operator must be square.

### Returns

**oper**

[*Qobj*] Matrix inverse of operator.

### Raises

**TypeError**

Quantum object is not square.

**property isbra**

Indicates if the *Qobj* represents a bra state.

**property isket**

Indicates if the *Qobj* represents a ket state.

**property isoper**

Indicates if the *Qobj* represents an operator.

**property isoperbra**

Indicates if the *Qobj* represents a operator-bra state.

**property isoperket**

Indicates if the *Qobj* represents a operator-ket state.

**property issuper**

Indicates if the *Qobj* represents a superoperator.

**logm**()

Matrix logarithm of quantum operator.

Input operator must be square.

### Returns

**oper**

[*Qobj*] Logarithm of the quantum operator.

### Raises

**TypeError**

Quantum operator is not square.

**matrix\_element**(*bra, ket*)

Calculates a matrix element.

Gives the matrix element for the quantum object sandwiched between a *bra* and *ket* vector.

### Parameters

**bra**

[*Qobj*] Quantum object of type 'bra' or 'ket'

**ket**

[*Qobj*] Quantum object of type 'ket'.

### Returns

### **elem**

[complex] Complex valued matrix element.

## **Notes**

It is slightly more computationally efficient to use a ket vector for the 'bra' input.

**norm**(*norm=None, kwargs=None*)

Norm of a quantum object.

Default norm is L2-norm for kets and trace-norm for operators. Other ket and operator norms may be specified using the *norm* parameter.

### **Parameters**

#### **norm**

[str] Which type of norm to use. Allowed values for vectors are 'l2' and 'max'. Allowed values for matrices are 'tr' for the trace norm, 'fro' for the Frobenius norm, 'one' and 'max'.

#### **kwargs**

[dict] Additional keyword arguments to pass on to the relevant norm solver. See details for each norm function in `data.norm`.

### **Returns**

#### **norm**

[float] The requested norm of the operator or state quantum object.

**overlap**(*other*)

Overlap between two state vectors or two operators.

Gives the overlap (inner product) between the current bra or ket Qobj and another bra or ket Qobj. It gives the Hilbert-Schmidt overlap when one of the Qobj is an operator/density matrix.

### **Parameters**

#### **other**

[Qobj] Quantum object for a state vector of type 'ket', 'bra' or density matrix.

### **Returns**

#### **overlap**

[complex] Complex valued overlap.

### **Raises**

#### **TypeError**

Can only calculate overlap between a bra, ket and density matrix quantum objects.

**permute**(*order*)

Permute the tensor structure of a quantum object. For example,

```
qutip.tensor(x, y).permute([1, 0])
```

will give the same result as

```
qutip.tensor(y, x)
```

and

```
qutip.tensor(a, b, c).permute([1, 2, 0])
```

will be the same as

```
qutip.tensor(b, c, a)
```

For regular objects (bras, kets and operators) we expect `order` to be a flat list of integers, which specifies the new order of the tensor product.

For superoperators, we expect `order` to be something like

```
[[0, 2], [1, 3]]
```

which tells us to permute according to [0, 2, 1, 3], and then group indices according to the length of each sublist. As another example, permuting a superoperator with dimensions of

```
[[[1, 2, 3], [1, 2, 3]], [[1, 2, 3], [1, 2, 3]]]
```

by an order

```
[[0, 3], [1, 4], [2, 5]]
```

should give a new object with dimensions

```
[[[1, 1], [2, 2], [3, 3]], [[1, 1], [2, 2], [3, 3]]].
```

### Parameters

#### **order**

[list] List of indices specifying the new tensor order.

### Returns

#### **P**

[*Qobj*] Permuted quantum object.

## **proj()**

Form the projector from a given ket or bra vector.

### Parameters

#### **Q**

[*Qobj*] Input bra or ket vector

### Returns

#### **P**

[*Qobj*] Projection operator.

## **ptrace(sel, dtype=None)**

Take the partial trace of the quantum object leaving the selected subspaces. In other words, trace out all subspaces which are `_not_` passed.

This is typically a function which acts on operators; bras and kets will be promoted to density matrices before the operation takes place since the partial trace is inherently undefined on pure states.

For operators which are currently being represented as states in the superoperator formalism (i.e. the object has type *operator-ket* or *operator-bra*), the partial trace is applied as if the operator were in the conventional form. This means that for any operator *x*, `operator_to_vector(x).ptrace(0) == operator_to_vector(x.ptrace(0))` and similar for *operator-bra*.

The story is different for full superoperators. In the formalism that QuTiP uses, if an operator has dimensions (*dims*) of `[[2, 3], [2, 3]]` then it can be represented as a state on a Hilbert space of dimensions `[2, 3, 2, 3]`, and a superoperator would be an operator which acts on this joint space. This function performs the partial trace on superoperators by letting the selected components refer to elements of the `_joint_space_`, and then returns a regular operator (of type *oper*).

### Parameters

#### **sel**

[int or iterable of int] An int or list of components to keep after partial trace. The selected subspaces will `_not_` be reordered, no matter order they are supplied to *ptrace*.

### Returns

**oper**

[*Qobj*] Quantum object representing partial trace with selected components remaining.

**purity()**

Calculate purity of a quantum object.

**Returns**

**state\_purity**

[float] Returns the purity of a quantum object. For a pure state, the purity is 1. For a mixed state of dimension  $d$ ,  $1/d \leq \text{purity} < 1$ .

**property shape**

Return the shape of the Qobj data.

**sinm()**

Sine of a quantum operator.

Operator must be square.

**Returns**

**oper**

[*Qobj*] Matrix sine of operator.

**Raises**

**TypeError**

Quantum object is not square.

## Notes

Uses the `Q.expm()` method.

**sqrtn**(*sparse=False, tol=0, maxiter=100000*)

Sqrt of a quantum operator. Operator must be square.

**Parameters**

**sparse**

[bool] Use sparse eigenvalue/vector solver.

**tol**

[float] Tolerance used by sparse solver (0 = machine precision).

**maxiter**

[int] Maximum number of iterations used by sparse solver.

**Returns**

**oper**

[*Qobj*] Matrix square root of operator.

**Raises**

**TypeError**

Quantum object is not square.



## Notes

The sparse eigensolver is much slower than the dense version. Use sparse only if memory requirements demand it.

**tidyup**(*atol=None*)

Removes small elements from the quantum object.

### Parameters

**atol**

[float] Absolute tolerance used by tidyup. Default is set via qutip global settings parameters.

### Returns

**oper**

[Qobj] Quantum object with small elements removed.

**to**(*data\_type*)

Convert the underlying data store of this *Qobj* into a different storage representation.

The different storage representations available are the “data-layer types” which are known to `qutip.core.data.to`. By default, these are CSR, Dense and Dia, which respectively construct a compressed sparse row matrix, diagonal matrix and a dense one. Certain algorithms and operations may be faster or more accurate when using a more appropriate data store.

If the data store is already in the format requested, the function returns *self*. Otherwise, it returns a copy of itself with the data store in the new type.

### Parameters

**data\_type**

[type] The data-layer type that the data of this *Qobj* should be converted to.

### Returns

**Qobj**

A new *Qobj* if a type conversion took place with the data stored in the requested format, or *self* if not.

**tr**()

Trace of a quantum object.

### Returns

**trace**

[float] Returns the trace of the quantum object.

**trans**()

Get the matrix transpose of the quantum operator.

### Returns

**oper**

[Qobj] Transpose of input operator.

**transform**(*inpt, inverse=False*)

Basis transform defined by input array.

Input array can be a matrix defining the transformation, or a list of kets that defines the new basis.

### Parameters

**inpt**

[array\_like] A matrix or list of kets defining the transformation.

**inverse**

[bool] Whether to return inverse transformation.

**Returns**

**oper**

[*Qobj*] Operator in new basis.

## Notes

This function is still in development.

**trunc\_neg**(*method*='clip')

Truncates negative eigenvalues and renormalizes.

Returns a new *Qobj* by removing the negative eigenvalues of this instance, then renormalizing to obtain a valid density operator.

**Parameters**

**method**

[str] Algorithm to use to remove negative eigenvalues. “clip” simply discards negative eigenvalues, then renormalizes. “sgs” uses the SGS algorithm (doi:10/bb76) to find the positive operator that is nearest in the Shatten 2-norm.

**Returns**

**oper**

[*Qobj*] A valid density operator.

**unit**(*inplace*=False, *norm*=None, *kwargs*=None)

Operator or state normalized to unity. Uses *norm* from *Qobj.norm()*.

**Parameters**

**inplace**

[bool] Do an in-place normalization

**norm**

[str] Requested norm for states / operators.

**kwargs**

[dict] Additional key-word arguments to be passed on to the relevant norm function (see *norm* for more details).

**Returns**

**obj**

[*Qobj*] Normalized quantum object. Will be the *self* object if in place.

## 5.1.2 QobjEvo

**class QobjEvo**

A class for representing time-dependent quantum objects, such as quantum operators and states.

Importantly, *QobjEvo* instances are used to represent such time-dependent quantum objects when working with QuTiP solvers.

A *QobjEvo* instance may be constructed from one of the following:

- a callable *f*(*t*: double, *args*: dict) -> *Qobj* that returns the value of the quantum object at time *t*.
- a [*Qobj*, *Coefficient*] pair, where the *Coefficient* may be any item that *coefficient* can accept (e.g. a function, a numpy array of coefficient values, a string expression).

- a *Qobj* (which creates a constant *QobjEvo* term).
- a list of such callables, pairs or *Qobjs*.
- a *QobjEvo* (in which case a copy is created, all other arguments are ignored except *args* which, if passed, replaces the existing arguments).

## Parameters

### **Q\_object**

[callable, list or *Qobj*] A specification of the time-dependent quantum object. See the paragraph above for a full description and the examples section below for examples.

### **args**

[dict, optional] A dictionary that contains the arguments for the coefficients. Arguments may be omitted if no function or string coefficients that require arguments are present.

### **tlist**

[array-like, optional] A list of times corresponding to the values of the coefficients supplied as numpy arrays. If no coefficients are supplied as numpy arrays, *tlist* may be omitted, otherwise it is required.

The times in *tlist* do not need to be equidistant, but must be sorted.

By default, a cubic spline interpolation will be used to interpolate the value of the (numpy array) coefficients at time *t*. If the coefficients are to be treated as step functions, pass the argument *order=0* (see below).

### **order**

[int, default=3] Order of the spline interpolation that is to be used to interpolate the value of the (numpy array) coefficients at time *t*. 0 use previous or left value.

### **copy**

[bool, default=True] Whether to make a copy of the *Qobj* instances supplied in the *Q\_object* parameter.

### **compress**

[bool, default=True] Whether to compress the *QobjEvo* instance terms after the instance has been created.

This sums the constant terms in a single term and combines [*Qobj*, *coefficient*] pairs with the same *Qobj* into a single pair containing the sum of the coefficients.

See *compress*.

### **function\_style**

[{None, "pythonic", "dict", "auto"}] The style of function signature used by callables in *Q\_object*. If style is *None*, the value of *qutip.settings.core["function\_coefficient\_style"]* is used. Otherwise the supplied value overrides the global setting.

### **boundary\_conditions**

[2-Tuple, str or None, optional] Boundary conditions for spline evaluation. Default value is *None*. Correspond to *bc\_type* of *scipy.interpolate.make\_interp\_spline*. Refer to Scipy's documentation for further details: [https://docs.scipy.org/doc/scipy/reference/generated/scipy.interpolate.make\\_interp\\_spline.html](https://docs.scipy.org/doc/scipy/reference/generated/scipy.interpolate.make_interp_spline.html)

## Examples

A *QobjEvo* constructed from a function:

```
def f(t, args):
    return qutip.qeye(N) * np.exp(args['w'] * t)

QobjEvo(f, args={'w': 1j})
```

For list based *QobjEvo*, the list must consist of *Qobj* or [*Qobj*, *Coefficient*] pairs:

```
QobjEvo([H0, [H1, coeff1], [H2, coeff2]], args=args)
```

The coefficients may be specified either using a *Coefficient* object or by a function, string, numpy array or any object that can be passed to the *coefficient* function. See the documentation of *coefficient* for a full description.

An example of a coefficient specified by a function:

```
def f1_t(t, args):
    return np.exp(-1j * t * args["w1"])

QobjEvo([H1, f1_t], args={"w1": 1.})
```

And of coefficients specified by string expressions:

```
H = QobjEvo(
    [H0, [H1, 'exp(-1j*w1*t)'], [H2, 'cos(w2*t)']],
    args={"w1": 1., "w2": 2.}
)
```

Coefficients maybe also be expressed as numpy arrays giving a list of the coefficient values:

```
tlist = np.logspace(-5, 0, 100)
H = QobjEvo(
    [H0, [H1, np.exp(-1j * tlist)], [H2, np.cos(2. * tlist)]],
    tlist=tlist
)
```

The coefficients array must have the same len as the tlist.

A *QobjEvo* may also be built using simple arithmetic operations combining *Qobj* with *Coefficient*, for example:

```
coeff = qutip.coefficient("exp(-1j*w1*t)", args={"w1": 1j})
qevo = H0 + H1 * coeff
```

## Attributes

### **dims**

[list] List of dimensions keeping track of the tensor structure.

### **shape**

[(int, int)] List of dimensions keeping track of the tensor structure.

### **type**

[str] Type of quantum object: 'bra', 'ket', 'oper', 'operator-ket', 'operator-bra', or 'super'.

### **superrep**

[str] Representation used if *type* is 'super'. One of 'super' (Liouville form) or 'choi' (Choi matrix with tr = dimension).

## `__call__()`

Get the *Qobj* at *t*.

### Parameters

**t**

[float] Time at which the *QobjEvo* is to be evaluated.

**\_args**

[dict [optional]] New arguments as a dict. Update args with `arguments(new_args)`.

**\*\*kwargs**

New arguments as a keywords. Update args with `arguments(**new_args)`.

### Notes

If both the positional `_args` and keywords are passed new values from both will be used. If a key is present with both, the `_args` dict value will take priority.

## `arguments(_args=None, **kwargs)`

Update the arguments.

### Parameters

**\_args**

[dict [optional]] New arguments as a dict. Update args with `arguments(new_args)`.

**\*\*kwargs**

New arguments as a keywords. Update args with `arguments(**new_args)`.

### Notes

If both the positional `_args` and keywords are passed new values from both will be used. If a key is present with both, the `_args` dict value will take priority.

## `compress()`

Look for redundance in the *QobjEvo* components:

Constant parts, (*Qobj* without Coefficient) will be summed. Pairs [*Qobj*, Coefficient] with the same *Qobj* are merged.

Example: `[[sigmax(), f1], [sigmax(), f2]] -> [[sigmax(), f1+f2]]`

The *QobjEvo* is transformed inplace.

### Returns

None

## `conj()`

Get the element-wise conjugation of the quantum object.

## `copy()`

Return a copy of this *QobjEvo*

## `dag()`

Get the Hermitian adjoint of the quantum object.

## `dtype`

Type of the data layers of the *QobjEvo*. When different data layers are used, we return the type of the sum of the parts.

**expect**(*t*, *state*, *check\_real=True*)

Expectation value of this operator at time *t* with the state.

**Parameters**

**t**

[float] Time of the operator to apply.

**state**

[Qobj] right matrix of the product

**check\_real**

[bool (True)] Whether to convert the result to a *real* when the imaginary part is smaller than the real part by a factor of `settings.core['rtol']`.

**Returns**

**expect**

[float or complex] `state.adjoint() @ self @ state` if `state` is a ket. `trace(self @ matrix)` if `state` is an operator or operator-ket.

**expect\_data**(*t*, *state*)

Expectation is defined as `state.adjoint() @ self @ state` if `state` is a vector, or `state` is an operator and `self` is a superoperator. If `state` is an operator and `self` is an operator, then expectation is `trace(self @ matrix)`.

**isbra**

Indicates if the system represents a bra state.

**isconstant**

Does the system change depending on *t*

**isket**

Indicates if the system represents a ket state.

**isoper**

Indicates if the system represents an operator.

**isoperbra**

Indicates if the system represents a operator-bra state.

**isoperket**

Indicates if the system represents a operator-ket state.

**issuper**

Indicates if the system represents a superoperator.

**linear\_map**(*op\_mapping*, \*, *\_skip\_check=False*)

Apply mapping to each Qobj contribution.

## Example

`QobjEvo([sigmax(), coeff]).linear_map(spre)`

gives the same result as

`QobjEvo([spre(sigmax()), coeff])`

**Parameters**

**op\_mapping: callable**

Function to apply to each elements.

**Returns**

## *QobjEvo*

Modified object

### Notes

Does not modify the coefficients, thus `linear_map(conj)` would not give the the conjugate of the *QobjEvo*. It's only valid for linear transformations.

**matmul**(*t, state*)

Product of this operator at time *t* to the state. `self(t) @ state`

#### Parameters

**t**

[float] Time of the operator to apply.

**state**

[Qobj] right matrix of the product

#### Returns

**product**

[Qobj] The result product as a Qobj

**matmul\_data**(*t, state, out=None*)

Compute `out += self(t) @ state`

**num\_elements**

Number of parts composing the system

**tidyup**(*atol=1e-12*)

Removes small elements from quantum object.

**to**(*data\_type*)

Convert the underlying data store of all component into the desired storage representation.

The different storage representations available are the “data-layer types”. By default, these are Dense, Dia and CSR, which respectively construct a dense matrix, diagonal sparse matrix and a compressed sparse row one.

The *QobjEvo* is transformed inplace.

#### Parameters

**data\_type**

[type] The data-layer type that the data of this *Qobj* should be converted to.

#### Returns

**None**

**to\_list**()

Restore the *QobjEvo* to a list form.

#### Returns

**list\_gevo: list**

The *QobjEvo* as a list, element are either *Qobj* for constant parts, [Qobj, Coefficient] for coefficient based term. The original format of the Coefficient is not restored. Lastly if the original *QobjEvo* is constructed with a function returning a Qobj, the term is returned as a pair of the original function and args (dict).

**trans**()

Transpose of the quantum object

### 5.1.3 Bloch sphere

**class Bloch**(*fig=None, axes=None, view=None, figsize=None, background=False*)

Class for plotting data on the Bloch sphere. Valid data can be either points, vectors, or Qobj objects.

#### Attributes

##### **axes**

[matplotlib.axes.Axes] User supplied Matplotlib axes for Bloch sphere animation.

##### **fig**

[matplotlib.figure.Figure] User supplied Matplotlib Figure instance for plotting Bloch sphere.

##### **font\_color**

[str, default 'black'] Color of font used for Bloch sphere labels.

##### **font\_size**

[int, default 20] Size of font used for Bloch sphere labels.

##### **frame\_alpha**

[float, default 0.1] Sets transparency of Bloch sphere frame.

##### **frame\_color**

[str, default 'gray'] Color of sphere wireframe.

##### **frame\_width**

[int, default 1] Width of wireframe.

##### **point\_color**

[list, default ["b", "r", "g", "#CC6600"]] List of colors for Bloch sphere point markers to cycle through, i.e. by default, points 0 and 4 will both be blue ('b').

##### **point\_marker**

[list, default ["o", "s", "d", "^"]] List of point marker shapes to cycle through.

##### **point\_size**

[list, default [25, 32, 35, 45]] List of point marker sizes. Note, not all point markers look the same size when plotted!

##### **sphere\_alpha**

[float, default 0.2] Transparency of Bloch sphere itself.

##### **sphere\_color**

[str, default '#FFDDDD'] Color of Bloch sphere.

##### **figsize**

[list, default [7, 7]] Figure size of Bloch sphere plot. Best to have both numbers the same; otherwise you will have a Bloch sphere that looks like a football.

##### **vector\_color**

[list, ["g", "#CC6600", "b", "r"]] List of vector colors to cycle through.

##### **vector\_width**

[int, default 5] Width of displayed vectors.

##### **vector\_style**

[str, default '->'] Vector arrowhead style (from matplotlib's arrow style).

##### **vector\_mutation**

[int, default 20] Width of vectors arrowhead.

##### **view**

[list, default [-60, 30]] Azimuthal and Elevation viewing angles.

##### **xlabel**

[list, default ["\$x\$", ""]] List of strings corresponding to +x and -x axes labels, respectively.



**xlpos**

[list, default [1.1, -1.1]] Positions of +x and -x labels respectively.

**ylabel**

[list, default ["\$y\$", ""]] List of strings corresponding to +y and -y axes labels, respectively.

**ylpos**

[list, default [1.2, -1.2]] Positions of +y and -y labels respectively.

**zlabel**

[list, default ['\$\left|0\right\rangle\$', '\$\left|1\right\rangle\$']] List of strings corresponding to +z and -z axes labels, respectively.

**zlpos**

[list, default [1.2, -1.2]] Positions of +z and -z labels respectively.

**add\_annotation**(*state\_or\_vector*, *text*, *\*\*kwargs*)

Add a text or LaTeX annotation to Bloch sphere, parametrized by a qubit state or a vector.

**Parameters**

**state\_or\_vector**

[*Qobj*/array/list/tuple] Position for the annotation. *Qobj* of a qubit or a vector of 3 elements.

**text**

[str] Annotation text. You can use LaTeX, but remember to use raw string e.g. `r"$\angle x \angle $"` or escape backslashes e.g. `"$\angle x \angle $"`.

**kwargs**

Options as for `mplot3d.axes3d.text`, including: `fontsize`, `color`, `horizontalalignment`, `verticalalignment`.

**add\_arc**(*start*, *end*, *fmt='b'*, *steps=None*, *\*\*kwargs*)

Adds an arc between two points on a sphere. The arc is set to be blue solid curve by default.

The start and end points must be on the same sphere (i.e. have the same radius) but need not be on the unit sphere.

**Parameters**

**start**

[*Qobj* or array-like] Array with cartesian coordinates of the first point, or a state vector or density matrix that can be mapped to a point on or within the Bloch sphere.

**end**

[*Qobj* or array-like] Array with cartesian coordinates of the second point, or a state vector or density matrix that can be mapped to a point on or within the Bloch sphere.

**fmt**

[str, default: "b"] A matplotlib format string for rendering the arc.

**steps**

[int, default: None] The number of segments to use when rendering the arc. The default uses 100 steps times the distance between the start and end points, with a minimum of 2 steps.

**\*\*kwargs**

[dict] Additional parameters to pass to the matplotlib `.plot` function when rendering this arc.

**add\_line**(*start*, *end*, *fmt='k'*, *\*\*kwargs*)

Adds a line segment connecting two points on the bloch sphere.

The line segment is set to be a black solid line by default.

### Parameters

#### start

[*Qobj* or array-like] Array with cartesian coordinates of the first point, or a state vector or density matrix that can be mapped to a point on or within the Bloch sphere.

#### end

[*Qobj* or array-like] Array with cartesian coordinates of the second point, or a state vector or density matrix that can be mapped to a point on or within the Bloch sphere.

#### fmt

[str, default: "k"] A matplotlib format string for rendering the line.

#### \*\*kwargs

[dict] Additional parameters to pass to the matplotlib .plot function when rendering this line.

**add\_points**(*points*, *meth*='s', *colors*=None, *alpha*=1.0)

Add a list of data points to bloch sphere.

### Parameters

#### points

[array\_like] Collection of data points.

#### meth

[{'s', 'm', 'l'}] Type of points to plot, use 'm' for multicolored, 'l' for points connected with a line.

#### colors

[array\_like] Optional array with colors for the points. A single color for meth 's', and list of colors for meth 'm'

#### alpha

[float, default=1.] Transparency value for the vectors. Values between 0 and 1.

### Notes

When using *meth*=1 in QuTiP 4.6, the line transparency defaulted to 0.75 and there was no way to alter it. When the *alpha* parameter was added in QuTiP 4.7, the default became *alpha*=1.0 for values of *meth*.

**add\_states**(*state*, *kind*='vector', *colors*=None, *alpha*=1.0)

Add a state vector *Qobj* to Bloch sphere.

### Parameters

#### state

[*Qobj*] Input state vector.

#### kind

[{'vector', 'point'}] Type of object to plot.

#### colors

[array\_like] Optional array with colors for the states.

#### alpha

[float, default=1.] Transparency value for the vectors. Values between 0 and 1.

**add\_vectors**(*vectors*, *colors*=None, *alpha*=1.0)

Add a list of vectors to Bloch sphere.

### Parameters

#### vectors

[array\_like] Array with vectors of unit length or smaller.

**colors**

[array\_like] Optional array with colors for the vectors.

**alpha**

[float, default=1.] Transparency value for the vectors. Values between 0 and 1.

**clear()**

Resets Bloch sphere data sets to empty.

**make\_sphere()**

Plots Bloch sphere and data sets.

**render()**

Render the Bloch sphere and its data sets in on given figure and axes.

**save(name=None, format='png', dirc=None, dpin=None)**

Saves Bloch sphere to file of type `format` in directory `dirc`.

**Parameters**

**name**

[str] Name of saved image. Must include path and format as well. i.e. `'/Users/Me/Desktop/bloch.png'` This overrides the `'format'` and `'dirc'` arguments.

**format**

[str] Format of output image.

**dirc**

[str] Directory for output images. Defaults to current working directory.

**dpin**

[int] Resolution in dots per inch.

**Returns**

**File containing plot of Bloch sphere.**

**set\_label\_convention(convention)**

Set x, y and z labels according to one of conventions.

**Parameters**

**convention**

[string] One of the following:

- “original”
- “xyz”
- “sx sy sz”
- “01”
- “polarization jones”
- “polarization jones letters” see also: [https://en.wikipedia.org/wiki/Jones\\_calculus](https://en.wikipedia.org/wiki/Jones_calculus)
- “polarization stokes” see also: [https://en.wikipedia.org/wiki/Stokes\\_parameters](https://en.wikipedia.org/wiki/Stokes_parameters)

**show()**

Display Bloch sphere and corresponding data sets.

## Notes

When using inline plotting in Jupyter notebooks, any figure created in a notebook cell is displayed after the cell executes. Thus if you create a figure yourself and use it create a Bloch sphere with `b = Bloch(..., fig=fig)` and then call `b.show()` in the same cell, then the figure will be displayed twice. If you do create your own figure, the simplest solution to this is to not call `.show()` in the cell you create the figure in.

## 5.1.4 Distributions

**class** `QFunc(xvec, yvec, g: float = 1.4142135623730951, memory: float = 1024)`

Class-based method of calculating the Husimi-Q function of many different quantum states at fixed phase-space points  $0.5 * g * (xvec + i * yvec)$ . This class has slightly higher first-usage costs than `qfunc`, but subsequent operations will be several times faster. However, it can require quite a lot of memory. Call the created object as a function to retrieve the Husimi-Q function.

### Parameters

**xvec, yvec**

[array\_like] x- and y-coordinates at which to calculate the Husimi-Q function.

**g**

[float, default:  $\sqrt{2}$ ] Scaling factor for  $a = 0.5 * g * (x + iy)$ . The value of  $g$  is related to the value of  $\hbar$  in the commutation relation  $[x, y] = i\hbar$  via  $\hbar = 2/g^2$ , so the default corresponds to  $\hbar = 1$ .

**memory**

[real, default: 1024] Size in MB that may be used internally as workspace. This class will raise `MemoryError` if subsequently passed a state of sufficiently large dimension that this bound would be exceeded. In those cases, use `qfunc` with `precompute_memory=None` instead to force using the slower, more memory-efficient algorithm.

See also:

### `qfunc`

A single function version, which will involve computing several quantities multiple times in order to use less memory.

## Examples

Initialise the class for a square set of coordinates, with some states we want to investigate.

```
>>> xvec = np.linspace(-2, 2, 101)
>>> states = [qutip.rand_dm(10) for _ in [None]*10]
>>> qfunc = qutip.QFunc(xvec, xvec)
```

Now we can calculate the Husimi-Q function over each of the states more efficiently with:

```
>>> husimiq = np.array([qfunc(state) for state in states])
```

## 5.1.5 Solvers

**class** `SESolver`(*H*, \*, *options=None*)

Bases: `Solver`

Schrodinger equation evolution of a state vector or unitary matrix for a given Hamiltonian.

### Parameters

#### **H**

[*Qobj*, *QobjEvo*] System Hamiltonian as a *Qobj* or *QobjEvo* for time-dependent Hamiltonians. List of [*Qobj*, *Coefficient*] or callable that can be made into *QobjEvo* are also accepted.

#### **options**

[dict, optional] Options for the solver, see `SESolver.options` and `Integrator` for a list of all options.

### Attributes

#### **stats: dict**

Diverse diagnostic statistics of the evolution.

**classmethod** `ExpectFeedback`(*operator*, *default=0.0*)

Expectation value of the instantaneous state of the evolution to be used by a time-dependent operator.

When used as an args:

```
QobjEvo([op, func], args={"E0": Solver.ExpectFeedback(oper)})
```

The func will receive `expect(oper, state)` as `E0` during the evolution.

### Parameters

#### **operator**

[*Qobj*, *QobjEvo*] Operator to compute the expectation values of.

#### **default**

[float, default][0.] Initial value to be used at setup.

**classmethod** `StateFeedback`(*default=None*, *raw\_data=False*, *prop=False*)

State of the evolution to be used in a time-dependent operator.

When used as an args:

```
QobjEvo([op, func], args={"state": SESolver.StateFeedback()})
```

The func will receive the ket as `state` during the evolution.

### Parameters

#### **default**

[*Qobj* or `qutip.core.data.Data`, default][None] Initial value to be used at setup of the system.

#### **prop**

[bool, default][False] Set to True when using `sesolve` for computing propagators.

#### **raw\_data**

[bool, default][False] If True, the raw matrix will be passed instead of a *Qobj*. For density matrices, the matrices can be column stacked or square depending on the integration method.

### property options

Solver's options:

**store\_final\_state: bool, default: False**

Whether or not to store the final state of the evolution in the result class.

**store\_states: bool, default: None**

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

**normalize\_output: bool, default: True**

Normalize output state to hide ODE numerical errors.

**progress\_bar: str {"text", "enhanced", "tqdm", ""}, default: ""**

How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.

**progress\_kwargs: dict, default: {"chunk\_size": 10}**

Arguments to pass to the progress\_bar. Qutip's bars use chunk\_size.

**method: str, default: "adams"**

Which ordinary differential equation integration method to use.

**run(state0, tlist, \*, args=None, e\_ops=None)**

Do the evolution of the Quantum system.

For a `state0` at time `tlist[0]` do the evolution as directed by `rhs` and for each time in `tlist` store the state and/or expectation values in a [Result](#). The evolution method and stored results are determined by options.

#### Parameters

**state0**

[[Qobj](#)] Initial state of the evolution.

**tlist**

[list of double] Time for which to save the results (state and/or expect) of the evolution. The first element of the list is the initial time of the evolution. Each times of the list must be increasing, but does not need to be uniformy distributed.

**args**

[dict, optional {None}] Change the args of the rhs for the evolution.

**e\_ops**

[list {None}] List of [Qobj](#), [QobjEvo](#) or callable to compute the expectation values. Function[s] must have the signature `f(t : float, state : Qobj) -> expect`.

#### Returns

**results**

[[Result](#)] Results of the evolution. States and/or expect will be saved. You can control the saved data in the options.

**start(state0, t0)**

Set the initial state and time for a step evolution.

#### Parameters

**state0**

[[Qobj](#)] Initial state of the evolution.

**t0**

[double] Initial time of the evolution.

**step(t, \*, args=None, copy=True)**

Evolve the state to `t` and return the state as a [Qobj](#).

#### Parameters

**t**

[double] Time to evolve to, must be higher than the last call.

**args**

[dict, optional {None}] Update the args of the system. The change is effective from the beginning of the interval. Changing args can slow the evolution.

**copy**

[bool, optional {True}] Whether to return a copy of the data or the data in the ODE solver.

**Notes**

The state must be initialized first by calling `start` or `run`. If `run` is called, `step` will continue from the last time and state obtained.

**property sys\_dims**

Dimensions of the space that the system use:

`qutip.basis(sovler.dims)` will create a state with proper dimensions for this solver.

**class MESolver**(*H*, *c\_ops*=None, \*, *options*=None)

Bases: [SESolver](#)

Master equation evolution of a density matrix for a given Hamiltonian and set of collapse operators, or a Liouvillian.

Evolve the density matrix (*rho0*) using a given Hamiltonian or Liouvillian (*H*) and an optional set of collapse operators (*c\_ops*), by integrating the set of ordinary differential equations that define the system.

If either *H* or the Qobj elements in *c\_ops* are superoperators, they will be treated as direct contributions to the total system Liouvillian. This allows the solution of master equations that are not in standard Lindblad form.

**Parameters**

**H**

[[Qobj](#), [QobjEvo](#)] Possibly time-dependent system Liouvillian or Hamiltonian as a Qobj or QobjEvo. List of [[Qobj](#), Coefficient] or callable that can be made into [QobjEvo](#) are also accepted.

**c\_ops**

[list of [Qobj](#), [QobjEvo](#)] Single collapse operator, or list of collapse operators, or a list of Liouvillian superoperators. None is equivalent to an empty list.

**options**

[dict, optional] Options for the solver, see [MESolver.options](#) and [Integrator](#) for a list of all options.

**Attributes**

**stats: dict**

Diverse diagnostic statistics of the evolution.

**classmethod ExpectFeedback**(*operator*, *default*=0.0)

Expectation value of the instantaneous state of the evolution to be used by a time-dependent operator.

When used as an args:

`QobjEvo([op, func], args={"E0": Solver.ExpectFeedback(oper)})`

The func will receive `expect(oper, state)` as `E0` during the evolution.

**Parameters**

**operator**

[[Qobj](#), [QobjEvo](#)] Operator to compute the expectation values of.

**default**

[float, default][0.] Initial value to be used at setup.

**classmethod** `StateFeedback`(*default=None, raw\_data=False, prop=False*)

State of the evolution to be used in a time-dependent operator.

When used as an args:

```
QobjEvo([op, func], args={"state": MESolver.StateFeedback()})
```

The func will receive the density matrix as `state` during the evolution.

#### Parameters

##### **default**

[Qobj or `qutip.core.data.Data`, default][None] Initial value to be used at setup of the system.

##### **prop**

[bool, default][False] Set to True when computing propagators. The default will take the shape of the propagator instead of a state.

##### **raw\_data**

[bool, default][False] If True, the raw matrix will be passed instead of a Qobj. For density matrices, the matrices can be column stacked or square depending on the integration method.

#### property options

Solver's options:

**store\_final\_state: bool, default: False**

Whether or not to store the final state of the evolution in the result class.

**store\_states: bool, default: None**

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

**normalize\_output: bool, default: True**

Normalize output state to hide ODE numerical errors.

**progress\_bar: str {"text", "enhanced", "tqdm", ""}, default: ""**

How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.

**progress\_kwargs: dict, default: {"chunk\_size": 10}**

Arguments to pass to the progress\_bar. Qutip's bars use `chunk_size`.

**method: str, default: "adams"**

Which ordinary differential equation integration method to use.

**run**(*state0, tlist, \*, args=None, e\_ops=None*)

Do the evolution of the Quantum system.

For a `state0` at time `tlist[0]` do the evolution as directed by `rhs` and for each time in `tlist` store the state and/or expectation values in a [Result](#). The evolution method and stored results are determined by options.

#### Parameters

##### **state0**

[Qobj] Initial state of the evolution.

##### **tlist**

[list of double] Time for which to save the results (state and/or expect) of the evolution. The first element of the list is the initial time of the evolution. Each times of the list must be increasing, but does not need to be uniform distributed.

##### **args**

[dict, optional {None}] Change the args of the rhs for the evolution.



**e\_ops**

[list {None}] List of Qobj, QobjEvo or callable to compute the expectation values. Function[s] must have the signature  $f(t : \text{float}, \text{state} : \text{Qobj}) \rightarrow \text{expect}$ .

**Returns**

**results**

[[Result](#)] Results of the evolution. States and/or expect will be saved. You can control the saved data in the options.

**start**(state0, t0)

Set the initial state and time for a step evolution.

**Parameters**

**state0**

[[Qobj](#)] Initial state of the evolution.

**t0**

[double] Initial time of the evolution.

**step**(t, \*, args=None, copy=True)

Evolve the state to t and return the state as a [Qobj](#).

**Parameters**

**t**

[double] Time to evolve to, must be higher than the last call.

**args**

[dict, optional {None}] Update the args of the system. The change is effective from the beginning of the interval. Changing args can slow the evolution.

**copy**

[bool, optional {True}] Whether to return a copy of the data or the data in the ODE solver.

**Notes**

The state must be initialized first by calling [start](#) or [run](#). If [run](#) is called, [step](#) will continue from the last time and state obtained.

**property sys\_dims**

Dimensions of the space that the system use:

`qutip.basis(sovler.dims)` will create a state with proper dimensions for this solver.

**class BRSolver**(H, a\_ops, c\_ops=None, sec\_cutoff=0.1, \*, options=None)

Bases: Solver

Bloch Redfield equation evolution of a density matrix for a given Hamiltonian and set of bath coupling operators.

**Parameters**

**H**

[[Qobj](#), [QobjEvo](#)] Possibly time-dependent system Liouvillian or Hamiltonian as a Qobj or QobjEvo. list of [[Qobj](#), Coefficient] or callable that can be made into [QobjEvo](#) are also accepted.

**a\_ops**

[list of (a\_op, spectra)] Nested list of system operators that couple to the environment, and the corresponding bath spectra.

**a\_op**

[[Qobj](#), [QobjEvo](#)] The operator coupling to the environment. Must be hermitian.

### spectra

[Coefficient] The corresponding bath spectra. As a *Coefficient* using an 'w' args. Can depend on t only if a\_op is a *QobjEvo*. *SpectraCoefficient* can be used to convert a coefficient depending on t to one depending on w.

Example:

```
a_ops = [
    (a+a.dag(), coefficient('w>0', args={'w':0})),
    (QobjEvo([b+b.dag(), lambda t: ...]),
     coefficient(lambda t, w: ...), args={"w": 0}),
    (c+c.dag(), SpectraCoefficient(coefficient(array, tlist=ws))),
]
```

### c\_ops

[list of *Qobj*, *QobjEvo*] Single collapse operator, or list of collapse operators, or a list of Lindblad dissipator. None is equivalent to an empty list.

### options

[dict, optional] Options for the solver, see *BRSSolver.options* and *Integrator* for a list of all options.

### sec\_cutoff

[float {0.1}] Cutoff for secular approximation. Use -1 if secular approximation is not used when evaluating bath-coupling terms.

### Attributes

#### stats: dict

Diverse diagnostic statistics of the evolution.

### classmethod ExpectFeedback(operator, default=0.0)

Expectation value of the instantaneous state of the evolution to be used by a time-dependent operator.

When used as an args:

```
QobjEvo([op, func], args={"E0": Solver.ExpectFeedback(oper)})
```

The func will receive `expect(oper, state)` as `E0` during the evolution.

### Parameters

#### operator

[Qobj, QobjEvo] Operator to compute the expectation values of.

#### default

[float, default][0.] Initial value to be used at setup.

### classmethod StateFeedback(default=None, raw\_data=False)

State of the evolution to be used in a time-dependent operator.

When used as an args:

```
QobjEvo([op, func], args={"state": BRMESolver.StateFeedback()})
```

The func will receive the density matrix as `state` during the evolution.

---

**Note:** The state will not be in the lab basis, but in the evolution basis.

---

### Parameters

#### default

[Qobj or qutip.core.data.Data, default][None] Initial value to be used at setup of the system.

### **raw\_data**

[bool, default][False] If True, the raw matrix will be passed instead of a Qobj. For density matrices, the matrices can be column stacked or square depending on the integration method.

### **property options**

Options for bloch redfield solver:

**store\_final\_state: bool, default: False**

Whether or not to store the final state of the evolution in the result class.

**store\_states: bool, default: None**

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

**normalize\_output: bool, default: False**

Normalize output state to hide ODE numerical errors.

**progress\_bar: str {'text', 'enhanced', 'tqdm', ''}, default: ""**

How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.

**progress\_kwargs: dict, default: {"chunk\_size":10}**

Arguments to pass to the progress\_bar. Qutip's bars use chunk\_size.

**tensor\_type: str ['sparse', 'dense', 'data'], default: "sparse"**

Which data type to use when computing the brtensor. With a cutoff 'sparse' is usually the most efficient.

**sparse\_eigsolver: bool, default: False**

Whether to use the sparse eigensolver

**method: str, default: "adams"**

Which ODE integrator methods are supported.

**run(state0, tlist, \*, args=None, e\_ops=None)**

Do the evolution of the Quantum system.

For a `state0` at time `tlist[0]` do the evolution as directed by `rhs` and for each time in `tlist` store the state and/or expectation values in a [Result](#). The evolution method and stored results are determined by options.

### **Parameters**

#### **state0**

[Qobj] Initial state of the evolution.

#### **tlist**

[list of double] Time for which to save the results (state and/or expect) of the evolution. The first element of the list is the initial time of the evolution. Each times of the list must be increasing, but does not need to be uniformy distributed.

#### **args**

[dict, optional {None}] Change the args of the rhs for the evolution.

#### **e\_ops**

[list {None}] List of Qobj, QobjEvo or callable to compute the expectation values. Function[s] must have the signature `f(t : float, state : Qobj) -> expect`.

### **Returns**

#### **results**

[[Result](#)] Results of the evolution. States and/or expect will be saved. You can control the saved data in the options.

**start**(state0, t0)

Set the initial state and time for a step evolution.

#### Parameters

**state0**

[*Qobj*] Initial state of the evolution.

**t0**

[double] Initial time of the evolution.

**step**(t, \*, args=None, copy=True)

Evolve the state to t and return the state as a *Qobj*.

#### Parameters

**t**

[double] Time to evolve to, must be higher than the last call.

**args**

[dict, optional {None}] Update the args of the system. The change is effective from the beginning of the interval. Changing args can slow the evolution.

**copy**

[bool, optional {True}] Whether to return a copy of the data or the data in the ODE solver.

#### Notes

The state must be initialized first by calling *start* or *run*. If *run* is called, *step* will continue from the last time and state obtained.

**property sys\_dims**

Dimensions of the space that the system use:

qutip.basis(sovler.dims) will create a state with proper dimensions for this solver.

**class FMESolver**(floquet\_basis, a\_ops, w\_th=0.0, \*, kmax=5, nT=None, options=None)

Bases: *MESolver*

Solver for the Floquet-Markov master equation.

---

**Note:** Operators (c\_ops and e\_ops) are in the laboratory basis.

---

#### Parameters

**floquet\_basis**

[*FloquetBasis*] The system Hamiltonian wrapped in a FloquetBasis object. Choosing a different integrator for the floquet\_basis than for the evolution of the floquet state can improve the performance.

**a\_ops**

[list of tuple(*Qobj*, callable)] List of collapse operators and the corresponding function for the noise power spectrum. The collapse operator must be a *Qobj* and cannot be time dependent. The spectrum function must take and return a numpy array.

**w\_th**

[float] The temperature of the environment in units of Hamiltonian frequency.

**kmax**

[int [5]] The truncation of the number of sidebands..

**nT**

[int [20\*kmax]] The number of integration steps (for calculating X) within one period.

### options

[dict, optional] Options for the solver, see [FMESolver.options](#) and [Integrator](#) for a list of all options.

### classmethod ExpectFeedback()

Expect of the state of the evolution to be used in a time-dependent operator.

Not implemented for FMESolver

### classmethod StateFeedback()

State of the evolution to be used in a time-dependent operator.

Not implemented for FMESolver

### property options

Solver's options:

#### store\_final\_state: bool, default: False

Whether or not to store the final state of the evolution in the result class.

#### store\_states: bool, default: None

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

#### normalize\_output: bool, default: True

Normalize output state to hide ODE numerical errors.

#### progress\_bar: str {"text", "enhanced", "tqdm", ""}, default: ""

How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.

#### progress\_kwargs: dict, default: {"chunk\_size": 10}

Arguments to pass to the progress\_bar. Qutip's bars use chunk\_size.

#### method: str, default: "adams"

Which ordinary differential equation integration method to use.

### run(state0, tlist, \*, floquet=False, args=None, e\_ops=None)

Calculate the evolution of the quantum system.

For a `state0` at time `tlist[0]` do the evolution as directed by `rhs` and for each time in `tlist` store the state and/or expectation values in a [Result](#). The evolution method and stored results are determined by options.

### Parameters

#### state0

[*Qobj*] Initial state of the evolution.

#### tlist

[list of double] Time for which to save the results (state and/or expect) of the evolution. The first element of the list is the initial time of the evolution. Each times of the list must be increasing, but does not need to be uniform distributed.

#### floquet

[bool, optional {False}] Whether the initial state in the floquet basis or laboratory basis.

#### args

[dict, optional {None}] Not supported

#### e\_ops

[list {None}] List of *Qobj*, *QobjEvo* or callable to compute the expectation values. Function[s] must have the signature `f(t : float, state : Qobj) -> expect`.

### Returns

#### results

[FloquetResult] Results of the evolution. States and/or expect will be saved. You can control the saved data in the options.

**start**(state0, t0, \*, floquet=False)

Set the initial state and time for a step evolution. options for the evolutions are read at this step.

#### Parameters

##### state0

[Qobj] Initial state of the evolution.

##### t0

[double] Initial time of the evolution.

##### floquet

[bool, optional {False}] Whether the initial state is in the floquet basis or laboratory basis.

**step**(t, \*, args=None, copy=True, floquet=False)

Evolve the state to t and return the state as a Qobj.

#### Parameters

##### t

[double] Time to evolve to, must be higher than the last call.

##### copy

[bool, optional {True}] Whether to return a copy of the data or the data in the ODE solver.

##### floquet

[bool, optional {False}] Whether to return the state in the floquet basis or laboratory basis.

##### args

[dict, optional {None}] Not supported

#### Notes

The state must be initialized first by calling start or run. If run is called, step will continue from the last time and state obtained.

#### property sys\_dims

Dimensions of the space that the system use:

qutip.basis(sovler.dims) will create a state with proper dimensions for this solver.

**class FloquetBasis**(H, T, args=None, options=None, sparse=False, sort=True, precompute=None)

Utility to compute floquet modes and states.

#### Attributes

##### U

[Propagator] The propagator of the Hamiltonian over one period.

##### evecs

[Data] Matrix where each column is an initial Floquet mode.

##### e\_quasi

[np.ndarray[float]] The quasi energies of the Hamiltonian.

**from\_floquet\_basis**(floquet\_basis, t=0)

Transform a ket or density matrix from the Floquet basis at time t to the lab basis.

#### Parameters

### **floquet\_basis**

[*Qobj*, Data] Initial state in the Floquet basis at time  $t$ . May be either a ket or density matrix.

**t**

[float [0]] The time at which to evaluate the Floquet states.

### **Returns**

#### **output**

[*Qobj*, Data] The state in the lab basis. The return type is the same as the type of the input state.

**mode**( $t$ ,  $data=False$ )

Calculate the Floquet modes at time  $t$ .

### **Parameters**

**t**

[float] The time for which to evaluate the Floquet mode.

**data**

[bool [False]] Whether to return the states as a single data matrix or a list of ket states.

### **Returns**

#### **output**

[list[*Qobj*], Data] A list of Floquet states for the time  $t$  or the states as column in a single matrix.

**state**( $t$ ,  $data=False$ )

Evaluate the floquet states at time  $t$ .

### **Parameters**

**t**

[float] The time for which to evaluate the Floquet states.

**data**

[bool [False]] Whether to return the states as a single data matrix or a list of ket states.

### **Returns**

#### **output**

[list[*Qobj*], Data] A list of Floquet states for the time  $t$  or the states as column in a single matrix.

**to\_floquet\_basis**( $lab\_basis$ ,  $t=0$ )

Transform a ket or density matrix in the lab basis to the Floquet basis at time  $t$ .

### **Parameters**

**lab\_basis**

[*Qobj*, Data] Initial state in the lab basis.

**t**

[float [0]] The time at which to evaluate the Floquet states.

### **Returns**

#### **output**

[*Qobj*, Data] The state in the Floquet basis. The return type is the same as the type of the input state.

**class Propagator**( $system$ , \*,  $c\_ops=()$ ,  $args=None$ ,  $options=None$ ,  $memoize=10$ ,  $tol=1e-14$ )

A generator of propagator for a system.

Usage:

```
U = Propagator(H, c_ops)
```

```
psi_t = U(t) @ psi_0
```

Save some previously computed propagator are stored to speed up subsequent computation. Changing args will erase these stored probagator.

### Parameters

#### system

[*Qobj*, *QobjEvo*, Solver] Possibly time-dependent system driving the evolution, either already packaged in a solver, such as *SESolver* or *BRSolver*, or the Liouvillian or Hamiltonian as a *Qobj*, *QobjEvo*. list of [*Qobj*, Coefficient] or callable that can be made into *QobjEvo* are also accepted.

Solvers that run non-deterministacilly, such as *MCSolver*, are not supported.

#### c\_ops

[list, optional] List of *Qobj* or *QobjEvo* collapse operators.

#### args

[dictionary, optional] Parameters to callback functions for time-dependent Hamiltonians and collapse operators.

#### options

[dict, optional] Options for the solver.

#### memoize

[int, default: 10] Max number of propagator to save.

#### tol

[float, default: 1e-14] Absolute tolerance for the time. If a previous propagator was computed at a time within tolerance, that propagator will be returned.

## Notes

The *Propagator* is not a *QobjEvo* so it cannot be used for operations with *Qobj* or *QobjEvo*. It can be made into a *QobjEvo* with

```
U = QobjEvo(Propagator(H))
```

```
__call__(t, t_start=0, **args)
```

Get the propagator from t\_start to t.

### Parameters

#### t

[float] Time at which to compute the propagator.

**t\_start: float [0]**

**Time at which the propagator start such that:**

```
psi[t] = U.prop(t, t_start) @ psi[t_start]
```

#### args

[dict] Argument to pass to a time dependent Hamiltonian. Updating args take effect since t=0 and the new args will be used in future call.

```
inv(t, **args)
```

**Get the inverse of the propagator at t, such that**

```
psi_0 = U.inv(t) @ psi_t
```

### Parameters



**t**  
[float] Time at which to compute the propagator.

**args**  
[dict] Argument to pass to a time dependent Hamiltonian. Updating args take effect since  $t=0$  and the new args will be used in future call.

### 5.1.6 Monte Carlo Solvers

**class MCSolver**(*H, c\_ops, \*, options=None*)

Bases: MultiTrajSolver

Monte Carlo Solver of a state vector  $|\psi\rangle$  for a given Hamiltonian and sets of collapse operators. Options for the underlying ODE solver are given by the Options class.

#### Parameters

**H**  
[Qobj, QobjEvo, list, callable.] System Hamiltonian as a Qobj, QobjEvo. It can also be any input type that QobjEvo accepts (see [QobjEvo's](#) documentation). H can also be a superoperator (liouvillian) if some collapse operators are to be treated deterministically.

**c\_ops**  
[list] A list of collapse operators in any input type that QobjEvo accepts (see [QobjEvo's](#) documentation). They must be operators even if H is a superoperator.

**options**  
[dict, [optional]] Options for the evolution.

**classmethod CollapseFeedback**(*default=None*)

Collapse of the trajectory argument for time dependent systems.

When used as an args:

```
QobjEvo([op, func], args={"cols": MCSolver.CollapseFeedback()})
```

The func will receive a list of (time, operator number) for each collapses of the trajectory as cols.

---

**Note:** CollapseFeedback can't be added to a running solver when updating arguments between steps: `solver.step(..., args={})`.

---

#### Parameters

**default**  
[callable, default][[]] Default function used outside the solver.

**classmethod ExpectFeedback**(*operator, default=0.0*)

Expectation value of the instantaneous state of the evolution to be used by a time-dependent operator.

When used as an args:

```
QobjEvo([op, func], args={"E0": Solver.ExpectFeedback(oper)})
```

The func will receive `expect(oper, state)` as E0 during the evolution.

#### Parameters

**operator**  
[Qobj, QobjEvo] Operator to compute the expectation values of.

**default**  
[float, default][0.] Initial value to be used at setup.

**classmethod** `StateFeedback`(*default=None, raw\_data=False, open=False*)

State of the evolution to be used in a time-dependent operator.

When used as an args:

```
QobjEvo([op, func], args={"state": MCSolver.StateFeedback()})
```

The func will receive the density matrix as `state` during the evolution.

#### Parameters

##### **default**

[Qobj or `qutip.core.data.Data`, default][None] Initial value to be used at setup of the system.

##### **open**

[bool, default False] Set to True when using the monte carlo solver for open systems.

##### **raw\_data**

[bool, default][False] If True, the raw matrix will be passed instead of a Qobj. For density matrices, the matrices can be column stacked or square depending on the integration method.

#### property options

Options for monte carlo solver:

**store\_final\_state: bool, default: False**

Whether or not to store the final state of the evolution in the result class.

**store\_states: bool, default: None**

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

**progress\_bar: str {'text', 'enhanced', 'tqdm', ''}, default: "text"**

How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.

**progress\_kwargs: dict, default: {"chunk\_size":10}**

Arguments to pass to the progress\_bar. Qutip's bars use `chunk_size`.

**keep\_runs\_results: bool, default: False**

Whether to store results from all trajectories or just store the averages.

**method: str, default: "adams"**

Which differential equation integration method to use.

**map: str {"serial", "parallel", "loky", "mpi"}, default: "serial"**

How to run the trajectories. "parallel" uses the multiprocessing module to run in parallel while "loky" and "mpi" use the "loky" and "mpi4py" modules to do so.

**mpi\_options: dict, default: {}**

Only applies if map is "mpi". This dictionary will be passed as keyword arguments to the `mpi4py.futures.MPIPoolExecutor` constructor. Note that the `max_workers` argument is provided separately through the `num_cpus` option.

**num\_cpus: None, int**

Number of cpus to use when running in parallel. None detect the number of available cpus.

**bitgenerator: {None, "MT19937", "PCG64", "PCG64DXSM", ...}**

Which of numpy.random's bitgenerator to use. With None, your numpy version's default is used.

**mc\_corr\_eps: float, default: 1e-10**

Small number used to detect non-physical collapse caused by numerical imprecision.

**norm\_t\_tol: float, default: 1e-6**

Tolerance in time used when finding the collapse.

**norm\_tol: float, default: 1e-4**

Tolerance in norm used when finding the collapse.

**norm\_steps: int, default: 5**

Maximum number of tries to find the collapse.

**improved\_sampling: Bool, default: False**

Whether to use the improved sampling algorithm of Abdelhafez et al. PRA (2019)

**run**(state, tlist, ntraj=1, \*, args=None, e\_ops=(), timeout=None, target\_tol=None, seeds=None)

Do the evolution of the Quantum system.

For a state at time `tlist[0]` do the evolution as directed by `rhs` and for each time in `tlist` store the state and/or expectation values in a [Result](#). The evolution method and stored results are determined by options.

#### Parameters

**state**

[[Qobj](#)] Initial state of the evolution.

**tlist**

[list of double] Time for which to save the results (state and/or expect) of the evolution. The first element of the list is the initial time of the evolution. Time in the list must be in increasing order, but does not need to be uniformly distributed.

**ntraj**

[int] Number of trajectories to add.

**args**

[dict, optional] Change the args of the rhs for the evolution.

**e\_ops**

[list] list of [Qobj](#) or [QobjEvo](#) to compute the expectation values. Alternatively, function[s] with the signature `f(t, state) -> expect` can be used.

**timeout**

[float, optional] Maximum time in seconds for the trajectories to run. Once this time is reached, the simulation will end even if the number of trajectories is less than `ntraj`. The map function, set in options, can interrupt the running trajectory or wait for it to finish. Set to an arbitrary high number to disable.

**target\_tol**

[{float, tuple, list}, optional] Target tolerance of the evolution. The evolution will compute trajectories until the error on the expectation values is lower than this tolerance. The maximum number of trajectories employed is given by `ntraj`. The error is computed using jackknife resampling. `target_tol` can be an absolute tolerance or a pair of absolute and relative tolerance, in that order. Lastly, it can be a list of pairs of (atol, rtol) for each `e_ops`.

**seeds**

[{int, [SeedSequence](#), list}, optional] Seed or list of seeds for each trajectories.

#### Returns

**results**

[[MultiTrajResult](#)] Results of the evolution. States and/or expect will be saved. You can control the saved data in the options.

**start**(state, t0, seed=None)

Set the initial state and time for a step evolution.

#### Parameters

**state**

[[Qobj](#)] Initial state of the evolution.

**t0**

[double] Initial time of the evolution.

**seed**

[int, SeedSequence, list, optional] Seed for the random number generator. It can be a single seed used to spawn seeds for each trajectory or a list of seed, one for each trajectory.

## Notes

When using step evolution, only one trajectory can be computed at once.

**step**(*t*, \*, *args*=None, *copy*=True)

Evolve the state to *t* and return the state as a [Qobj](#).

## Parameters

**t**

[double] Time to evolve to, must be higher than the last call.

**args**

[dict, optional] Update the args of the system. The change is effective from the beginning of the interval. Changing args can slow the evolution.

**copy**

[bool, default: True] Whether to return a copy of the data or the data in the ODE solver.

**property sys\_dims**

Dimensions of the space that the system use:

`qutip.basis(sovler.dims)` will create a state with proper dimensions for this solver.

**class NonMarkovianMCSolver**(*H*, *ops\_and\_rates*, *args*=None, *options*=None)

Bases: [MCSolver](#)

Monte Carlo Solver for Lindblad equations with “rates” that may be negative. The `c_ops` parameter of [MCSolver](#) is replaced by an `ops_and_rates` parameter to allow for negative rates. Options for the underlying ODE solver are given by the Options class.

## Parameters

**H**

[[Qobj](#), [QobjEvo](#), list, callable.] System Hamiltonian as a [Qobj](#), [QobjEvo](#). It can also be any input type that [QobjEvo](#) accepts (see [QobjEvo](#) documentation). *H* can also be a superoperator (liouvillian) if some collapse operators are to be treated deterministically.

**ops\_and\_rates**

[list] A list of tuples (*L*, *Gamma*), where the Lindblad operator *L* is a [Qobj](#) and *Gamma* represents the corresponding rate, which is allowed to be negative. The Lindblad operators must be operators even if *H* is a superoperator. Each rate *Gamma* may be just a number (in the case of a constant rate) or, otherwise, specified using any format accepted by `qutip.coefficient`.

**args**

[None / dict] Arguments for time-dependent Hamiltonian and collapse operator terms.

**options**

[SolverOptions, [optional]] Options for the evolution.

**classmethod CollapseFeedback**(*default*=None)

Collapse of the trajectory argument for time dependent systems.

When used as an args:

```
QobjEvo([op, func], args={"cols": MCSolver.CollapseFeedback()})
```

The func will receive a list of (time, operator number) for each collapses of the trajectory as cols.

---

**Note:** CollapseFeedback can't be added to a running solver when updating arguments between steps: solver.step(..., args={}).

---

### Parameters

#### default

[callable, default][[]] Default function used outside the solver.

**classmethod ExpectFeedback**(operator, default=0.0)

Expectation value of the instantaneous state of the evolution to be used by a time-dependent operator.

When used as an args:

QobjEvo([op, func], args={"E0": Solver.ExpectFeedback(oper)})

The func will receive expect(oper, state) as E0 during the evolution.

### Parameters

#### operator

[Qobj, QobjEvo] Operator to compute the expectation values of.

#### default

[float, default][0.] Initial value to be used at setup.

**classmethod StateFeedback**(default=None, raw\_data=False, open=False)

State of the evolution to be used in a time-dependent operator.

When used as an args:

QobjEvo([op, func], args={"state": MCSolver.StateFeedback()})

The func will receive the density matrix as state during the evolution.

### Parameters

#### default

[Qobj or qutip.core.data.Data, default][None] Initial value to be used at setup of the system.

#### open

[bool, default False] Set to True when using the monte carlo solver for open systems.

#### raw\_data

[bool, default][False] If True, the raw matrix will be passed instead of a Qobj. For density matrices, the matrices can be column stacked or square depending on the integration method.

**current\_martingale**()

Returns the value of the influence martingale along the current trajectory. The value of the martingale is the product of the continuous and the discrete contribution. The current time and the collapses that have happened are read out from the internal integrator.

### property options

Options for non-Markovian Monte Carlo solver:

**store\_final\_state: bool, default: False**

Whether or not to store the final state of the evolution in the result class.

**store\_states: bool, default: None**

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

**progress\_bar:** str {'text', 'enhanced', 'tqdm', ''}, default: "text"

How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.

**progress\_kwargs:** dict, default: {"chunk\_size":10}

Arguments to pass to the progress\_bar. Qutip's bars use chunk\_size.

**keep\_runs\_results:** bool, default: False

Whether to store results from all trajectories or just store the averages.

**method:** str, default: "adams"

Which differential equation integration method to use.

**map:** str {"serial", "parallel", "loky", "mpi"}, default: "serial"

How to run the trajectories. "parallel" uses the multiprocessing module to run in parallel while "loky" and "mpi" use the "loky" and "mpi4py" modules to do so.

**mpi\_options:** dict, default: {}

Only applies if map is "mpi". This dictionary will be passed as keyword arguments to the *mpi4py.futures.MPIPoolExecutor* constructor. Note that the *max\_workers* argument is provided separately through the *num\_cpus* option.

**num\_cpus:** None, int

Number of cpus to use when running in parallel. None detect the number of available cpus.

**bitgenerator:** {None, "MT19937", "PCG64", "PCG64DXSM", ...}

Which of numpy.random's bitgenerator to use. With None, your numpy version's default is used.

**mc\_corr\_eps:** float, default: 1e-10

Small number used to detect non-physical collapse caused by numerical imprecision.

**norm\_t\_tol:** float, default: 1e-6

Tolerance in time used when finding the collapse.

**norm\_tol:** float, default: 1e-4

Tolerance in norm used when finding the collapse.

**norm\_steps:** int, default: 5

Maximum number of tries to find the collapse.

**completeness\_rtol:** float, default: 1e-5

Used in determining whether the given Lindblad operators satisfy a certain completeness relation. If they do not, an additional Lindblad operator is added automatically (with zero rate).

**completeness\_atol:** float, default: 1e-8

Used in determining whether the given Lindblad operators satisfy a certain completeness relation. If they do not, an additional Lindblad operator is added automatically (with zero rate).

**martingale\_quad\_limit:** float or int, default: 100

An upper bound on the number of subintervals used in the adaptive integration of the martingale.

Note that the 'improved\_sampling' option is not currently supported.

**rate**(*t*, *i*)

Return the *i*'th unshifted rate at time *t*.

#### Parameters

**t**

[float] The time at which to calculate the rate.

**i**

[int] Which rate to calculate.

#### Returns

**rate**

[float] The value of rate *i* at time *t*.

### **rate\_shift(*t*)**

Return the rate shift at time *t*.

The rate shift is  $2 * \text{abs}(\min([0, \text{rate\_1}(t), \text{rate\_2}(t), \dots]))$ .

#### **Parameters**

**t**

[float] The time at which to calculate the rate shift.

#### **Returns**

**rate\_shift**

[float] The rate shift amount.

### **run(*state, tlist, ntraj=1, \*, args=None, \*\*kwargs*)**

Do the evolution of the Quantum system.

For a *state* at time *tlist*[0] do the evolution as directed by *rhs* and for each time in *tlist* store the state and/or expectation values in a *Result*. The evolution method and stored results are determined by options.

#### **Parameters**

**state**

[*Qobj*] Initial state of the evolution.

**tlist**

[list of double] Time for which to save the results (state and/or expect) of the evolution. The first element of the list is the initial time of the evolution. Time in the list must be in increasing order, but does not need to be uniformly distributed.

**ntraj**

[int] Number of trajectories to add.

**args**

[dict, optional] Change the args of the rhs for the evolution.

**e\_ops**

[list] list of *Qobj* or *QobjEvo* to compute the expectation values. Alternatively, function[s] with the signature *f(t, state) -> expect* can be used.

**timeout**

[float, optional] Maximum time in seconds for the trajectories to run. Once this time is reached, the simulation will end even if the number of trajectories is less than *ntraj*. The map function, set in options, can interrupt the running trajectory or wait for it to finish. Set to an arbitrary high number to disable.

**target\_tol**

[{float, tuple, list}, optional] Target tolerance of the evolution. The evolution will compute trajectories until the error on the expectation values is lower than this tolerance. The maximum number of trajectories employed is given by *ntraj*. The error is computed using jackknife resampling. *target\_tol* can be an absolute tolerance or a pair of absolute and relative tolerance, in that order. Lastly, it can be a list of pairs of (atol, rtol) for each *e\_ops*.

**seeds**

[{int, SeedSequence, list}, optional] Seed or list of seeds for each trajectories.

#### **Returns**

**results**

[*MultiTrajResult*] Results of the evolution. States and/or expect will be saved. You can control the saved data in the options.

### **sqrt\_shifted\_rate(*t*, *i*)**

Return the square root of the *i*'th shifted rate at time *t*.

#### **Parameters**

**t**

[float] The time at which to calculate the shifted rate.

**i**

[int] Which shifted rate to calculate.

#### **Returns**

**rate**

[float] The square root of the shifted value of rate *i* at time *t*.

### **start(*state*, *t0*, *seed*=None)**

Set the initial state and time for a step evolution.

#### **Parameters**

**state**

[*Qobj*] Initial state of the evolution.

**t0**

[double] Initial time of the evolution.

**seed**

[int, SeedSequence, list, optional] Seed for the random number generator. It can be a single seed used to spawn seeds for each trajectory or a list of seed, one for each trajectory.

## **Notes**

When using step evolution, only one trajectory can be computed at once.

### **step(*t*, \*, *args*=None, *copy*=True)**

Evolve the state to *t* and return the state as a *Qobj*.

#### **Parameters**

**t**

[double] Time to evolve to, must be higher than the last call.

**args**

[dict, optional] Update the args of the system. The change is effective from the beginning of the interval. Changing args can slow the evolution.

**copy**

[bool, default: True] Whether to return a copy of the data or the data in the ODE solver.

### **property sys\_dims**

Dimensions of the space that the system use:

`utip.basis(solver.dims)` will create a state with proper dimensions for this solver.



### 5.1.7 Non-Markovian HEOM Solver

**class** `HEOMSolver`(*H, bath, max\_depth, \*, options=None*)

HEOM solver that supports multiple baths.

The baths must be all either bosonic or fermionic baths.

#### Parameters

##### **H**

[*Qobj*, *QobjEvo*] Possibly time-dependent system Liouvillian or Hamiltonian as a *Qobj* or *QobjEvo*. list of [*Qobj*, *Coefficient*] or callable that can be made into *QobjEvo* are also accepted.

##### **bath**

[Bath or list of Bath] A *Bath* containing the exponents of the expansion of the bath correlation function and their associated coefficients and coupling operators, or a list of baths.

If multiple baths are given, they must all be either fermionic or bosonic baths.

##### **max\_depth**

[int] The maximum depth of the hierarchy (i.e. the maximum number of bath exponent “excitations” to retain).

##### **options**

[dict, optional] Generic solver options. If set to *None* the default options will be used. Keyword only. Default: *None*.

#### Attributes

##### **ados**

[*HierarchyADOs*] The description of the hierarchy constructed from the given bath and maximum depth.

##### **rhs**

[*QobjEvo*] The right-hand side (RHS) of the hierarchy evolution ODE. Internally the system and bath coupling operators are converted to `qutip.data.CSR` instances during construction of the RHS, so the operators in the `rhs` will all be sparse.

#### property options

Options for `HEOMSolver`:

**store\_final\_state: bool, default: False**

Whether or not to store the final state of the evolution in the result class.

**store\_states: bool, default: None**

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

**normalize\_output: bool, default: False**

Normalize output state to hide ODE numerical errors.

**progress\_bar: str {'text', 'enhanced', 'tqdm', ''}, default: “text”**

How to present the solver progress. ‘tqdm’ uses the python module of the same name and raise an error if not installed. Empty string or *False* will disable the bar.

**progress\_kwargs: dict, default: {"chunk\_size": 10}**

Arguments to pass to the `progress_bar`. Qutip’s bars use `chunk_size`.

**method: str, default: “adams”**

Which ordinary differential equation integration method to use.

**state\_data\_type: str, default: “dense”**

Name of the data type of the state used during the ODE evolution. Use an empty string to keep the input state type. Many integrators support only work with *Dense*.

### store\_ados

[bool, default: False] Whether or not to store the HEOM ADOs. Only relevant when using the HEOM solver.

**run**(state0, tlist, \*, args=None, e\_ops=None)

Solve for the time evolution of the system.

### Parameters

#### state0

[Qobj or *HierarchyADOsState* or array-like] If rho0 is a Qobj the it is the initial state of the system (i.e. a Qobj density matrix).

If it is a *HierarchyADOsState* or array-like, then rho0 gives the initial state of all ADOs.

Usually the state of the ADOs would be determine from a previous call to .run(..) with the solver results option store\_ados set to True. For example, result = solver.run(...) could be followed by solver.run(result.ado\_states[-1], tlist).

If a numpy array-like is passed its shape must be (number\_of\_ados, n, n) where (n, n) is the system shape (i.e. shape of the system density matrix) and the ADOs must be in the same order as in .ados.labels.

#### tlist

[list] An ordered list of times at which to return the value of the state.

#### args

[dict, optional {None}] Change the args of the RHS for the evolution.

#### e\_ops

[Qobj / QobjEvo / callable / list / dict / None, optional] A list or dictionary of operators as Qobj, QobjEvo and/or callable functions (they can be mixed) or a single operator or callable function. For an operator op, the result will be computed using (state \* op).tr() and the state at each time t. For callable functions, f, the result is computed using f(t, ado\_state). The values are stored in the expect and e\_data attributes of the result (see the return section below).

### Returns

#### HEOMResult

The results of the simulation run, with the following important attributes:

- times: the times t (i.e. the tlist).
- states: the system state at each time t (only available if e\_ops was None or if the solver option store\_states was set to True).
- ado\_states: the full ADO state at each time (only available if the results option ado\_return was set to True). Each element is an instance of *HierarchyADOsState*. The state of a particular ADO may be extracted from result.ado\_states[i] by calling extract.
- expect: a list containing the values of each e\_ops at time t.
- e\_data: a dictionary containing the values of each e\_ops at time t. The keys are those given by e\_ops if it was a dict, otherwise they are the indexes of the supplied e\_ops.

See *HEOMResult* and *Result* for the complete list of attributes.

**start**(state0, t0)

Set the initial state and time for a step evolution.

### Parameters

**state0**

[*Qobj*] Initial state of the evolution. This may provide either just the initial density matrix of the system, or the full set of ADOs for the hierarchy. See the documentation for `rho0` in the `.run(...)` method for details.

**t0**

[double] Initial time of the evolution.

**steady\_state**(*use\_mkl=True, mkl\_max\_iter\_refine=100, mkl\_weighted\_matching=False*)

Compute the steady state of the system.

#### Parameters

**use\_mkl**

[bool, default=False] Whether to use mkl or not. If mkl is not installed or if this is false, use the scipy splu solver instead.

**mkl\_max\_iter\_refine**

[int] Specifies the the maximum number of iterative refinement steps that the MKL PARDISO solver performs.

For a complete description, see `iparm(7)` in <https://www.intel.com/content/www/us/en/docs/onemkl/developer-reference-c/2023-0/pardiso-iparm-parameter.html>

**mkl\_weighted\_matching**

[bool] MKL PARDISO can use a maximum weighted matching algorithm to permute large elements close the diagonal. This strategy adds an additional level of reliability to the factorization methods.

For a complete description, see `iparm(12)` in <https://www.intel.com/content/www/us/en/docs/onemkl/developer-reference-c/2023-0/pardiso-iparm-parameter.html>

#### Returns

**steady\_state**

[*Qobj*] The steady state density matrix of the system.

**steady\_ados**

[*HierarchyADOsState*] The steady state of the full ADO hierarchy. A particular ADO may be extracted from the full state by calling `extract`.

**property sys\_dims**

Dimensions of the space that the system use, excluding any environment:

`qutip.basis(sovler.dims)` will create a state with proper dimensions for this solver.

**class HSolverDL**(*H\_sys, coup\_op, coup\_strength, temperature, N\_cut, N\_exp, cut\_freq, \*, bnd\_cut\_approx=False, options=None, combine=True*)

A helper class for creating an *HEOMSolver* that is backwards compatible with the *HSolverDL* provided in `qutip.nonmarkov.heom` in QuTiP 4.6 and below.

See *HEOMSolver* and *DrudeLorentzBath* for more descriptions of the underlying solver and bath construction.

An exact copy of the QuTiP 4.6 *HSolverDL* is provided in `qutip.nonmarkov.dlheom_solver` for cases where the functionality of the older solver is required. The older solver will be completely removed in QuTiP 5.

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**Note:** Unlike the version of *HSolverDL* in QuTiP 4.6, this solver supports supplying a time-dependent or Liouvillian *H\_sys*.

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**Note:** For compatibility with *HSolverDL* in QuTiP 4.6 and below, the parameter *N\_exp* specifying the number of exponents to keep in the expansion of the bath correlation function is one more than the equivalent

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$N_k$  used in the [DrudeLorentzBath](#). I.e.,  $N_k = N_{\text{exp}} - 1$ . The  $N_k$  parameter in the [DrudeLorentzBath](#) does not count the zeroeth exponent in order to better match common usage in the literature.

---

**Note:** The `stats` and `renorm` arguments accepted in QuTiP 4.6 and below are no longer supported.

---

## Parameters

### **H\_sys**

[Qobj or QobjEvo or list] The system Hamiltonian or Liouvillian. See [HEOMSolver](#) for a complete description.

### **coup\_op**

[Qobj] Operator describing the coupling between system and bath. See parameter `Q` in [BosonicBath](#) for a complete description.

### **coup\_strength**

[float] Coupling strength. Referred to as  $\lambda$  in [DrudeLorentzBath](#).

### **temperature**

[float] Bath temperature. Referred to as  $T$  in [DrudeLorentzBath](#).

### **N\_cut**

[int] The maximum depth of the hierarchy. See `max_depth` in [HEOMSolver](#) for a full description.

### **N\_exp**

[int] Number of exponential terms used to approximate the bath correlation functions. The equivalent  $N_k$  in [DrudeLorentzBath](#) is one less than  $N_{\text{exp}}$  (see note above).

### **cut\_freq**

[float] Bath spectral density cutoff frequency. Referred to as  $\gamma$  in [DrudeLorentzBath](#).

### **bnd\_cut\_approx**

[bool] Use boundary cut off approximation. If true, the Matsubara terminator is added to the system Liouvillian (and `H_sys` is promoted to a Liouvillian if it was a Hamiltonian). Keyword only. Default: False.

### **options**

[dict, optional] Generic solver options. If set to None the default options will be used. Keyword only. Default: None.

### **combine**

[bool, default: True] Whether to combine exponents with the same frequency (and coupling operator). See [BosonicBath.combine](#) for details. Keyword only. Default: True.

**class BathExponent**(*type, dim, Q, ck, vk, ck2=None, sigma\_bar\_k\_offset=None, tag=None*)

Represents a single exponent (naively, an excitation mode) within the decomposition of the correlation functions of a bath.

## Parameters

### **type**

[{"R", "I", "RI", "+", "-"} or BathExponent.ExponentType] The type of bath exponent.

"R" and "I" are bosonic bath exponents that appear in the real and imaginary parts of the correlation expansion.

"RI" is combined bosonic bath exponent that appears in both the real and imaginary parts of the correlation expansion. The combined exponent has a single  $v_k$ . The  $ck$  is the coefficient in the real expansion and  $ck2$  is the coefficient in the imaginary expansion.

“+” and “-” are fermionic bath exponents. These fermionic bath exponents must specify `sigma_bar_k_offset` which specifies the amount to add to `k` (the exponent index within the bath of this exponent) to determine the `k` of the corresponding exponent with the opposite sign (i.e. “-” or “+”).

**dim**

[int or None] The dimension (i.e. maximum number of excitations for this exponent). Usually 2 for fermionic exponents or None (i.e. unlimited) for bosonic exponents.

**Q**

[Qobj] The coupling operator for this excitation mode.

**vk**

[complex] The frequency of the exponent of the excitation term.

**ck**

[complex] The coefficient of the excitation term.

**ck2**

[optional, complex] For exponents of type “RI” this is the coefficient of the term in the imaginary expansion (and `ck` is the coefficient in the real expansion).

**sigma\_bar\_k\_offset**

[optional, int] For exponents of type “+” this gives the offset (within the list of exponents within the bath) of the corresponding “-” bath exponent. For exponents of type “-” it gives the offset of the corresponding “+” exponent.

**tag**

[optional, str, tuple or any other object] A label for the exponent (often the name of the bath). It defaults to None.

**Attributes**

**fermionic**

[bool] True if the type of the exponent is a Fermionic type (i.e. either “+” or “-”) and False otherwise.

**All of the parameters are also available as attributes.**

**types**

alias of `ExponentType`

**class Bath**(*exponents*)

Represents a list of bath expansion exponents.

**Parameters**

**exponents**

[list of `BathExponent`] The exponents of the correlation function describing the bath.

**Attributes**

**All of the parameters are available as attributes.**

**class BosonicBath**(*Q, ck\_real, vk\_real, ck\_imag, vk\_imag, combine=True, tag=None*)

A helper class for constructing a bosonic bath from the expansion coefficients and frequencies for the real and imaginary parts of the bath correlation function.

If the correlation functions  $C(t)$  is split into real and imaginary parts:

$$C(t) = C_{\text{real}}(t) + i * C_{\text{imag}}(t)$$

then:

$$\begin{aligned} C_{\text{real}}(t) &= \text{sum}(ck_{\text{real}} * \exp(- vk_{\text{real}} * t)) \\ C_{\text{imag}}(t) &= \text{sum}(ck_{\text{imag}} * \exp(- vk_{\text{imag}} * t)) \end{aligned}$$

Defines the coefficients  $ck$  and the frequencies  $vk$ .

Note that the  $ck$  and  $vk$  may be complex, even through  $C\_real(t)$  and  $C\_imag(t)$  (i.e. the sum) is real.

#### Parameters

**Q**

[Qobj] The coupling operator for the bath.

**ck\_real**

[list of complex] The coefficients of the expansion terms for the real part of the correlation function. The corresponding frequencies are passed as  $vk\_real$ .

**vk\_real**

[list of complex] The frequencies (exponents) of the expansion terms for the real part of the correlation function. The corresponding coefficients are passed as  $ck\_real$ .

**ck\_imag**

[list of complex] The coefficients of the expansion terms in the imaginary part of the correlation function. The corresponding frequencies are passed as  $vk\_imag$ .

**vk\_imag**

[list of complex] The frequencies (exponents) of the expansion terms for the imaginary part of the correlation function. The corresponding coefficients are passed as  $ck\_imag$ .

**combine**

[bool, default True] Whether to combine exponents with the same frequency (and coupling operator). See [combine](#) for details.

**tag**

[optional, str, tuple or any other object] A label for the bath exponents (for example, the name of the bath). It defaults to None but can be set to help identify which bath an exponent is from.

**classmethod combine**(*exponents*, *rtol*=1e-05, *atol*=1e-07)

Group bosonic exponents with the same frequency and return a single exponent for each frequency present.

Exponents with the same frequency are only combined if they share the same coupling operator  $.Q$ .

Note that combined exponents take their tag from the first exponent in the group being combined (i.e. the one that occurs first in the given exponents list).

#### Parameters

**exponents**

[list of BathExponent] The list of exponents to combine.

**rtol**

[float, default 1e-5] The relative tolerance to use to when comparing frequencies and coupling operators.

**atol**

[float, default 1e-7] The absolute tolerance to use to when comparing frequencies and coupling operators.

#### Returns

**list of BathExponent**

The new reduced list of exponents.

**class DrudeLorentzBath**(*Q*, *lam*, *gamma*, *T*, *Nk*, *combine*=True, *tag*=None)

A helper class for constructing a Drude-Lorentz bosonic bath from the bath parameters (see parameters below).

#### Parameters

**Q**

[Qobj] Operator describing the coupling between system and bath.

**lam**

[float] Coupling strength.

**gamma**

[float] Bath spectral density cutoff frequency.

**T**

[float] Bath temperature.

**Nk**

[int] Number of exponential terms used to approximate the bath correlation functions.

**combine**

[bool, default True] Whether to combine exponents with the same frequency (and coupling operator). See *BosonicBath.combine* for details.

**tag**

[optional, str, tuple or any other object] A label for the bath exponents (for example, the name of the bath). It defaults to None but can be set to help identify which bath an exponent is from.

**terminator()**

Return the Matsubara terminator for the bath and the calculated approximation discrepancy.

**Returns**

**delta: float**

The approximation discrepancy. That is, the difference between the true correlation function of the Drude-Lorentz bath and the sum of the *Nk* exponential terms is approximately  $2 * \text{delta} * \text{dirac}(t)$ , where  $\text{dirac}(t)$  denotes the Dirac delta function.

**terminator**

[Qobj] The Matsubara terminator – i.e. a liouvillian term representing the contribution to the system-bath dynamics of all exponential expansion terms beyond *Nk*. It should be used by adding it to the system liouvillian (i.e. `liouvillian(H_sys)`).

**class DrudeLorentzPadeBath(Q, lam, gamma, T, Nk, combine=True, tag=None)**

A helper class for constructing a Padé expansion for a Drude-Lorentz bosonic bath from the bath parameters (see parameters below).

A Padé approximant is a sum-over-poles expansion ( see [https://en.wikipedia.org/wiki/Pad%C3%A9\\_approximant](https://en.wikipedia.org/wiki/Pad%C3%A9_approximant)).

The application of the Padé method to spectrum decompositions is described in “Padé spectrum decompositions of quantum distribution functions and optimal hierarchical equations of motion construction for quantum open systems” [1].

The implementation here follows the approach in the paper.

[1] J. Chem. Phys. 134, 244106 (2011); <https://doi.org/10.1063/1.3602466>

This is an alternative to the *DrudeLorentzBath* which constructs a simpler exponential expansion.

**Parameters**

**Q**

[Qobj] Operator describing the coupling between system and bath.

**lam**

[float] Coupling strength.

**gamma**

[float] Bath spectral density cutoff frequency.

**T**

[float] Bath temperature.

**Nk**

[int] Number of Padé exponentials terms used to approximate the bath correlation functions.

**combine**

[bool, default True] Whether to combine exponents with the same frequency (and coupling operator). See [BosonicBath.combine](#) for details.

**tag**

[optional, str, tuple or any other object] A label for the bath exponents (for example, the name of the bath). It defaults to None but can be set to help identify which bath an exponent is from.

**terminator()**

Return the Padé terminator for the bath and the calculated approximation discrepancy.

**Returns**

**delta: float**

The approximation discrepancy. That is, the difference between the true correlation function of the Drude-Lorentz bath and the sum of the  $N_k$  exponential terms is approximately  $2 * \text{delta} * \text{dirac}(t)$ , where  $\text{dirac}(t)$  denotes the Dirac delta function.

**terminator**

[Qobj] The Padé terminator – i.e. a liouvillian term representing the contribution to the system-bath dynamics of all exponential expansion terms beyond  $N_k$ . It should be used by adding it to the system liouvillian (i.e. `liouvillian(H_sys)`).

**class UnderDampedBath(*Q, lam, gamma, w0, T, Nk, combine=True, tag=None*)**

A helper class for constructing an under-damped bosonic bath from the bath parameters (see parameters below).

**Parameters**

**Q**

[Qobj] Operator describing the coupling between system and bath.

**lam**

[float] Coupling strength.

**gamma**

[float] Bath spectral density cutoff frequency.

**w0**

[float] Bath spectral density resonance frequency.

**T**

[float] Bath temperature.

**Nk**

[int] Number of exponential terms used to approximate the bath correlation functions.

**combine**

[bool, default True] Whether to combine exponents with the same frequency (and coupling operator). See [BosonicBath.combine](#) for details.

**tag**

[optional, str, tuple or any other object] A label for the bath exponents (for example, the name of the bath). It defaults to None but can be set to help identify which bath an exponent is from.



**class FermionicBath**(*Q, ck\_plus, vk\_plus, ck\_minus, vk\_minus, tag=None*)

A helper class for constructing a fermionic bath from the expansion coefficients and frequencies for the + and - modes of the bath correlation function.

There must be the same number of + and - modes and their coefficients must be specified in the same order so that `ck_plus[i]`, `vk_plus[i]` are the plus coefficient and frequency corresponding to the minus mode `ck_minus[i]`, `vk_minus[i]`.

In the fermionic case the order in which excitations are created or destroyed is important, resulting in two different correlation functions labelled `C_plus(t)` and `C_minus(t)`:

```
C_plus(t) = sum(ck_plus * exp(- vk_plus * t))
C_minus(t) = sum(ck_minus * exp(- vk_minus * t))
```

where the expansions above define the coefficients `ck` and the frequencies `vk`.

#### Parameters

**Q**

[Qobj] The coupling operator for the bath.

**ck\_plus**

[list of complex] The coefficients of the expansion terms for the + part of the correlation function. The corresponding frequencies are passed as `vk_plus`.

**vk\_plus**

[list of complex] The frequencies (exponents) of the expansion terms for the + part of the correlation function. The corresponding coefficients are passed as `ck_plus`.

**ck\_minus**

[list of complex] The coefficients of the expansion terms for the - part of the correlation function. The corresponding frequencies are passed as `vk_minus`.

**vk\_minus**

[list of complex] The frequencies (exponents) of the expansion terms for the - part of the correlation function. The corresponding coefficients are passed as `ck_minus`.

**tag**

[optional, str, tuple or any other object] A label for the bath exponents (for example, the name of the bath). It defaults to `None` but can be set to help identify which bath an exponent is from.

**class LorentzianBath**(*Q, gamma, w, mu, T, Nk, tag=None*)

A helper class for constructing a Lorentzian fermionic bath from the bath parameters (see parameters below).

**Note:** This Matsubara expansion used in this bath converges very slowly and `Nk > 20` may be required to get good convergence. The Padé expansion used by [LorentzianPadeBath](#) converges much more quickly.

#### Parameters

**Q**

[Qobj] Operator describing the coupling between system and bath.

**gamma**

[float] The coupling strength between the system and the bath.

**w**

[float] The width of the environment.

**mu**

[float] The chemical potential of the bath.

**T**

[float] Bath temperature.

**Nk**

[int] Number of exponential terms used to approximate the bath correlation functions.

**tag**

[optional, str, tuple or any other object] A label for the bath exponents (for example, the name of the bath). It defaults to None but can be set to help identify which bath an exponent is from.

**class LorentzianPadeBath**(*Q, gamma, w, mu, T, Nk, tag=None*)

A helper class for constructing a Padé expansion for Lorentzian fermionic bath from the bath parameters (see parameters below).

A Padé approximant is a sum-over-poles expansion ( see [https://en.wikipedia.org/wiki/Pad%C3%A9\\_approximant](https://en.wikipedia.org/wiki/Pad%C3%A9_approximant)).

The application of the Padé method to spectrum decompositions is described in “Padé spectrum decompositions of quantum distribution functions and optimal hierarchical equations of motion construction for quantum open systems” [1].

The implementation here follows the approach in the paper.

[1] J. Chem. Phys. 134, 244106 (2011); <https://doi.org/10.1063/1.3602466>

This is an alternative to the *LorentzianBath* which constructs a simpler exponential expansion that converges much more slowly in this particular case.

#### Parameters

**Q**

[Qobj] Operator describing the coupling between system and bath.

**gamma**

[float] The coupling strength between the system and the bath.

**w**

[float] The width of the environment.

**mu**

[float] The chemical potential of the bath.

**T**

[float] Bath temperature.

**Nk**

[int] Number of exponential terms used to approximate the bath correlation functions.

**tag**

[optional, str, tuple or any other object] A label for the bath exponents (for example, the name of the bath). It defaults to None but can be set to help identify which bath an exponent is from.

**class HierarchyADOs**(*exponents, max\_depth*)

A description of ADOs (auxilliary density operators) with the hierarchical equations of motion.

The list of ADOs is constructed from a list of bath exponents (corresponding to one or more baths). Each ADO is referred to by a label that lists the number of “excitations” of each bath exponent. The level of a label within the hierarchy is the sum of the “excitations” within the label.

For example the label (0, 0, ..., 0) represents the density matrix of the system being solved and is the only 0th level label.

The labels with a single 1, i.e. (1, 0, ..., 0), (0, 1, 0, ..., 0), etc. are the 1st level labels.

The second level labels all have either two 1s or a single 2, and so on for the third and higher levels of the hierarchy.

#### Parameters

**exponents**

[list of BathExponent] The exponents of the correlation function describing the bath or baths.

**max\_depth**

[int] The maximum depth of the hierarchy (i.e. the maximum sum of “excitations” in the hierarchy ADO labels or maximum ADO level).

**Attributes**

**exponents**

[list of BathExponent] The exponents of the correlation function describing the bath or baths.

**max\_depth**

[int] The maximum depth of the hierarchy (i.e. the maximum sum of “excitations” in the hierarchy ADO labels).

**dims**

[list of int] The dimensions of each exponent within the bath(s).

**vk**

[list of complex] The frequency of each exponent within the bath(s).

**ck**

[list of complex] The coefficient of each exponent within the bath(s).

**ck2: list of complex**

For exponents of type “RI”, the coefficient of the exponent within the imaginary expansion. For other exponent types, the entry is None.

**sigma\_bar\_k\_offset: list of int**

For exponents of type “+” or “-” the offset within the list of modes of the corresponding “-” or “+” exponent. For other exponent types, the entry is None.

**labels: list of tuples**

A list of the ADO labels within the hierarchy.

**exps(*label*)**

Converts an ADO label into a tuple of exponents, with one exponent for each “excitation” within the label.

The number of exponents returned is always equal to the level of the label within the hierarchy (i.e. the sum of the indices within the label).

**Parameters**

**label**

[tuple] The ADO label to convert to a list of exponents.

**Returns**

**tuple of BathExponent**

A tuple of BathExponents.

## Examples

`ados.exps((1, 0, 0))` would return `[ados.exponents[0]]`

`ados.exps((2, 0, 0))` would return `[ados.exponents[0], ados.exponents[0]]`.

`ados.exps((1, 2, 1))` would return `[ados.exponents[0], ados.exponents[1], ados.exponents[1], ados.exponents[2]]`.

**filter**(*level=None, tags=None, dims=None, types=None*)

Return a list of ADO labels for ADOs whose “excitations” match the given patterns.

Each of the filter parameters (*tags*, *dims*, *types*) may be either unspecified (*None*) or a list. Unspecified parameters are excluded from the filtering.

All specified filter parameters must be lists of the same length. Each position in the lists describes a particular excitation and any exponent that matches the filters may supply that excitation. The level of all labels returned is thus equal to the length of the filter parameter lists.

Within a filter parameter list, items that are *None* represent wildcards and match any value of that exponent attribute

### Parameters

#### level

[int] The hierarchy depth to return ADOs from.

#### tags

[list of object or None] Filter parameter that matches the `.tag` attribute of exponents.

#### dims

[list of int] Filter parameter that matches the `.dim` attribute of exponents.

#### types

[list of BathExponent types or list of str] Filter parameter that matches the `.type` attribute of exponents. Types may be supplied by name (e.g. “R”, “I”, “+”) instead of by the actual type (e.g. `BathExponent.types.R`).

### Returns

#### list of tuple

The ADO label for each ADO whose exponent excitations (i.e. label) match the given filters or level.

**idx**(*label*)

Return the index of the ADO label within the list of labels, i.e. within `self.labels`.

### Parameters

#### label

[tuple] The label to look up.

### Returns

#### int

The index of the label within the list of ADO labels.

## Notes

This implementation of the `.idx(...)` method is just for reference and documentation. To avoid the cost of a Python function call, it is replaced with `self._label_idx.__getitem__` when the instance is created.

**next**(*label*, *k*)

Return the ADO label with one more excitation in the *k*'th exponent dimension or None if adding the excitation would exceed the dimension or maximum depth of the hierarchy.

### Parameters

**label**

[tuple] The ADO label to add an excitation to.

**k**

[int] The exponent to add the excitation to.

### Returns

**tuple or None**

The next label.

**prev**(*label*, *k*)

Return the ADO label with one fewer excitation in the *k*'th exponent dimension or None if the label has no excitations in the *k*'th exponent.

### Parameters

**label**

[tuple] The ADO label to remove the excitation from.

**k**

[int] The exponent to remove the excitation from.

### Returns

**tuple or None**

The previous label.

**class HierarchyADOsState**(*rho*, *ados*, *ado\_state*)

Provides convenient access to the full hierarchy ADO state at a particular point in time, *t*.

### Parameters

**rho**

[Qobj] The current state of the system (i.e. the 0th component of the hierarchy).

**ados**

[HierarchyADOs] The description of the hierarchy.

**ado\_state**

[numpy.array] The full state of the hierarchy.

### Attributes

**rho**

[Qobj] The system state.

In addition, all of the attributes of the hierarchy description, i.e. ```HierarchyADOs```, are provided directly on this class for convenience. E.g. one can access ```.labels```, or ```.exponents``` or call ```.idx(label)``` directly.

See `:class:`HierarchyADOs`` for a full list of the available attributes and methods.

**extract**(*idx\_or\_label*)

Extract a Qobj representing the specified ADO from a full representation of the ADO states.

**Parameters**

**idx**

[int or label] The index of the ADO to extract. If an ADO label, e.g. (0, 1, 0, ...) is supplied instead, then the ADO is extracted by label instead.

**Returns**

**Qobj**

A Qobj representing the state of the specified ADO.

**class HEOMResult**(*e\_ops, options: ResultOptions, \*, solver=None, stats=None, \*\*kw*)

## 5.1.8 Stochastic Solver

**class SMESolver**(*H, sc\_ops, heterodyne, \*, c\_ops=(), options=None*)

Stochastic Master Equation Solver.

**Parameters**

**H**

[Qobj, QobjEvo, QobjEvo compatible format.] System Hamiltonian as a Qobj or QobjEvo for time-dependent Hamiltonians. List of [Qobj, Coefficient] or callable that can be made into QobjEvo are also accepted.

**sc\_ops**

[list of (QobjEvo, QobjEvo compatible format)] List of stochastic collapse operators.

**heterodyne**

[bool, default: False] Whether to use heterodyne or homodyne detection.

**options**

[dict, optional] Options for the solver, see [SMESolver.options](#) and [SIntegrator](#) for a list of all options.

**classmethod ExpectFeedback**(*operator, default=0.0*)

Expectation value of the instantaneous state of the evolution to be used by a time-dependent operator.

When used as an args:

QobjEvo([op, func], args={"E0": Solver.ExpectFeedback(oper)})

The func will receive `expect(oper, state)` as E0 during the evolution.

**Parameters**

**operator**

[Qobj, QobjEvo] Operator to compute the expectation values of.

**default**

[float, default][0.] Initial value to be used at setup.

**classmethod StateFeedback**(*default=None, raw\_data=False*)

State of the evolution to be used in a time-dependent operator.

When used as an args:

QobjEvo([op, func], args={"state": SMESolver.StateFeedback()})

The func will receive the density matrix as `state` during the evolution.

---

**Note:** Not supported by the `rouchon` method.

---

## Parameters

### default

[Qobj or qutip.core.data.Data, default][None] Initial value to be used at setup of the system.

### raw\_data

[bool, default][False] If True, the raw matrix will be passed instead of a Qobj. For density matrices, the matrices can be column stacked or square depending on the integration method.

## classmethod WienerFeedback(default=None)

Wiener function of the trajectory argument for time dependent systems.

When used as an args:

```
QobjEvo([op, func], args={"W": SMESolver.WienerFeedback()})
```

The func will receive a function as W that return an array of wiener processes values at t. The wiener process for the i-th sc\_ops is the i-th element for homodyne detection and the (2i, 2i+1) pairs of process in heterodyne detection. The process is a step function with step of length options["dt"].

---

**Note:** WienerFeedback can't be added to a running solver when updating arguments between steps: solver.step(..., args={}).

---

## Parameters

### default

[callable, optional] Default function used outside the solver. When not passed, a function returning np.array([0]) is used.

## property options

Options for stochastic solver:

### store\_final\_state: bool, default: False

Whether or not to store the final state of the evolution in the result class.

### store\_states: None, bool, default: None

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

### store\_measurement: bool, default: False

Whether to store the measurement for each trajectories. Storing measurements will also store the wiener process, or brownian noise for each trajectories.

### progress\_bar: str {'text', 'enhanced', 'tqdm', ''}, default: "text"

How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.

### progress\_kwargs: dict, default: {"chunk\_size":10}

Arguments to pass to the progress\_bar. Qutip's bars use chunk\_size.

### keep\_runs\_results: bool, default: False

Whether to store results from all trajectories or just store the averages.

### normalize\_output: bool

Normalize output state to hide ODE numerical errors.

### method: str, default: "platen"

Which differential equation integration method to use.

### map: str {"serial", "parallel", "loky", "mpi"}, default: "serial"

How to run the trajectories. "parallel" uses the multiprocessing module to run in parallel while "loky" and "mpi" use the "loky" and "mpi4py" modules to do so.

**mpi\_options: dict, default: {}**

Only applies if map is “mpi”. This dictionary will be passed as keyword arguments to the *mpi4py.futures.MPIPoolExecutor* constructor. Note that the *max\_workers* argument is provided separately through the *num\_cpus* option.

**num\_cpus: None, int, default: None**

Number of cpus to use when running in parallel. None detect the number of available cpus.

**bitgenerator: {None, “MT19937”, “PCG64DXSM”, ...}, default: None**

Which of numpy.random’s bitgenerator to use. With None, your numpy version’s default is used.

**run**(state, tlist, ntraj=1, \*, args=None, e\_ops=(), timeout=None, target\_tol=None, seeds=None)

Do the evolution of the Quantum system.

For a state at time *tlist*[0] do the evolution as directed by *rhs* and for each time in *tlist* store the state and/or expectation values in a *Result*. The evolution method and stored results are determined by options.

**Parameters**

**state**

[*Qobj*] Initial state of the evolution.

**tlist**

[list of double] Time for which to save the results (state and/or expect) of the evolution. The first element of the list is the initial time of the evolution. Time in the list must be in increasing order, but does not need to be uniformly distributed.

**ntraj**

[int] Number of trajectories to add.

**args**

[dict, optional] Change the args of the rhs for the evolution.

**e\_ops**

[list] list of *Qobj* or *QobjEvo* to compute the expectation values. Alternatively, function[s] with the signature *f*(*t*, *state*) -> *expect* can be used.

**timeout**

[float, optional] Maximum time in seconds for the trajectories to run. Once this time is reached, the simulation will end even if the number of trajectories is less than *ntraj*. The map function, set in options, can interrupt the running trajectory or wait for it to finish. Set to an arbitrary high number to disable.

**target\_tol**

[{float, tuple, list}, optional] Target tolerance of the evolution. The evolution will compute trajectories until the error on the expectation values is lower than this tolerance. The maximum number of trajectories employed is given by *ntraj*. The error is computed using jackknife resampling. *target\_tol* can be an absolute tolerance or a pair of absolute and relative tolerance, in that order. Lastly, it can be a list of pairs of (*atol*, *rtol*) for each *e\_ops*.

**seeds**

[{int, SeedSequence, list}, optional] Seed or list of seeds for each trajectories.

**Returns**

**results**

[*MultiTrajResult*] Results of the evolution. States and/or expect will be saved. You can control the saved data in the options.

**start**(state, t0, seed=None)

Set the initial state and time for a step evolution.

**Parameters**



**state**

[[Qobj](#)] Initial state of the evolution.

**t0**

[double] Initial time of the evolution.

**seed**

[int, SeedSequence, list, optional] Seed for the random number generator. It can be a single seed used to spawn seeds for each trajectory or a list of seed, one for each trajectory.

## Notes

When using step evolution, only one trajectory can be computed at once.

**step**(*t*, \*, *args=None*, *copy=True*)

Evolve the state to *t* and return the state as a [Qobj](#).

### Parameters

**t**

[double] Time to evolve to, must be higher than the last call.

**args**

[dict, optional] Update the *args* of the system. The change is effective from the beginning of the interval. Changing *args* can slow the evolution.

**copy**

[bool, default: True] Whether to return a copy of the data or the data in the ODE solver.

### property sys\_dims

Dimensions of the space that the system use:

`qutip.basis(sovler.dims)` will create a state with proper dimensions for this solver.

**class SSERsolver**(*H*, *sc\_ops*, *heterodyne*, \*, *c\_ops=()*, *options=None*)

Stochastic Schrodinger Equation Solver.

### Parameters

**H**

[[Qobj](#), [QobjEvo](#), [QobjEvo](#) compatible format.] System Hamiltonian as a [Qobj](#) or [QobjEvo](#) for time-dependent Hamiltonians. List of [[Qobj](#), Coefficient] or callable that can be made into [QobjEvo](#) are also accepted.

**c\_ops**

[list of ([QobjEvo](#), [QobjEvo](#) compatible format)] Deterministic collapse operator which will contribute with a standard Lindblad type of dissipation.

**sc\_ops**

[list of ([QobjEvo](#), [QobjEvo](#) compatible format)] List of stochastic collapse operators.

**heterodyne**

[bool, default: False] Whether to use heterodyne or homodyne detection.

**options**

[dict, optional] Options for the solver, see [SSERsolver.options](#) and [SIntegrator](#) for a list of all options.

**classmethod ExpectFeedback**(*operator*, *default=0.0*)

Expectation value of the instantaneous state of the evolution to be used by a time-dependent operator.

When used as an *args*:

`QobjEvo([op, func], args={"E0": Solver.ExpectFeedback(oper)})`

The func will receive `expect(operator, state)` as `E0` during the evolution.

#### Parameters

##### operator

[Qobj, QobjEvo] Operator to compute the expectation values of.

##### default

[float, default][0.] Initial value to be used at setup.

**classmethod** `StateFeedback`(*default=None, raw\_data=False*)

State of the evolution to be used in a time-dependent operator.

When used as an args:

```
QobjEvo([op, func], args={"state": SMESolver.StateFeedback()})
```

The func will receive the density matrix as `state` during the evolution.

---

**Note:** Not supported by the `rouchon` method.

---

#### Parameters

##### default

[Qobj or `qutip.core.data.Data`, default][None] Initial value to be used at setup of the system.

##### raw\_data

[bool, default][False] If True, the raw matrix will be passed instead of a Qobj. For density matrices, the matrices can be column stacked or square depending on the integration method.

**classmethod** `WienerFeedback`(*default=None*)

Wiener function of the trajectory argument for time dependent systems.

When used as an args:

```
QobjEvo([op, func], args={"W": SMESolver.WienerFeedback()})
```

The func will receive a function as `W` that return an array of wiener processes values at `t`. The wiener process for the `i`-th `sc_ops` is the `i`-th element for homodyne detection and the `(2i, 2i+1)` pairs of process in heterodyne detection. The process is a step function with step of length `options["dt"]`.

---

**Note:** `WienerFeedback` can't be added to a running solver when updating arguments between steps: `solver.step(..., args={})`.

---

#### Parameters

##### default

[callable, optional] Default function used outside the solver. When not passed, a function returning `np.array([0])` is used.

#### property options

Options for stochastic solver:

**store\_final\_state: bool, default: False**

Whether or not to store the final state of the evolution in the result class.

**store\_states: None, bool, default: None**

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

**store\_measurement: bool, default: False**

Whether to store the measurement for each trajectories. Storing measurements will also store the wiener process, or brownian noise for each trajectories.

**progress\_bar: str {'text', 'enhanced', 'tqdm', ''}, default: "text"**

How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.

**progress\_kwargs: dict, default: {"chunk\_size":10}**

Arguments to pass to the progress\_bar. Qutip's bars use chunk\_size.

**keep\_runs\_results: bool, default: False**

Whether to store results from all trajectories or just store the averages.

**normalize\_output: bool**

Normalize output state to hide ODE numerical errors.

**method: str, default: "platen"**

Which differential equation integration method to use.

**map: str {"serial", "parallel", "loky", "mpi"}, default: "serial"**

How to run the trajectories. "parallel" uses the multiprocessing module to run in parallel while "loky" and "mpi" use the "loky" and "mpi4py" modules to do so.

**mpi\_options: dict, default: {}**

Only applies if map is "mpi". This dictionary will be passed as keyword arguments to the *mpi4py.futures.MPIPoolExecutor* constructor. Note that the *max\_workers* argument is provided separately through the *num\_cpus* option.

**num\_cpus: None, int, default: None**

Number of cpus to use when running in parallel. None detect the number of available cpus.

**bitgenerator: {None, "MT19937", "PCG64DXSM", ...}, default: None**

Which of numpy.random's bitgenerator to use. With None, your numpy version's default is used.

**run(state, tlist, ntraj=1, \*, args=None, e\_ops=(), timeout=None, target\_tol=None, seeds=None)**

Do the evolution of the Quantum system.

For a state at time `tlist[0]` do the evolution as directed by `rhs` and for each time in `tlist` store the state and/or expectation values in a *Result*. The evolution method and stored results are determined by options.

#### Parameters

**state**

[*Qobj*] Initial state of the evolution.

**tlist**

[list of double] Time for which to save the results (state and/or expect) of the evolution. The first element of the list is the initial time of the evolution. Time in the list must be in increasing order, but does not need to be uniformly distributed.

**ntraj**

[int] Number of trajectories to add.

**args**

[dict, optional] Change the args of the rhs for the evolution.

**e\_ops**

[list] list of *Qobj* or *QobjEvo* to compute the expectation values. Alternatively, function[s] with the signature `f(t, state) -> expect` can be used.

**timeout**

[float, optional] Maximum time in seconds for the trajectories to run. Once this time is reached, the simulation will end even if the number of trajectories is less than `ntraj`. The map function, set in options, can interrupt the running trajectory or wait for it to finish. Set to an arbitrary high number to disable.

**target\_tol**

[{float, tuple, list}, optional] Target tolerance of the evolution. The evolution will compute trajectories until the error on the expectation values is lower than this tolerance. The maximum number of trajectories employed is given by `ntraj`. The error is computed using jackknife resampling. `target_tol` can be an absolute tolerance or a pair of absolute and relative tolerance, in that order. Lastly, it can be a list of pairs of (atol, rtol) for each `e_ops`.

**seeds**

[{int, SeedSequence, list}, optional] Seed or list of seeds for each trajectories.

**Returns**

**results**

[[MultiTrajResult](#)] Results of the evolution. States and/or expect will be saved. You can control the saved data in the options.

**start**(*state*, *t0*, *seed=None*)

Set the initial state and time for a step evolution.

**Parameters**

**state**

[[Qobj](#)] Initial state of the evolution.

**t0**

[double] Initial time of the evolution.

**seed**

[int, SeedSequence, list, optional] Seed for the random number generator. It can be a single seed used to spawn seeds for each trajectory or a list of seed, one for each trajectory.

**Notes**

When using step evolution, only one trajectory can be computed at once.

**step**(*t*, \*, *args=None*, *copy=True*)

Evolve the state to *t* and return the state as a [Qobj](#).

**Parameters**

**t**

[double] Time to evolve to, must be higher than the last call.

**args**

[dict, optional] Update the `args` of the system. The change is effective from the beginning of the interval. Changing `args` can slow the evolution.

**copy**

[bool, default: True] Whether to return a copy of the data or the data in the ODE solver.

**property sys\_dims**

Dimensions of the space that the system use:

`qutip.basis(sovler.dims)` will create a state with proper dimensions for this solver.

### 5.1.9 Integrator

**class IntegratorScipyAdams**(*system, options*)

Integrator using Scipy *ode* with zvode integrator using adams method. Ordinary Differential Equation solver by netlib (<https://www.netlib.org/odepack>).

Usable with method="adams"

**property options**

Supported options by zvode integrator:

**atol**

[float, default: 1e-8] Absolute tolerance.

**rtol**

[float, default: 1e-6] Relative tolerance.

**order**

[int, default: 12, 'adams' or 5, 'bdf'] Order of integrator <=12 'adams', <=5 'bdf'

**nsteps**

[int, default: 2500] Max. number of internal steps/call.

**first\_step**

[float, default: 0] Size of initial step (0 = automatic).

**min\_step**

[float, default: 0] Minimum step size (0 = automatic).

**max\_step**

[float, default: 0] Maximum step size (0 = automatic) When using pulses, change to half the thinnest pulse otherwise it may be skipped.

**class IntegratorScipyBDF**(*system, options*)

Integrator using Scipy *ode* with zvode integrator using bdf method. Ordinary Differential Equation solver by netlib (<https://www.netlib.org/odepack>).

Usable with method="bdf"

**property options**

Supported options by zvode integrator:

**atol**

[float, default: 1e-8] Absolute tolerance.

**rtol**

[float, default: 1e-6] Relative tolerance.

**order**

[int, default: 12, 'adams' or 5, 'bdf'] Order of integrator <=12 'adams', <=5 'bdf'

**nsteps**

[int, default: 2500] Max. number of internal steps/call.

**first\_step**

[float, default: 0] Size of initial step (0 = automatic).

**min\_step**

[float, default: 0] Minimum step size (0 = automatic).

**max\_step**

[float, default: 0] Maximum step size (0 = automatic) When using pulses, change to half the thinnest pulse otherwise it may be skipped.

**class IntegratorScipyIlsoda**(*system, options*)

Integrator using Scipy *ode* with lsoda integrator. ODE solver by netlib (<https://www.netlib.org/odepack>)  
Automatically choose between 'Adams' and 'BDF' methods to solve both stiff and non-stiff systems.

Usable with `method="lsoda"`

**property options**

Supported options by lsoda integrator:

**atol**

[float, default: 1e-8] Absolute tolerance.

**rtol**

[float, default: 1e-6] Relative tolerance.

**nsteps**

[int, default: 2500] Max. number of internal steps/call.

**max\_order\_ns**

[int, default: 12] Maximum order used in the nonstiff case ( $\leq 12$ ).

**max\_order\_s**

[int, default: 5] Maximum order used in the stiff case ( $\leq 5$ ).

**first\_step**

[float, default: 0] Size of initial step (0 = automatic).

**max\_step**

[float, default: 0] Maximum step size (0 = automatic) When using pulses, change to half the thinnest pulse otherwise it may be skipped.

**min\_step**

[float, default: 0] Minimum step size (0 = automatic)

**class IntegratorScipyDop853**(*system, options*)

Integrator using Scipy *ode* with dop853 integrator. Eight order runge-kutta method by Dormand & Prince. Use fortran implementation from [E. Hairer, S.P. Norsett and G. Wanner, Solving Ordinary Differential Equations i. Nonstiff Problems. 2nd edition. Springer Series in Computational Mathematics, Springer-Verlag (1993)].

Usable with `method="dop853"`

**property options**

Supported options by dop853 integrator:

**atol**

[float, default: 1e-8] Absolute tolerance.

**rtol**

[float, default: 1e-6] Relative tolerance.

**nsteps**

[int, default: 2500] Max. number of internal steps/call.

**first\_step**

[float, default: 0] Size of initial step (0 = automatic).

**max\_step**

[float, default: 0] Maximum step size (0 = automatic)

**ifactor, dfactor**

[float, default: 6., 0.3] Maximum factor to increase/decrease step size by in one step

**beta**

[float, default: 0] Beta parameter for stabilised step size control.

See `scipy.integrate.ode` for more detail

### **class IntegratorVern7**(*system, options*)

QuTiP's implementation of Verner's "most efficient" Runge-Kutta method of order 7. These are Runge-Kutta methods with variable steps and dense output.

The implementation uses QuTiP's Data objects for the state, allowing sparse, GPU or other data layer objects to be used efficiently by the solver in their native formats.

See <https://www.sfu.ca/~jverner/> for a detailed description of the methods.

Usable with `method="vern7"`

#### **property options**

Supported options by verner method:

##### **atol**

[float, default: 1e-8] Absolute tolerance.

##### **rtol**

[float, default: 1e-6] Relative tolerance.

##### **nsteps**

[int, default: 1000] Max. number of internal steps/call.

##### **first\_step**

[float, default: 0] Size of initial step (0 = automatic).

##### **min\_step**

[float, default: 0] Minimum step size (0 = automatic).

##### **max\_step**

[float, default: 0] Maximum step size (0 = automatic) When using pulses, change to half the thinnest pulse otherwise it may be skipped.

##### **interpolate**

[bool, default: True] Whether to use interpolation step, faster most of the time.

### **class IntegratorVern9**(*system, options*)

QuTiP's implementation of Verner's "most efficient" Runge-Kutta method of order 9. These are Runge-Kutta methods with variable steps and dense output.

The implementation uses QuTiP's Data objects for the state, allowing sparse, GPU or other data layer objects to be used efficiently by the solver in their native formats.

See <https://www.sfu.ca/~jverner/> for a detailed description of the methods.

Usable with `method="vern9"`

#### **property options**

Supported options by verner method:

##### **atol**

[float, default: 1e-8] Absolute tolerance.

##### **rtol**

[float, default: 1e-6] Relative tolerance.

##### **nsteps**

[int, default: 1000] Max. number of internal steps/call.

##### **first\_step**

[float, default: 0] Size of initial step (0 = automatic).

##### **min\_step**

[float, default: 0] Minimum step size (0 = automatic).

##### **max\_step**

[float, default: 0] Maximum step size (0 = automatic) When using pulses, change to half the thinnest pulse otherwise it may be skipped.

**interpolate**

[bool, default: True] Whether to use interpolation step, faster most of the time.

**class IntegratorDiag**(*system, options*)

Integrator solving the ODE by diagonalizing the system and solving analytically. It can only solve constant system and has a long preparation time, but the integration is fast.

Usable with `method="diag"`

**property options**

Supported options by “diag” method:

**eigensolver\_dtype**

[str, default: “dense”] Qutip data type { “dense”, “csr”, etc. } to use when computing the eigenstates. The dense eigen solver is usually faster and more stable.

**class IntegratorKrylov**(*system, options*)

Evolve the state vector (“psi0”) finding an approximation for the time evolution operator of Hamiltonian (“H”) by obtaining the projection of the time evolution operator on a set of small dimensional Krylov subspaces ( $m \ll \dim(H)$ ).

**property options**

Supported options by krylov method:

**atol**

[float, default: 1e-7] Absolute tolerance.

**nsteps**

[int, default: 100] Max. number of internal steps/call.

**min\_step, max\_step**

[float, default: (1e-5, 1e5)] Minimum and maximum step size.

**krylov\_dim: int, default: 0**

Dimension of Krylov approximation subspaces used for the time evolution approximation. If the default 0 is given, the dimension is calculated from the system size  $N$ , using  $\min(\text{int}((N + 100) * 0.5), N - 1)$ .

**sub\_system\_tol: float, default: 1e-7**

Tolerance to detect a happy breakdown. A happy breakdown occurs when the initial ket is in a subspace of the Hamiltonian smaller than `krylov_dim`.

**always\_compute\_step: bool, default: False**

If True, the step length is computed each time a new Krylov subspace is computed. Otherwise it is computed only once when creating the integrator.

## 5.1.10 Stochastic Integrator

**class RouchonSODE**(*rhs, options*)

Stochastic integration method keeping the positivity of the density matrix. See eq. (4) Pierre Rouchon and Jason F. Ralph, *Efficient Quantum Filtering for Quantum Feedback Control*, [arXiv:1410.5345](https://arxiv.org/abs/1410.5345) [quant-ph], Phys. Rev. A 91, 012118, (2015).

- Order: strong 1



## Notes

This method should be used with very small `dt`. Unlike other methods that will return unphysical state (negative eigenvalues, Nans) when the time step is too large, this method will return state that seems normal.

### property options

Supported options by Rouchon Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-7] Relative tolerance.

**class EulerSODE**(*rhs, options*)

A simple generalization of the Euler method for ordinary differential equations to stochastic differential equations. Only solver which could take non-commuting `sc_ops`.

- Order: 0.5

### property options

Supported options by Explicit Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-10] Tolerance for the time steps.

**class Milstein\_SODE**(*rhs, options*)

An order 1.0 strong Taylor scheme. Better approximate numerical solution to stochastic differential equations. See eq. (3.12) of chapter 10.3 of Peter E. Kloeden and Exkhard Platen, *Numerical Solution of Stochastic Differential Equations*.

- Order strong 1.0

### property options

Supported options by Explicit Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-10] Tolerance for the time steps.

**class Taylor1\_5\_SODE**(*rhs, options*)

Order 1.5 strong Taylor scheme. Solver with more terms of the Ito-Taylor expansion. See eq. (4.6) of chapter 10.4 of Peter E. Kloeden and Exkhard Platen, *Numerical Solution of Stochastic Differential Equations*.

- Order strong 1.5

### property options

Supported options by Order 1.5 strong Taylor Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-10] Relative tolerance.

**derr\_dt**

[float, default: 1e-6] Finite time difference used to compute the derrivative of the hamiltonian and `sc_ops`.

**class Implicit\_Milstein\_SODE**(*rhs, options*)

An order 1.0 implicit strong Taylor scheme. Implicit Milstein scheme for the numerical simulation of stiff stochastic differential equations. Eq. (2.11) with  $\alpha=0.5$  of chapter 12.2 of Peter E. Kloeden and Exkhard Platen, *Numerical Solution of Stochastic Differential Equations*.

- Order strong 1.0

**property options**

Supported options by Implicit Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-10] Tolerance for the time steps.

**solve\_method**

[str, default: None] Method used for solver the  $Ax=b$  of the implicit step. Accept methods supported by `qutip.core.data.solve`. When the system is constant, the inverse of the matrix  $A$  can be used by entering `inv`.

**solve\_options**

[dict, default: {}] Options to pass to the call to `qutip.core.data.solve`.

**class Implicit\_Taylor1\_5\_SODE**(*rhs, options*)

Order 1.5 implicit strong Taylor scheme. Solver with more terms of the Ito-Taylor expansion. Eq. (2.18) with  $\alpha=0.5$  of chapter 12.2 of Peter E. Kloeden and Exkhard Platen, *Numerical Solution of Stochastic Differential Equations*.

- Order strong 1.5

**property options**

Supported options by Implicit Order 1.5 strong Taylor Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-10] Tolerance for the time steps.

**solve\_method**

[str, default: None] Method used for solver the  $Ax=b$  of the implicit step. Accept methods supported by `qutip.core.data.solve`. When the system is constant, the inverse of the matrix  $A$  can be used by entering `inv`.

**solve\_options**

[dict, default: {}] Options to pass to the call to `qutip.core.data.solve`.

**derr\_dt**

[float, default: 1e-6] Finite time difference used to compute the derrivative of the hamiltonian and `sc_ops`.

**class PlatenSODE**(*rhs, options*)

Explicit scheme, creates the Milstein using finite differences instead of analytic derivatives. Also contains some higher order terms, thus converges better than Milstein while staying strong order 1.0. Does not require derivatives. See eq. (7.47) of chapter 7 of H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*.

- Order: strong 1, weak 2

**property options**

Supported options by Explicit Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-10] Tolerance for the time steps.

**class Explicit1\_5\_SODE**(*rhs, options*)

Explicit order 1.5 strong schemes. Reproduce the order 1.5 strong Taylor scheme using finite difference instead of derivatives. Slower than `taylor15` but usable when derivatives cannot be analytically obtained. See eq. (2.13) of chapter 11.2 of Peter E. Kloeden and Exkhard Platen, *Numerical Solution of Stochastic Differential Equations*.

- Order: strong 1.5

**property options**

Supported options by Explicit Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-10] Tolerance for the time steps.

**class PredCorr\_SODE**(*rhs, options*)

Generalization of the trapezoidal method to stochastic differential equations. More stable than explicit methods. See eq. (5.4) of chapter 15.5 of Peter E. Kloeden and Exkhard Platen, *Numerical Solution of Stochastic Differential Equations*.

- Order strong 0.5, weak 1.0
- Codes to only correct the stochastic part ( $\alpha = 0, \eta = 1/2$ ): 'pred-corr', 'predictor-corrector' or 'pc-euler'
- Codes to correct both the stochastic and deterministic parts ( $\alpha = 1/2, \eta = 1/2$ ): 'pc-euler-imp', 'pc-euler-2' or 'pred-corr-2'

**property options**

Supported options by Explicit Stochastic Integrators:

**dt**

[float, default: 0.001] Internal time step.

**tol**

[float, default: 1e-10] Tolerance for the time steps.

**alpha**

[float, default: 0.] Implicit factor to the drift.  $\text{eff\_drift} \sim \text{drift}(t) * (1-\alpha) + \text{drift}(t+dt) * \alpha$

**eta**

[float, default: 0.5] Implicit factor to the diffusion.  $\text{eff\_diffusion} \sim \text{diffusion}(t) * (1-\eta) + \text{diffusion}(t+dt) * \eta$

### 5.1.11 Solver Options and Results

**class Result**(*e\_ops, options: ResultOptions, \*, solver=None, stats=None, \*\*kw*)

Base class for storing solver results.

**Parameters**

**e\_ops**

[*Qobj*, *QobjEvo*, function or list or dict of these] The `e_ops` parameter defines the set of values to record at each time step `t`. If an element is a *Qobj* or *QobjEvo* the value recorded is the expectation value of that operator given the state at `t`. If the element is a function, `f`, the value recorded is `f(t, state)`.

The values are recorded in the `e_data` and `expect` attributes of this result object. `e_data` is a dictionary and `expect` is a list, where each item contains the values of the corresponding `e_op`.

**options**

[dict] The options for this result class.

**solver**

[str or None] The name of the solver generating these results.

**stats**

[dict or None] The stats generated by the solver while producing these results. Note that the solver may update the stats directly while producing results.

**kw**

[dict] Additional parameters specific to a result sub-class.

**Attributes**

**times**

[list] A list of the times at which the expectation values and states were recorded.

**states**

[list of *Qobj*] The state at each time  $t$  (if the recording of the state was requested).

**final\_state**

[*Qobj*:] The final state (if the recording of the final state was requested).

**expect**

[list of arrays of expectation values] A list containing the values of each *e\_op*. The list is in the same order in which the *e\_ops* were supplied and empty if no *e\_ops* were given.

Each element is itself a list and contains the values of the corresponding *e\_op*, with one value for each time in *.times*.

The same lists of values may be accessed via the *.e\_data* dictionary and the original *e\_ops* are available via the *.e\_ops* attribute.

**e\_data**

[dict] A dictionary containing the values of each *e\_op*. If the *e\_ops* were supplied as a dictionary, the keys are the same as in that dictionary. Otherwise the keys are the index of the *e\_op* in the *.expect* list.

The lists of expectation values returned are the *same* lists as those returned by *.expect*.

**e\_ops**

[dict] A dictionary containing the supplied *e\_ops* as *ExpectOp* instances. The keys of the dictionary are the same as for *.e\_data*. Each value is object where *.e\_ops[k](t, state)* calculates the value of *e\_op k* at time  $t$  and the given state, and *.e\_ops[k].op* is the original object supplied to create the *e\_op*.

**solver**

[str or None] The name of the solver generating these results.

**stats**

[dict or None] The stats generated by the solver while producing these results.

**options**

[dict] The options for this result class.

**class MultiTrajResult**(*e\_ops, options: MultiTrajResultOptions, \*, solver=None, stats=None, \*\*kw*)

Base class for storing results for solver using multiple trajectories.

**Parameters**

**e\_ops**

[*Qobj*, *QobjEvo*, function or list or dict of these] The *e\_ops* parameter defines the set of values to record at each time step  $t$ . If an element is a *Qobj* or *QobjEvo* the value recorded is the expectation value of that operator given the state at  $t$ . If the element is a function, *f*, the value recorded is *f(t, state)*.

The values are recorded in the `.expect` attribute of this result object. `.expect` is a list, where each item contains the values of the corresponding `e_op`.

Function `e_ops` must return a number so the average can be computed.

**options**

[dict] The options for this result class.

**solver**

[str or None] The name of the solver generating these results.

**stats**

[dict or None] The stats generated by the solver while producing these results. Note that the solver may update the stats directly while producing results.

**kw**

[dict] Additional parameters specific to a result sub-class.

**Attributes**

**times**

[list] A list of the times at which the expectation values and states were recorded.

**average\_states**

[list of *Qobj*] States averages as density matrices.

**runs\_states**

[list of list of *Qobj*] States of every runs as `states[run][t]`.

**final\_state**

[*Qobj*:] Runs final states if available, average otherwise.

**runs\_final\_state**

[list of *Qobj*] The final state for each trajectory (if the recording of the final state and trajectories was requested).

**average\_expect**

[list of array of expectation values] A list containing the values of each `e_op` averaged over each trajectories. The list is in the same order in which the `e_ops` were supplied and empty if no `e_ops` were given.

Each element is itself an array and contains the values of the corresponding `e_op`, with one value for each time in `.times`.

**std\_expect**

[list of array of expectation values] A list containing the standard derivation of each `e_op` over each trajectories. The list is in the same order in which the `e_ops` were supplied and empty if no `e_ops` were given.

Each element is itself an array and contains the values of the corresponding `e_op`, with one value for each time in `.times`.

**runs\_expect**

[list of array of expectation values] A list containing the values of each `e_op` for each trajectories. The list is in the same order in which the `e_ops` were supplied and empty if no `e_ops` were given. Only available if the storing of trajectories was requested.

The order of the elements is `runs_expect[e_ops][trajectory][time]`.

Each element is itself an array and contains the values of the corresponding `e_op`, with one value for each time in `.times`.

**average\_e\_data**

[dict] A dictionary containing the values of each `e_op` averaged over each trajectories. If the `e_ops` were supplied as a dictionary, the keys are the same as in that dictionary. Otherwise the keys are the index of the `e_op` in the `.expect` list.

The lists of expectation values returned are the *same* lists as those returned by `.expect`.

**average\_e\_data**

[dict] A dictionary containing the standard derivation of each `e_op` over each trajectories. If the `e_ops` were supplied as a dictionary, the keys are the same as in that dictionary. Otherwise the keys are the index of the `e_op` in the `.expect` list.

The lists of expectation values returned are the *same* lists as those returned by `.expect`.

**runs\_e\_data**

[dict] A dictionary containing the values of each `e_op` for each trajectories. If the `e_ops` were supplied as a dictionary, the keys are the same as in that dictionary. Otherwise the keys are the index of the `e_op` in the `.expect` list. Only available if the storing of trajectories was requested.

The order of the elements is `runs_expect[e_ops][trajectory][time]`.

The lists of expectation values returned are the *same* lists as those returned by `.expect`.

**solver**

[str or None] The name of the solver generating these results.

**stats**

[dict or None] The stats generated by the solver while producing these results.

**options**

[SolverResultsOptions] The options for this result class.

**property average\_final\_state**

Last states of each trajectories averaged into a density matrix.

**property average\_states**

States averages as density matrices.

**property final\_state**

Runs final states if available, average otherwise.

**property runs\_final\_states**

Last states of each trajectories.

**property runs\_states**

States of every runs as `states[run][t]`.

**property states**

Runs final states if available, average otherwise.

**steady\_state(N=0)**

Average the states of the last N times of every runs as a density matrix. Should converge to the steady state in the right circumstances.

**Parameters**

**N**

[int [optional]] Number of states from the end of `tlist` to average. Per default all states will be averaged.

**class McResult**(*e\_ops*, *options*: MultiTrajResultOptions, \*, *solver*=None, *stats*=None, \*\*kw)

Class for storing Monte-Carlo solver results.

**Parameters**

**e\_ops**

[Qobj, QobjEvo, function or list or dict of these] The `e_ops` parameter defines the set of values to record at each time step `t`. If an element is a `Qobj` or `QobjEvo` the value recorded is the expectation value of that operator given the state at `t`. If the element is a function, `f`, the value recorded is `f(t, state)`.

The values are recorded in the `.expect` attribute of this result object. `.expect` is a list, where each item contains the values of the corresponding `e_op`.

**options**

[SolverResultsOptions] The options for this result class.

**solver**

[str or None] The name of the solver generating these results.

**stats**

[dict] The stats generated by the solver while producing these results. Note that the solver may update the stats directly while producing results. Must include a value for “num\_collapse”.

**kw**

[dict] Additional parameters specific to a result sub-class.

**Attributes**

**collapse**

[list] For each runs, a list of every collapse as a tuple of the time it happened and the corresponding `c_ops` index.

**property average\_final\_state**

Last states of each trajectories averaged into a density matrix.

**property average\_states**

States averages as density matrices.

**property col\_times**

List of the times of the collapses for each runs.

**property col\_which**

List of the indexes of the collapses for each runs.

**property final\_state**

Runs final states if available, average otherwise.

**property photocurrent**

Average photocurrent or measurement of the evolution.

**property runs\_final\_states**

Last states of each trajectories.

**property runs\_photocurrent**

Photocurrent or measurement of each runs.

**property runs\_states**

States of every runs as `states[run][t]`.

**property states**

Runs final states if available, average otherwise.

**steady\_state( $N=0$ )**

Average the states of the last  $N$  times of every runs as a density matrix. Should converge to the steady state in the right circumstances.

**Parameters**

**N**

[int [optional]] Number of states from the end of `tlist` to average. Per default all states will be averaged.

**class NmmcResult**(*e\_ops*, *options*: MultiTrajResultOptions, \*, *solver*=None, *stats*=None, \*\**kw*)

Class for storing the results of the non-Markovian Monte-Carlo solver.

**Parameters**

#### **e\_ops**

[*Qobj*, *QobjEvo*, function or list or dict of these] The `e_ops` parameter defines the set of values to record at each time step `t`. If an element is a *Qobj* or *QobjEvo* the value recorded is the expectation value of that operator given the state at `t`. If the element is a function, `f`, the value recorded is `f(t, state)`.

The values are recorded in the `.expect` attribute of this result object. `.expect` is a list, where each item contains the values of the corresponding `e_op`.

#### **options**

[*SolverResultsOptions*] The options for this result class.

#### **solver**

[str or None] The name of the solver generating these results.

#### **stats**

[dict] The stats generated by the solver while producing these results. Note that the solver may update the stats directly while producing results. Must include a value for “num\_collapse”.

#### **kw**

[dict] Additional parameters specific to a result sub-class.

### **Attributes**

#### **average\_trace**

[list] The average trace (i.e., averaged over all trajectories) at each time.

#### **std\_trace**

[list] The standard deviation of the trace at each time.

#### **runs\_trace**

[list of lists] For each recorded trajectory, the trace at each time. Only present if `keep_runs_results` is set in the options.

#### **property average\_final\_state**

Last states of each trajectories averaged into a density matrix.

#### **property average\_states**

States averages as density matrices.

#### **property col\_times**

List of the times of the collapses for each runs.

#### **property col\_which**

List of the indexes of the collapses for each runs.

#### **property final\_state**

Runs final states if available, average otherwise.

#### **property photocurrent**

Average photocurrent or measurement of the evolution.

#### **property runs\_final\_states**

Last states of each trajectories.

#### **property runs\_photocurrent**

Photocurrent or measurement of each runs.

#### **property runs\_states**

States of every runs as `states[run][t]`.

#### **property states**

Runs final states if available, average otherwise.



### **steady\_state( $N=0$ )**

Average the states of the last  $N$  times of every runs as a density matrix. Should converge to the steady state in the right circumstances.

#### **Parameters**

**N**

[int [optional]] Number of states from the end of `tlist` to average. Per default all states will be averaged.

### **property trace**

Refers to `average_trace` or `runs_trace`, depending on whether `keep_runs_results` is set in the options.

## 5.1.12 Permutational Invariance

**class Dicke( $N$ , *hamiltonian=None*, *emission=0.0*, *dephasing=0.0*, *pumping=0.0*, *collective\_emission=0.0*, *collective\_dephasing=0.0*, *collective\_pumping=0.0*)**

The Dicke class which builds the Lindbladian and Liouvillian matrix.

#### **Parameters**

**N: int**

The number of two-level systems.

**hamiltonian**

[*Qobj*] A Hamiltonian in the Dicke basis.

The matrix dimensions are (nds, nds), with nds being the number of Dicke states. The Hamiltonian can be built with the operators given by the *jspin* functions.

**emission: float**

Incoherent emission coefficient (also nonradiative emission). default: 0.0

**dephasing: float**

Local dephasing coefficient. default: 0.0

**pumping: float**

Incoherent pumping coefficient. default: 0.0

**collective\_emission: float**

Collective (superradiant) emission coefficient. default: 0.0

**collective\_pumping: float**

Collective pumping coefficient. default: 0.0

**collective\_dephasing: float**

Collective dephasing coefficient. default: 0.0

### Examples

```
>>> from qutip.piqs import Dicke, jspin
>>> N = 2
>>> jx, jy, jz = jspin(N)
>>> jp = jspin(N, "+")
>>> jm = jspin(N, "-")
>>> ensemble = Dicke(N, emission=1.)
>>> L = ensemble.liouvillian()
```

#### **Attributes**

**N: int**

The number of two-level systems.

**hamiltonian**

[*Qobj*] A Hamiltonian in the Dicke basis.

The matrix dimensions are (nds, nds), with nds being the number of Dicke states. The Hamiltonian can be built with the operators given by the *jspin* function in the “dicke” basis.

**emission: float**

Incoherent emission coefficient (also nonradiative emission). default: 0.0

**dephasing: float**

Local dephasing coefficient. default: 0.0

**pumping: float**

Incoherent pumping coefficient. default: 0.0

**collective\_emission: float**

Collective (superradiant) emission coefficient. default: 0.0

**collective\_dephasing: float**

Collective dephasing coefficient. default: 0.0

**collective\_pumping: float**

Collective pumping coefficient. default: 0.0

**nds: int**

The number of Dicke states.

**dshape: tuple**

The shape of the Hilbert space in the Dicke or uncoupled basis. default: (nds, nds).

**c\_ops()**

Build collapse operators in the full Hilbert space  $2^N$ .

**Returns**

**c\_ops\_list: list**

The list with the collapse operators in the  $2^N$  Hilbert space.

**coefficient\_matrix()**

Build coefficient matrix for ODE for a diagonal problem.

**Returns**

**M: ndarray**

The matrix M of the coefficients for the ODE  $dp/dt = Mp$ . p is the vector of the diagonal matrix elements of the density matrix rho in the Dicke basis.

**lindbladian()**

Build the Lindbladian superoperator of the dissipative dynamics.

**Returns**

**lindbladian**

[*Qobj*] The Lindbladian matrix as a *qutip.Qobj*.

**liouvillian()**

Build the total Liouvillian using the Dicke basis.

**Returns**

**liouv**

[*Qobj*] The Liouvillian matrix for the system.

**pisolve**(*initial\_state*, *tlist*)

Solve for diagonal Hamiltonians and initial states faster.

**Parameters**

**initial\_state**

[*Qobj*] An initial state specified as a density matrix of *qutip.Qobj* type.

**tlist: ndarray**

A 1D numpy array of list of timesteps to integrate

**Returns**

**result: list**

A dictionary of the type *qutip.piqs.Result* which holds the results of the evolution.

**class Pim**(*N*, *emission*=0.0, *dephasing*=0, *pumping*=0, *collective\_emission*=0, *collective\_pumping*=0, *collective\_dephasing*=0)

The Permutation Invariant Matrix class.

Initialize the class with the parameters for generating a Permutation Invariant matrix which evolves a given diagonal initial state *p* as:

$dp/dt = Mp$

**Parameters**

**N: int**

The number of two-level systems.

**emission: float**

Incoherent emission coefficient (also nonradiative emission). default: 0.0

**dephasing: float**

Local dephasing coefficient. default: 0.0

**pumping: float**

Incoherent pumping coefficient. default: 0.0

**collective\_emission: float**

Collective (superradiant) emission coefficient. default: 0.0

**collective\_pumping: float**

Collective pumping coefficient. default: 0.0

**collective\_dephasing: float**

Collective dephasing coefficient. default: 0.0

**Attributes**

**N: int**

The number of two-level systems.

**emission: float**

Incoherent emission coefficient (also nonradiative emission). default: 0.0

**dephasing: float**

Local dephasing coefficient. default: 0.0

**pumping: float**

Incoherent pumping coefficient. default: 0.0

**collective\_emission: float**

Collective (superradiant) emission coefficient. default: 0.0

**collective\_dephasing: float**

Collective dephasing coefficient. default: 0.0

**collective\_pumping:** float

Collective pumping coefficient. default: 0.0

**M:** dict

A nested dictionary of the structure {row: {col: val}} which holds non zero elements of the matrix M

**calculate\_j\_m**(dicke\_row, dicke\_col)

Get the value of j and m for the particular Dicke space element.

**Parameters**

**dicke\_row, dicke\_col:** int

The row and column from the Dicke space matrix

**Returns**

**j, m:** float

The j and m values.

**calculate\_k**(dicke\_row, dicke\_col)

Get k value from the current row and column element in the Dicke space.

**Parameters**

**dicke\_row, dicke\_col:** int

The row and column from the Dicke space matrix.

**Returns**

**k:** int

The row index for the matrix M for given Dicke space element.

**coefficient\_matrix**()

Generate the matrix M governing the dynamics for diagonal cases.

If the initial density matrix and the Hamiltonian is diagonal, the evolution of the system is given by the simple ODE:  $dp/dt = Mp$ .

**isdicke**(dicke\_row, dicke\_col)

Check if an element in a matrix is a valid element in the Dicke space. Dicke row: j value index. Dicke column: m value index. The function returns True if the element exists in the Dicke space and False otherwise.

**Parameters**

**dicke\_row, dicke\_col**

[int] Index of the element in Dicke space which needs to be checked

**solve**(rho0, tlist)

Solve the ODE for the evolution of diagonal states and Hamiltonians.

**tau1**(j, m)

Calculate coefficient matrix element relative to (j, m, m).

**tau2**(j, m)

Calculate coefficient matrix element relative to (j, m+1, m+1).

**tau3**(j, m)

Calculate coefficient matrix element relative to (j+1, m+1, m+1).

**tau4**(j, m)

Calculate coefficient matrix element relative to (j-1, m+1, m+1).

**tau5**(*j, m*)

Calculate coefficient matrix element relative to (*j*+1, *m*, *m*).

**tau6**(*j, m*)

Calculate coefficient matrix element relative to (*j*-1, *m*, *m*).

**tau7**(*j, m*)

Calculate coefficient matrix element relative to (*j*+1, *m*-1, *m*-1).

**tau8**(*j, m*)

Calculate coefficient matrix element relative to (*j*, *m*-1, *m*-1).

**tau9**(*j, m*)

Calculate coefficient matrix element relative to (*j*-1, *m*-1, *m*-1).

**tau\_valid**(*dicke\_row, dicke\_col*)

Find the Tau functions which are valid for this value of (*dicke\_row*, *dicke\_col*) given the number of TLS. This calculates the valid tau values and returns a dictionary specifying the tau function name and the value.

#### Parameters

**dicke\_row, dicke\_col**

[int] Index of the element in Dicke space which needs to be checked.

#### Returns

**taus: dict**

A dictionary of key, val as {tau: value} consisting of the valid taus for this row and column of the Dicke space element.

### 5.1.13 Distribution functions

**class Distribution**(*data=None, xvecs=[], xlabel=[]*)

A class for representation spatial distribution functions.

The Distribution class can be used to represent spatial distribution functions of arbitrary dimension (although only 1D and 2D distributions are used so far).

It is intended as a base class for specific distribution function, and provide implementation of basic functions that are shared among all Distribution functions, such as visualization, calculating marginal distributions, etc.

#### Parameters

**data**

[array\_like] Data for the distribution. The dimensions must match the lengths of the coordinate arrays in *xvecs*.

**xvecs**

[list] List of arrays that spans the space for each coordinate.

**xlabels**

[list] List of labels for each coordinate.

**marginal**(*dim=0*)

Calculate the marginal distribution function along the dimension *dim*. Return a new Distribution instance describing this reduced- dimensionality distribution.

#### Parameters

**dim**

[int] The dimension (coordinate index) along which to obtain the marginal distribution.

#### Returns

**d**

[Distributions] A new instances of Distribution that describes the marginal distribution.

**project**(*dim=0*)

Calculate the projection (max value) distribution function along the dimension *dim*. Return a new Distribution instance describing this reduced-dimensionality distribution.

**Parameters**

**dim**

[int] The dimension (coordinate index) along which to obtain the projected distribution.

**Returns**

**d**

[Distributions] A new instances of Distribution that describes the projection.

**visualize**(*fig=None, ax=None, figsize=(8, 6), colorbar=True, cmap=None, style='colormap', show\_xlabel=True, show\_ylabel=True*)

Visualize the data of the distribution in 1D or 2D, depending on the dimensionality of the underlying distribution.

Parameters:

**fig**

[matplotlib Figure instance] If given, use this figure instance for the visualization,

**ax**

[matplotlib Axes instance] If given, render the visualization using this axis instance.

**figsize**

[tuple] Size of the new Figure instance, if one needs to be created.

**colorbar: Bool**

Whether or not the colorbar (in 2D visualization) should be used.

**cmap: matplotlib colormap instance**

If given, use this colormap for 2D visualizations.

**style**

[string] Type of visualization: 'colormap' (default) or 'surface'.

**Returns**

**fig, ax**

[tuple] A tuple of matplotlib figure and axes instances.

## 5.2 Functions

### 5.2.1 Manipulation and Creation of States and Operators

#### Quantum States

**basis**(*dimensions, n=None, offset=None, \*, dtype=None*)

Generates the vector representation of a Fock state.

**Parameters**

**dimensions**

[int or list of ints, Space] Number of basis states in Hilbert space. If a list, then the resultant object will be a tensor product over spaces with those dimensions.

**n**  
[int or list of ints, optional (default 0 for all dimensions)] Integer corresponding to desired number state, defaults to 0 for all dimensions if omitted. The shape must match dimensions, e.g. if dimensions is a list, then n must either be omitted or a list of equal length.

**offset**  
[int or list of ints, optional (default 0 for all dimensions)] The lowest number state that is included in the finite number state representation of the state in the relevant dimension.

**dtype**  
[type or str, optional] storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

**state**  
[*Qobj*] *Qobj* representing the requested number state  $|n\rangle$ .

### Notes

A subtle incompatibility with the quantum optics toolbox: In QuTiP:

```
basis(N, 0) = ground state
```

but in the qotoolbox:

```
basis(N, 1) = ground state
```

### Examples

```
>>> basis(5,2)
Quantum object: dims = [[5], [1]], shape = (5, 1), type = ket
Qobj data =
[[ 0.+0.j]
 [ 0.+0.j]
 [ 1.+0.j]
 [ 0.+0.j]
 [ 0.+0.j]]
>>> basis([2,2,2], [0,1,0])
Quantum object: dims = [[2, 2, 2], [1, 1, 1]], shape = (8, 1), type = ket
Qobj data =
[[0.]
 [0.]
 [1.]
 [0.]
 [0.]
 [0.]
 [0.]
 [0.]]
```

**bell\_state**(state='00', \*, dtype=None)

Returns the selected Bell state:

$$\begin{aligned} |B_{00}\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ |B_{01}\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \\ |B_{10}\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \\ |B_{11}\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \end{aligned}$$

### Parameters

**state**

[str ['00', '01', '10', '11']] Which bell state to return

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

**Bell\_state**

[qobj] Bell state

**bra**(seq, dim=2, \*, dtype=None)

Produces a multiparticle bra state for a list or string, where each element stands for state of the respective particle.

### Parameters

**seq**

[str / list of ints or characters] Each element defines state of the respective particle. (e.g. [1,1,0,1] or a string "1101"). For qubits it is also possible to use the following conventions:

- 'g'/'e' (ground and excited state)
- 'u'/'d' (spin up and down)
- 'H'/'V' (horizontal and vertical polarization)

Note: for dimension > 9 you need to use a list.

**dim**

[int (default: 2) / list of ints] Space dimension for each particle: int if there are the same, list if they are different.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

**bra**

[qobj]



## Examples

```
>>> bra("10")
Quantum object: dims = [[1, 1], [2, 2]], shape = [1, 4], type = bra
Qobj data =
[[ 0.  0.  1.  0.]]
```

```
>>> bra("Hue")
Quantum object: dims = [[1, 1, 1], [2, 2, 2]], shape = [1, 8], type = bra
Qobj data =
[[ 0.  1.  0.  0.  0.  0.  0.  0.]]
```

```
>>> bra("12", 3)
Quantum object: dims = [[1, 1], [3, 3]], shape = [1, 9], type = bra
Qobj data =
[[ 0.  0.  0.  0.  0.  1.  0.  0.  0.]]
```

```
>>> bra("31", [5, 2])
Quantum object: dims = [[1, 1], [5, 2]], shape = [1, 10], type = bra
Qobj data =
[[ 0.  0.  0.  0.  0.  0.  0.  1.  0.  0.]]
```

**coherent** (*N*, *alpha*, *offset*=0, *method*=None, \*, *dtype*=None)

Generates a coherent state with eigenvalue *alpha*.

Constructed using displacement operator on vacuum state.

### Parameters

**N**

[int] Number of Fock states in Hilbert space.

**alpha**

[float/complex] Eigenvalue of coherent state.

**offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the state. Using a non-zero offset will make the default method 'analytic'.

**method**

[string {'operator', 'analytic'}, optional] Method for generating coherent state.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

**state**

[qobj] Qobj quantum object for coherent state

## Notes

Select method ‘operator’ (default) or ‘analytic’. With the ‘operator’ method, the coherent state is generated by displacing the vacuum state using the displacement operator defined in the truncated Hilbert space of size ‘N’. This method guarantees that the resulting state is normalized. With ‘analytic’ method the coherent state is generated using the analytical formula for the coherent state coefficients in the Fock basis. This method does not guarantee that the state is normalized if truncated to a small number of Fock states, but would in that case give more accurate coefficients.

## Examples

```
>>> coherent(5,0.25j)
Quantum object: dims = [[5], [1]], shape = [5, 1], type = ket
Qobj data =
[[ 9.69233235e-01+0.j          ]
 [ 0.00000000e+00+0.24230831j]
 [ -4.28344935e-02+0.j          ]
 [ 0.00000000e+00-0.00618204j]
 [ 7.80904967e-04+0.j          ]]
```

**coherent\_dm**(*N*, *alpha*, *offset=0*, *method='operator'*, \*, *dtype=None*)

Density matrix representation of a coherent state.

Constructed via outer product of [coherent](#)

### Parameters

**N**

[int] Number of basis states in Hilbert space.

**alpha**

[float/complex] Eigenvalue for coherent state.

**offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the state.

**method**

[string { ‘operator’, ‘analytic’ }, optional] Method for generating coherent density matrix.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

**dm**

[qobj] Density matrix representation of coherent state.

## Notes

Select method ‘operator’ (default) or ‘analytic’. With the ‘operator’ method, the coherent density matrix is generated by displacing the vacuum state using the displacement operator defined in the truncated Hilbert space of size ‘N’. This method guarantees that the resulting density matrix is normalized. With ‘analytic’ method the coherent density matrix is generated using the analytical formula for the coherent state coefficients in the Fock basis. This method does not guarantee that the state is normalized if truncated to a small number of Fock states, but would in that case give more accurate coefficients.

## Examples

```
>>> coherent_dm(3,0.25j)
Quantum object: dims = [[3], [3]], shape = [3, 3], type = oper, isHerm = True
Qobj data =
[[ 0.93941695+0.j          0.00000000-0.23480733j -0.04216943+0.j          ]
 [ 0.00000000+0.23480733j  0.05869011+0.j          0.00000000-0.01054025j]
 [-0.04216943+0.j          0.00000000+0.01054025j  0.00189294+0.j          ]]
```

**fock**(*dimensions*, *n=None*, *offset=None*, \*, *dtype=None*)

Bosonic Fock (number) state.

Same as *basis*.

### Parameters

#### **dimensions**

[int or list of ints, Space] Number of basis states in Hilbert space. If a list, then the resultant object will be a tensor product over spaces with those dimensions.

#### **n**

[int or list of ints, default: 0 for all dimensions] Integer corresponding to desired number state, defaults to 0 for all dimensions if omitted. The shape must match *dimensions*, e.g. if *dimensions* is a list, then *n* must either be omitted or a list of equal length.

#### **offset**

[int or list of ints, default: 0 for all dimensions] The lowest number state that is included in the finite number state representation of the state in the relevant dimension.

#### **dtype**

[type or str, optional] Storage representation. Any data-layer known to *qutip.data.to* is accepted.

### Returns

Requested number state  $|n\rangle$ .

## Examples

```
>>> fock(4,3)
Quantum object: dims = [[4], [1]], shape = [4, 1], type = ket
Qobj data =
[[ 0.+0.j]
 [ 0.+0.j]
 [ 0.+0.j]
 [ 1.+0.j]]
```

**fock\_dm**(*dimensions*, *n=None*, *offset=None*, \*, *dtype=None*)

Density matrix representation of a Fock state

Constructed via outer product of *basis*.

### Parameters

#### **dimensions**

[int or list of ints, Space] Number of basis states in Hilbert space. If a list, then the resultant object will be a tensor product over spaces with those dimensions.

#### **n**

[int or list of ints, default: 0 for all dimensions] Integer corresponding to desired number state, defaults to 0 for all dimensions if omitted. The shape must match *dimensions*, e.g. if *dimensions* is a list, then *n* must either be omitted or a list of equal length.

**offset**

[int or list of ints, default: 0 for all dimensions] The lowest number state that is included in the finite number state representation of the state in the relevant dimension.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**dm**

[qobj] Density matrix representation of Fock state.

## Examples

```
>>> fock_dm(3,1)
Quantum object: dims = [[3], [3]], shape = [3, 3], type = oper, isHerm = True
Qobj data =
[[ 0.+0.j  0.+0.j  0.+0.j]
 [ 0.+0.j  1.+0.j  0.+0.j]
 [ 0.+0.j  0.+0.j  0.+0.j]]
```

**ghz\_state**(*N\_qubit*, \*, *dtype=None*)

**Returns the N-qubit GHZ-state:**

$[|00\dots00\rangle + |11\dots11\rangle] / \sqrt{2}$

**Parameters**

**N\_qubit**

[int] Number of qubits in state

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**G**

[qobj] N-qubit GHZ-state

**ket**(*seq*, *dim=2*, \*, *dtype=None*)

Produces a multiparticle ket state for a list or string, where each element stands for state of the respective particle.

**Parameters**

**seq**

[str / list of ints or characters] Each element defines state of the respective particle. (e.g. [1,1,0,1] or a string "1101"). For qubits it is also possible to use the following conventions: - 'g'/'e' (ground and excited state) - 'u'/'d' (spin up and down) - 'H'/'V' (horizontal and vertical polarization) Note: for dimension > 9 you need to use a list.

**dim**

[int or list of ints, default: 2] Space dimension for each particle: int if there are the same, list if they are different.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**ket**  
[qobj]

## Examples

```
>>> ket("10")
Quantum object: dims = [[2, 2], [1, 1]], shape = [4, 1], type = ket
Qobj data =
[[ 0.]
 [ 0.]
 [ 1.]
 [ 0.]]
```

```
>>> ket("Hue")
Quantum object: dims = [[2, 2, 2], [1, 1, 1]], shape = [8, 1], type = ket
Qobj data =
[[ 0.]
 [ 1.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]]
```

```
>>> ket("12", 3)
Quantum object: dims = [[3, 3], [1, 1]], shape = [9, 1], type = ket
Qobj data =
[[ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 1.]
 [ 0.]
 [ 0.]
 [ 0.]]
```

```
>>> ket("31", [5, 2])
Quantum object: dims = [[5, 2], [1, 1]], shape = [10, 1], type = ket
Qobj data =
[[ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 1.]
 [ 0.]
 [ 0.]]
```

### ket2dm(Q)

Takes input ket or bra vector and returns density matrix formed by outer product. This is completely identical to calling `Q.proj()`.

### Parameters

**Q**

[*Qobj*] Ket or bra type quantum object.

### Returns

**dm**

[*Qobj*] Density matrix formed by outer product of *Q*.

### Examples

```
>>> x=basis(3,2)
>>> ket2dm(x)
Quantum object: dims = [[3], [3]], shape = [3, 3], type = oper, isHerm = True
Qobj data =
[[ 0.+0.j  0.+0.j  0.+0.j]
 [ 0.+0.j  0.+0.j  0.+0.j]
 [ 0.+0.j  0.+0.j  1.+0.j]]
```

**maximally\_mixed\_dm**(*dimensions*, \*, *dtype=None*)

Returns the maximally mixed density matrix for a Hilbert space of dimension *N*.

### Parameters

**dimensions**

[int or list of ints, Space] Number of basis states in Hilbert space. If a list, then the resultant object will be a tensor product over spaces with those dimensions.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

**dm**

[*Qobj*] Thermal state density matrix.

**phase\_basis**(*N*, *m*, *phi0=0*, \*, *dtype=None*)

Basis vector for the *m*th phase of the Pegg-Barnett phase operator.

### Parameters

**N**

[int] Number of basis states in Hilbert space.

**m**

[int] Integer corresponding to the *m*th discrete phase  $\phi_m = \phi_0 + 2 * \pi * m / N$

**phi0**

[float, default: 0] Reference phase angle.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

**state**

[*qobj*] Ket vector for *m*th Pegg-Barnett phase operator basis state.

## Notes

The Pegg-Barnett basis states form a complete set over the truncated Hilbert space.

**projection**(*dimensions, n, m, offset=None, \*, dtype=None*)

The projection operator that projects state  $|m\rangle$  on state  $|n\rangle$ .

### Parameters

#### **dimensions**

[int or list of ints, Space] Number of basis states in Hilbert space. If a list, then the resultant object will be a tensor product over spaces with those dimensions.

#### **n, m**

[int] The number states in the projection.

#### **offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the projector.

#### **dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

#### **oper**

[qobj] Requested projection operator.

**qutrit\_basis**(*\*, dtype=None*)

Basis states for a three level system (qutrit)

#### **dtype**

[type or str, optional] storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

#### **qstates**

[array] Array of qutrit basis vectors

**singlet\_state**(*\*, dtype=None*)

Returns the two particle singlet-state:

$$|S\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

that is identical to the fourth bell state.

### Parameters

#### **dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

#### **Bell\_state**

[qobj]  $|B_{11}\rangle$  Bell state

**spin\_coherent**(*j, theta, phi, type='ket', \*, dtype=None*)

Generate the coherent spin state  $|\theta, \phi\rangle$ .

### Parameters

#### **j**

[float] The spin of the state.

**theta**

[float] Angle from z axis.

**phi**

[float] Angle from x axis.

**type**

[string { 'ket', 'bra', 'dm' }, default: 'ket'] Type of state to generate.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**state**

[qobj] Qobj quantum object for spin coherent state

**spin\_state**(*j, m, type='ket', \*, dtype=None*)

Generates the spin state  $|j, m\rangle$ , i.e. the eigenstate of the spin-*j* Sz operator with eigenvalue *m*.

**Parameters**

**j**

[float] The spin of the state ().

**m**

[int] Eigenvalue of the spin-*j* Sz operator.

**type**

[string { 'ket', 'bra', 'dm' }, default: 'ket'] Type of state to generate.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**state**

[qobj] Qobj quantum object for spin state

**state\_index\_number**(*dims, index*)

Return a quantum number representation given a state index, for a system of composite structure defined by *dims*.

**Example**

```
>>> state_index_number([2, 2, 2], 6)
[1, 1, 0]
```

**Parameters**

**dims**

[list or array] The quantum state dimensions array, as it would appear in a Qobj.

**index**

[integer] The index of the state in standard enumeration ordering.

**Returns**

**state**

[tuple] The state number tuple corresponding to index *index* in standard enumeration ordering.



**state\_number\_enumerate**(*dims*, *excitations=None*)

An iterator that enumerates all the state number tuples (quantum numbers of the form (n1, n2, n3, ...)) for a system with dimensions given by *dims*.

### Example

```
>>> for state in state_number_enumerate([2,2]):
>>>     print(state)
( 0  0 )
( 0  1 )
( 1  0 )
( 1  1 )
```

### Parameters

#### **dims**

[list or array] The quantum state dimensions array, as it would appear in a Qobj.

#### **excitations**

[integer, optional] Restrict state space to states with excitation numbers below or equal to this value.

### Returns

#### **state\_number**

[tuple] Successive state number tuples that can be used in loops and other iterations, using standard state enumeration *by definition*.

**state\_number\_index**(*dims*, *state*)

Return the index of a quantum state corresponding to *state*, given a system with dimensions given by *dims*.

### Example

```
>>> state_number_index([2, 2, 2], [1, 1, 0])
6
```

### Parameters

#### **dims**

[list or array] The quantum state dimensions array, as it would appear in a Qobj.

#### **state**

[list] State number array.

### Returns

#### **idx**

[int] The index of the state given by *state* in standard enumeration ordering.

**state\_number\_qobj**(*dims*, *state*, \*, *dtype=None*)

Return a Qobj representation of a quantum state specified by the state array *state*.

---

**Note:** Deprecated in QuTiP 5.0, use *basis* instead.

---

## Example

```
>>> state_number_qobj([2, 2, 2], [1, 0, 1])
Quantum object: dims = [[2, 2, 2], [1, 1, 1]], shape = [8, 1], type = ket
Qobj data =
[[ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 0.]
 [ 1.]
 [ 0.]
 [ 0.]]
```

### Parameters

#### **dims**

[list or array] The quantum state dimensions array, as it would appear in a Qobj.

#### **state**

[list] State number array.

#### **dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

#### **state**

[Qobj] The state as a *Qobj* instance.

**thermal\_dm**(*N*, *n*, *method*='operator', \*, *dtype*=None)

Density matrix for a thermal state of *n* particles

### Parameters

#### **N**

[int] Number of basis states in Hilbert space.

#### **n**

[float] Expectation value for number of particles in thermal state.

#### **method**

[string { 'operator', 'analytic' }, default: 'operator'] string that sets the method used to generate the thermal state probabilities

#### **dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

#### **dm**

[qobj] Thermal state density matrix.

## Notes

The ‘operator’ method (default) generates the thermal state using the truncated number operator `num(N)`. This is the method that should be used in computations. The ‘analytic’ method uses the analytic coefficients derived in an infinite Hilbert space. The analytic form is not necessarily normalized, if truncated too aggressively.

## Examples

```
>>> thermal_dm(5, 1)
Quantum object: dims = [[5], [5]], shape = [5, 5], type = oper, isHerm = True
Qobj data =
[[ 0.51612903  0.          0.          0.          0.          ]
 [ 0.          0.25806452  0.          0.          0.          ]
 [ 0.          0.          0.12903226  0.          0.          ]
 [ 0.          0.          0.          0.06451613  0.          ]
 [ 0.          0.          0.          0.          0.03225806]]
```

```
>>> thermal_dm(5, 1, 'analytic')
Quantum object: dims = [[5], [5]], shape = [5, 5], type = oper, isHerm = True
Qobj data =
[[ 0.5      0.      0.      0.      0.      ]
 [ 0.      0.25    0.      0.      0.      ]
 [ 0.      0.      0.125   0.      0.      ]
 [ 0.      0.      0.      0.0625  0.      ]
 [ 0.      0.      0.      0.      0.03125]]
```

**triplet\_states**(\*, dtype=None)

Returns a list of the two particle triplet-states:

$$|T_1\rangle = |11\rangle|T_2\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)|T_3\rangle = |00\rangle$$

### Parameters

#### dtype

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

#### trip\_states

[list] 2 particle triplet states

**w\_state**(N\_qubit, \*, dtype=None)

Returns the N-qubit W-state:

$$[ |100\dots0\rangle + |010\dots0\rangle + |001\dots0\rangle + \dots |000\dots1\rangle ] / \text{sqrt}(n)$$

### Parameters

#### N\_qubit

[int] Number of qubits in state

#### dtype

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

#### W

[Qobj] N-qubit W-state

**zero\_ket**(*dimensions*, \*, *dtype=None*)

Creates the zero ket vector with shape Nx1 and dimensions *dims*.

**Parameters**

**dimensions**

[int or list of ints, Space] Number of basis states in Hilbert space. If a list, then the resultant object will be a tensor product over spaces with those dimensions.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**zero\_ket**

[qobj] Zero ket on given Hilbert space.

## Quantum Operators

This module contains functions for generating Qobj representation of a variety of commonly occurring quantum operators.

**charge**(*Nmax*, *Nmin=None*, *frac=1*, \*, *dtype=None*)

Generate the diagonal charge operator over charge states from *Nmin* to *Nmax*.

**Parameters**

**Nmax**

[int] Maximum charge state to consider.

**Nmin**

[int, default: -Nmax] Lowest charge state to consider.

**frac**

[float, default: 1] Specify fractional charge if needed.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**C**

[Qobj] Charge operator over [Nmin, Nmax].

## Notes

New in version 3.2.

**commutator**(*A*, *B*, *kind='normal'*)

Return the commutator of kind *kind* (normal, anti) of the two operators *A* and *B*.

**Parameters**

**A, B**

[Qobj, QobjEvo] The operators to compute the commutator of.

**kind: str {"normal", "anti"}, default: "anti"**

Which kind of commutator to compute.

**create**(*N*, *offset=0*, \*, *dtype=None*)

Creation (raising) operator.

**Parameters**

**N**

[int] Number of basis states in the Hilbert space.

**offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the operator.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper**

[qobj] Qobj for raising operator.

## Examples

```
>>> create(4)
Quantum object: dims=[[4], [4]], shape=(4, 4), type='oper', isherm=False
Qobj data =
[[ 0.00000000+0.j  0.00000000+0.j  0.00000000+0.j  0.00000000+0.j]
 [ 1.00000000+0.j  0.00000000+0.j  0.00000000+0.j  0.00000000+0.j]
 [ 0.00000000+0.j  1.41421356+0.j  0.00000000+0.j  0.00000000+0.j]
 [ 0.00000000+0.j  0.00000000+0.j  1.73205081+0.j  0.00000000+0.j]]
```

**destroy**(*N*, *offset*=0, \*, *dtype*=None)

Destruction (lowering) operator.

**Parameters**

**N**

[int] Number of basis states in the Hilbert space.

**offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the operator.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper**

[qobj] Qobj for lowering operator.

## Examples

```
>>> destroy(4)
Quantum object: dims=[[4], [4]], shape=(4, 4), type='oper', isherm=False
Qobj data =
[[ 0.00000000+0.j  1.00000000+0.j  0.00000000+0.j  0.00000000+0.j]
 [ 0.00000000+0.j  0.00000000+0.j  1.41421356+0.j  0.00000000+0.j]
 [ 0.00000000+0.j  0.00000000+0.j  0.00000000+0.j  1.73205081+0.j]
 [ 0.00000000+0.j  0.00000000+0.j  0.00000000+0.j  0.00000000+0.j]]
```

**displace**(*N*, *alpha*, *offset*=0, \*, *dtype*=None)

Single-mode displacement operator.

**Parameters**

**N**

[int] Number of basis states in the Hilbert space.

**alpha**

[float/complex] Displacement amplitude.

**offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the operator.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

## Returns

**oper**

[qobj] Displacement operator.

## Examples

```
>>> displace(4,0.25)
Quantum object: dims = [[4], [4]], shape = [4, 4], type = oper, isHerm = False
Qobj data =
[[ 0.96923323+0.j -0.24230859+0.j 0.04282883+0.j -0.00626025+0.j]
 [ 0.24230859+0.j 0.90866411+0.j -0.33183303+0.j 0.07418172+0.j]
 [ 0.04282883+0.j 0.33183303+0.j 0.84809499+0.j -0.41083747+0.j]
 [ 0.00626025+0.j 0.07418172+0.j 0.41083747+0.j 0.90866411+0.j]]
```

**fcreate**(*n\_sites*, *site*, *dtype=None*)

Fermionic creation operator. We use the Jordan-Wigner transformation, making use of the Jordan-Wigner ZZ..Z strings, to construct this as follows:

$$a_j = \sigma_z^{\otimes j} \otimes \left( \frac{\sigma_x - i\sigma_y}{2} \right) \otimes I^{\otimes N-j-1}$$

## Parameters

**n\_sites**

[int] Number of sites in Fock space.

**site**

[int] The site in Fock space to add a fermion to. Corresponds to *j* in the above JW transform.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

## Returns

**oper**

[qobj] Qobj for raising operator.

## Examples

```
>>> fcreate(2)
Quantum object: dims = [[2, 2], [2, 2]], shape = (4, 4),      type = oper, isherm=False
Qobj data =
[[0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [1. 0. 0. 0.]
 [0. 1. 0. 0.]]
```

**fdestroy**(*n\_sites*, *site*, *dtype=None*)

Fermionic destruction operator. We use the Jordan-Wigner transformation, making use of the Jordan-Wigner ZZ..Z strings, to construct this as follows:

$$a_j = \sigma_z^{\otimes j} \otimes \left( \frac{\sigma_x + i\sigma_y}{2} \right) \otimes I^{\otimes N-j-1}$$

### Parameters

**n\_sites**

[int] Number of sites in Fock space.

**site**

[int, default: 0] The site in Fock space to add a fermion to. Corresponds to *j* in the above JW transform.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

**oper**

[qobj] Qobj for destruction operator.

## Examples

```
>>> fdestroy(2)
Quantum object: dims=[[2 2], [2 2]], shape=(4, 4),      type='oper', isherm=False
Qobj data =
[[0. 0. 1. 0.]
 [0. 0. 0. 1.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]]
```

**identity**(*dimensions*, \*, *dtype=None*)

Identity operator.

### Parameters

**dimensions**

[(int) or (list of int) or (list of list of int), Space] Number of basis states in the Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new Qobj are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

### oper

[qobj] Identity operator Qobj.

### Examples

```
>>> qeye(3)
Quantum object: dims = [[3], [3]], shape = (3, 3), type = oper, isherm = True
Qobj data =
[[ 1.  0.  0.]
 [ 0.  1.  0.]
 [ 0.  0.  1.]]
>>> qeye([2,2])
Quantum object: dims = [[2, 2], [2, 2]], shape = (4, 4), type = oper, isherm = True
Qobj data =
[[1. 0. 0. 0.]
 [0. 1. 0. 0.]
 [0. 0. 1. 0.]
 [0. 0. 0. 1.]]
```

**jmat**(j, which=None, \*, dtype=None)

Higher-order spin operators:

#### Parameters

##### j

[float] Spin of operator

##### which

[str, optional] Which operator to return 'x','y','z','+','-'. If not given, then output is ['x','y','z']

##### dtype

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

#### Returns

##### jmat

[Qobj or tuple of Qobj] qobj for requested spin operator(s).

### Examples

```
>>> jmat(1)
[ Quantum object: dims = [[3], [3]], shape = [3, 3], type = oper, isHerm = True
Qobj data =
[[ 0.          0.70710678  0.          ]
 [ 0.70710678  0.          0.70710678]
 [ 0.          0.70710678  0.          ]]
Quantum object: dims = [[3], [3]], shape = [3, 3], type = oper, isHerm = True
Qobj data =
[[ 0.+0.j          0.-0.70710678j  0.+0.j          ]
 [ 0.+0.70710678j  0.+0.j          0.-0.70710678j]
 [ 0.+0.j          0.+0.70710678j  0.+0.j          ]]
Quantum object: dims = [[3], [3]], shape = [3, 3], type = oper, isHerm = True
Qobj data =
[[ 1.  0.  0.]
```

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```
[ 0.  0.  0.]
[ 0.  0. -1.]]
```

**momentum**(*N*, *offset*=0, \*, *dtype*=None)

Momentum operator  $p = -1j/\sqrt{2}*(a - a.dag())$

#### Parameters

**N**

[int] Number of basis states in the Hilbert space.

**offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the operator.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

#### Returns

**oper**

[qobj] Momentum operator as Qobj.

**num**(*N*, *offset*=0, \*, *dtype*=None)

Quantum object for number operator.

#### Parameters

**N**

[int] Number of basis states in the Hilbert space.

**offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the operator.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

#### Returns

**oper: qobj**

Qobj for number operator.

### Examples

```
>>> num(4)
Quantum object: dims=[[4], [4]], shape=(4, 4), type='oper', isherm=True
Qobj data =
[[0 0 0 0]
 [0 1 0 0]
 [0 0 2 0]
 [0 0 0 3]]
```

**phase**(*N*, *phi0*=0, \*, *dtype*=None)

Single-mode Pegg-Barnett phase operator.

#### Parameters

**N**

[int] Number of basis states in the Hilbert space.

**phi0**

[float, default: 0] Reference phase.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper**

[qobj] Phase operator with respect to reference phase.

**Notes**

The Pegg-Barnett phase operator is Hermitian on a truncated Hilbert space.

**position**(*N*, *offset*=0, \*, *dtype*=None)

Position operator  $x = 1/\sqrt{2} * (a + a.dag())$

**Parameters**

**N**

[int] Number of basis states in the Hilbert space.

**offset**

[int, default: 0] The lowest number state that is included in the finite number state representation of the operator.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper**

[qobj] Position operator as Qobj.

**qdiags**(*diagonals*, *offsets*=None, *dims*=None, *shape*=None, \*, *dtype*=None)

Constructs an operator from an array of diagonals.

**Parameters**

**diagonals**

[sequence of array\_like] Array of elements to place along the selected diagonals.

**offsets**

[sequence of ints, optional]

**Sequence for diagonals to be set:**

- k=0 main diagonal
- k>0 kth upper diagonal
- k<0 kth lower diagonal

**dims**

[list, optional] Dimensions for operator

**shape**

[list, tuple, optional] Shape of operator. If omitted, a square operator large enough to contain the diagonals is generated.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

## Examples

```
>>> qdiags(sqrt(range(1, 4)), 1)
Quantum object: dims = [[4], [4]], shape = [4, 4], type = oper, isherm = False
Qobj data =
[[ 0.      1.      0.      0.      ]
 [ 0.      0.      1.41421356  0.      ]
 [ 0.      0.      0.      1.73205081]
 [ 0.      0.      0.      0.      ]]
```

**qeye**(*dimensions*, \*, *dtype*=None)

Identity operator.

### Parameters

#### **dimensions**

[(int) or (list of int) or (list of list of int), Space] Number of basis states in the Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the *dims* property of the new Qobj are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

#### **dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

### Returns

#### **oper**

[qobj] Identity operator Qobj.

## Examples

```
>>> qeye(3)
Quantum object: dims = [[3], [3]], shape = (3, 3), type = oper, isherm = True
Qobj data =
[[ 1.  0.  0.]
 [ 0.  1.  0.]
 [ 0.  0.  1.]]
>>> qeye([2,2])
Quantum object: dims = [[2, 2], [2, 2]], shape = (4, 4), type = oper, isherm = True
Qobj data =
[[1. 0. 0. 0.]
 [0. 1. 0. 0.]
 [0. 0. 1. 0.]
 [0. 0. 0. 1.]]
```

**qeye\_like**(*qobj*)

Identity operator with the same dims and type as the reference quantum object.

### Parameters

#### **qobj**

[Qobj, QobjEvo] Reference quantum object to copy the dims from.

### Returns

#### **oper**

[qobj] Identity operator Qobj.

**qutrit\_ops**(\*, dtype=None)

Operators for a three level system (qutrit).

**Parameters**

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**opers:** array

array of qutrit operators.

**qzero**(dimensions, dims\_right=None, \*, dtype=None)

Zero operator.

**Parameters**

**dimensions**

[int, list of int, list of list of int, Space] Number of basis states in the Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new Qobj are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

**dims\_right**

[int, list of int, list of list of int, Space, optional] Number of basis states in the right Hilbert space when the operator is rectangular.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**qzero**

[qobj] Zero operator Qobj.

**qzero\_like**(qobj)

Zero operator of the same dims and type as the reference.

**Parameters**

**qobj**

[Qobj, QobjEvo] Reference quantum object to copy the dims from.

**Returns**

**qzero**

[qobj] Zero operator Qobj.

**sigmam**()

Annihilation operator for Pauli spins.

## Examples

```
>>> sigmam()
Quantum object: dims = [[2], [2]], shape = [2, 2], type = oper, isHerm = False
Qobj data =
[[ 0.  0.]
 [ 1.  0.]]
```

**sigmap**()

Creation operator for Pauli spins.

### Examples

```
>>> sigmap()
Quantum object: dims = [[2], [2]], shape = [2, 2], type = oper, isHerm = False
Qobj data =
[[ 0.  1.]
 [ 0.  0.]]
```

#### **sigmax()**

Pauli spin 1/2 sigma-x operator

### Examples

```
>>> sigmax()
Quantum object: dims = [[2], [2]], shape = [2, 2], type = oper, isHerm = False
Qobj data =
[[ 0.  1.]
 [ 1.  0.]]
```

#### **sigmay()**

Pauli spin 1/2 sigma-y operator.

### Examples

```
>>> sigmay()
Quantum object: dims = [[2], [2]], shape = [2, 2], type = oper, isHerm = True
Qobj data =
[[ 0.+0.j  0.-1.j]
 [ 0.+1.j  0.+0.j]]
```

#### **sigmaz()**

Pauli spin 1/2 sigma-z operator.

### Examples

```
>>> sigmaz()
Quantum object: dims = [[2], [2]], shape = [2, 2], type = oper, isHerm = True
Qobj data =
[[ 1.  0.]
 [ 0. -1.]]
```

#### **spin\_Jm(j, \*, dtype=None)**

Spin-j annihilation operator

##### **Parameters**

**j**

[float] Spin of operator

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

##### **Returns**

**op**

[Qobj] qobj representation of the operator.

**spin\_Jp**(*j*, \*, *dtype=None*)

Spin-j creation operator

**Parameters**

**j**

[float] Spin of operator

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**op**

[Qobj] qobj representation of the operator.

**spin\_Jx**(*j*, \*, *dtype=None*)

Spin-j x operator

**Parameters**

**j**

[float] Spin of operator

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**op**

[Qobj] qobj representation of the operator.

**spin\_Jy**(*j*, \*, *dtype=None*)

Spin-j y operator

**Parameters**

**j**

[float] Spin of operator

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**op**

[Qobj] qobj representation of the operator.

**spin\_Jz**(*j*, \*, *dtype=None*)

Spin-j z operator

**Parameters**

**j**

[float] Spin of operator

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**op**  
[Qobj] qobj representation of the operator.

**squeeze**(*N*, *z*, *offset*=0, \*, *dtype*=None)

Single-mode squeezing operator.

#### Parameters

**N**  
[int] Dimension of hilbert space.

**z**  
[float/complex] Squeezing parameter.

**offset**  
[int, default: 0] The lowest number state that is included in the finite number state representation of the operator.

**dtype**  
[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

#### Returns

**oper**  
[Qobj] Squeezing operator.

### Examples

```
>>> squeeze(4, 0.25)
Quantum object: dims = [[4], [4]], shape = [4, 4], type = oper, isHerm = False
Qobj data =
[[ 0.98441565+0.j  0.00000000+0.j  0.17585742+0.j  0.00000000+0.j]
 [ 0.00000000+0.j  0.95349007+0.j  0.00000000+0.j  0.30142443+0.j]
 [-0.17585742+0.j  0.00000000+0.j  0.98441565+0.j  0.00000000+0.j]
 [ 0.00000000+0.j -0.30142443+0.j  0.00000000+0.j  0.95349007+0.j]]
```

**squeezing**(*a1*, *a2*, *z*)

Generalized squeezing operator.

$$S(z) = \exp\left(\frac{1}{2}\left(z^* a_1 a_2 - z a_1^\dagger a_2^\dagger\right)\right)$$

#### Parameters

**a1**  
[Qobj] Operator 1.

**a2**  
[Qobj] Operator 2.

**z**  
[float/complex] Squeezing parameter.

#### Returns

**oper**  
[Qobj] Squeezing operator.

**tunneling**(*N*, *m*=1, \*, *dtype*=None)

Tunneling operator with elements of the form  
 $\sum |N\rangle\langle N+m| + |N+m\rangle\langle N|$ .

#### Parameters

**N**

[int] Number of basis states in the Hilbert space.

**m**

[int, default: 1] Number of excitations in tunneling event.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**T**

[Qobj] Tunneling operator.

## Energy Restricted Operators

**enr\_destroy**(*dims*, *excitations*, \*, *dtype=None*)

Generate annihilation operators for modes in a excitation-number-restricted state space. For example, consider a system consisting of 4 modes, each with 5 states. The total hilbert space size is  $5^{**}4 = 625$ . If we are only interested in states that contain up to 2 excitations, we only need to include states such as

(0, 0, 0, 0) (0, 0, 0, 1) (0, 0, 0, 2) (0, 0, 1, 0) (0, 0, 1, 1) (0, 0, 2, 0) ...

This function creates annihilation operators for the 4 modes that act within this state space:

`a1, a2, a3, a4 = enr_destroy([5, 5, 5, 5], excitations=2)`

From this point onwards, the annihilation operators `a1`, ..., `a4` can be used to setup a Hamiltonian, collapse operators and expectation-value operators, etc., following the usual pattern.

**Parameters**

**dims**

[list] A list of the dimensions of each subsystem of a composite quantum system.

**excitations**

[integer] The maximum number of excitations that are to be included in the state space.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**a\_ops**

[list of qobj] A list of annihilation operators for each mode in the composite quantum system described by `dims`.

**enr\_fock**(*dims*, *excitations*, *state*, \*, *dtype=None*)

Generate the Fock state representation in a excitation-number restricted state space. The *dims* argument is a list of integers that define the number of quantum states of each component of a composite quantum system, and the *excitations* specifies the maximum number of excitations for the basis states that are to be included in the state space. The *state* argument is a tuple of integers that specifies the state (in the number basis representation) for which to generate the Fock state representation.

**Parameters**

**dims**

[list] A list of the dimensions of each subsystem of a composite quantum system.

**excitations**

[integer] The maximum number of excitations that are to be included in the state space.

**state**

[list of integers] The state in the number basis representation.



**dtype**

[type or str, optional] Storage representation. Any data-layer known to *qutip.data.to* is accepted.

**Returns**

**ket**

[Qobj] A Qobj instance that represent a Fock state in the excitation-number- restricted state space defined by *dims* and *excitations*.

**enr\_identity**(*dims*, *excitations*, \*, *dtype=None*)

Generate the identity operator for the excitation-number restricted state space defined by the *dims* and *excitations* arguments. See the docstring for *enr\_fock* for a more detailed description of these arguments.

**Parameters**

**dims**

[list] A list of the dimensions of each subsystem of a composite quantum system.

**excitations**

[integer] The maximum number of excitations that are to be included in the state space.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to *qutip.data.to* is accepted.

**Returns**

**op**

[Qobj] A Qobj instance that represent the identity operator in the excitation-number- restricted state space defined by *dims* and *excitations*.

**enr\_state\_dictionaries**(*dims*, *excitations*)

Return the number of states, and lookup-dictionaries for translating a state tuple to a state index, and vice versa, for a system with a given number of components and maximum number of excitations.

**Parameters**

**dims: list**

A list with the number of states in each sub-system.

**excitations**

[integer] The maximum numbers of dimension

**Returns**

**nstates, state2idx, idx2state: integer, dict, dict**

The number of states *nstates*, a dictionary for looking up state indices from a state tuple, and a dictionary for looking up state state tuples from state indices. *state2idx* and *idx2state* are reverses of each other, i.e., *state2idx[idx2state[idx]] = idx* and *idx2state[state2idx[state]] = state*.

**enr\_thermal\_dm**(*dims*, *excitations*, *n*, \*, *dtype=None*)

Generate the density operator for a thermal state in the excitation-number- restricted state space defined by the *dims* and *excitations* arguments. See the documentation for *enr\_fock* for a more detailed description of these arguments. The temperature of each mode in *dims* is specified by the average number of excitatons *n*.

**Parameters**

**dims**

[list] A list of the dimensions of each subsystem of a composite quantum system.

**excitations**

[integer] The maximum number of excitations that are to be included in the state space.

**n**

[integer] The average number of exciations in the thermal state. *n* can be a float (which

then applies to each mode), or a list/array of the same length as `dims`, in which each element corresponds specifies the temperature of the corresponding mode.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to *qutip.data.to* is accepted.

**Returns**

**dm**

[Qobj] Thermal state density matrix.

## Quantum Objects

The Quantum Object (Qobj) class, for representing quantum states and operators, and related functions.

**ptrace(*Q*, *sel*)**

Partial trace of the Qobj with selected components remaining.

**Parameters**

**Q**

[Qobj] Composite quantum object.

**sel**

[int/list] An int or list of components to keep after partial trace.

**Returns**

**oper**

[Qobj] Quantum object representing partial trace with selected components remaining.

## Notes

This function is for legacy compatibility only. It is recommended to use the `ptrace()` Qobj method.

## Random Operators and States

This module is a collection of random state and operator generators.

**rand\_dm(*dimensions*, *density*=0.75, *distribution*='ginibre', \*, *eigenvalues*=(), *rank*=None, *seed*=None, *dtype*=None)**

Creates a random density matrix of the desired dimensions.

**Parameters**

**dimensions**

[(int) or (list of int) or (list of list of int)]

Dimension of Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new Qobj are set to this list. This can produce either `oper` or `super` depending on the passed `dimensions`.

**density**

[float, default: 0.75] Density between [0,1] of output density matrix. Used by the “pure”, “eigen” and “herm”.

`distribution` : str {“ginibre”, “hs”, “pure”, “eigen”, “uniform”},

**default: “ginibre”**

Method used to obtain the density matrices.

- “ginibre” : Ginibre random density operator of rank `rank` by using the algorithm of [BCSZ08].
- “hs” : Hilbert-Schmidt ensemble, equivalent to a full rank ginibre operator.
- “pure” : Density matrix created from a random ket.
- “eigen” : A density matrix with the given `eigenvalues`.
- “herm” : Build from a random hermitian matrix using `rand_herm`.

#### **eigenvalues**

[array\_like, optional] Eigenvalues of the output Hermitian matrix. The len must match the shape of the matrix.

#### **rank**

[int, optional] When using the “ginibre” distribution, rank of the density matrix. Will default to a full rank operator when not provided.

#### **seed**

[int, SeedSequence, Generator, optional] Seed to create the random number generator or a pre prepared generator. When none is supplied, a default generator is used.

#### **dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data` to is accepted.

### **Returns**

#### **oper**

[qobj] Density matrix quantum operator.

**rand\_herm**(*dimensions*, *density*=0.3, *distribution*='fill', \*, *eigenvalues*=(), *seed*=None, *dtype*=None)

Creates a random sparse Hermitian quantum object.

### **Parameters**

#### **dimensions**

[(int) or (list of int) or (list of list of int)] Dimension of Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new Qobj are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

#### **density**

[float, default: 0.30] Density between [0,1] of output Hermitian operator.

#### **distribution**

[str {“fill”, “pos\_def”, “eigen”}, default: “fill”] Method used to obtain the density matrices.

- “fill” : Uses  $H = 0.5 * (X + X^+)$  where  $X$  is a randomly generated quantum operator with elements uniformly distributed between  $[-1, 1] + [-1j, 1j]$ .
- “eigen” : A density matrix with the given `eigenvalues`. It uses random complex Jacobi rotations to shuffle the operator.
- “pos\_def” : Return a positive semi-definite matrix by diagonal dominance.

#### **eigenvalues**

[array\_like, optional] Eigenvalues of the output Hermitian matrix. The len must match the shape of the matrix.

#### **seed**

[int, SeedSequence, Generator, optional] Seed to create the random number generator or a pre prepared generator. When none is supplied, a default generator is used.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper**

[*Qobj*] Hermitian quantum operator.

**Notes**

If given a list of eigenvalues the object is created using complex Jacobi rotations. While this method is fast for small matrices, it should not be repeatedly used for generating matrices larger than ~1000x1000.

**rand\_ket**(*dimensions*, *density*=1, *distribution*='haar', \*, *seed*=None, *dtype*=None)

Creates a random ket vector.

**Parameters**

**dimensions**

[(int) or (list of int) or (list of list of int)] Dimension of Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new *Qobj* are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

**density**

[float, default: 1] Density between [0,1] of output ket state when using the `fill` method.

**distribution**

[str {"haar", "fill"}, default: "haar"] Method used to obtain the kets.

- haar : Haar random pure state obtained by applying a Haar random unitary to a fixed pure state.
- fill : Fill the ket with uniformly distributed random complex number.

**seed**

[int, SeedSequence, Generator, optional] Seed to create the random number generator or a pre prepared generator. When none is supplied, a default generator is used.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper**

[*qobj*] Ket quantum state vector.

**rand\_kraus\_map**(*dimensions*, \*, *seed*=None, *dtype*=None)

Creates a random CPTP map on an N-dimensional Hilbert space in Kraus form.

**Parameters**

**dimensions**

[(int) or (list of int) or (list of list of int)] Dimension of Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new *Qobj* are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

**seed**

[int, SeedSequence, Generator, optional] Seed to create the random number generator or a pre prepared generator. When none is supplied, a default generator is used.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper\_list**

[list of qobj]  $N^2 \times N \times N$  qobj operators.

**rand\_stochastic**(*dimensions*, *density*=0.75, *kind*='left', \*, *seed*=None, *dtype*=None)

Generates a random stochastic matrix.

**Parameters**

**dimensions**

[(int) or (list of int) or (list of list of int)] Dimension of Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new Qobj are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

**density**

[float, default: 0.75] Density between [0,1] of output density matrix.

**kind**

[str {"left", "right"}, default: "left"] Generate 'left' or 'right' stochastic matrix.

**seed**

[int, SeedSequence, Generator, optional] Seed to create the random number generator or a pre prepared generator. When none is supplied, a default generator is used.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper**

[qobj] Quantum operator form of stochastic matrix.

**rand\_super**(*dimensions*, \*, *superrep*='super', *seed*=None, *dtype*=None)

Returns a randomly drawn superoperator acting on operators acting on  $N$  dimensions.

**Parameters**

**dimensions**

[(int) or (list of int) or (list of list of int)] Dimension of Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new Qobj are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

**superrep**

[str, default: "super"] Representation of the super operator

**seed**

[int, SeedSequence, Generator, optional] Seed to create the random number generator or a pre prepared generator. When none is supplied, a default generator is used.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**rand\_super\_bcsz**(*dimensions*, *enforce\_tp*=True, *rank*=None, \*, *superrep*='super', *seed*=None, *dtype*=None)

Returns a random superoperator drawn from the Bruzda et al ensemble for CPTP maps [BCSZ08]. Note that due to finite numerical precision, for ranks less than full-rank, zero eigenvalues may become slightly negative, such that the returned operator is not actually completely positive.

**Parameters**

**dimensions**

[(int) or (list of int) or (list of list of int)] Dimension of Hilbert space. If an int is provided, it is understood as the Square root of the dimension of the superoperator to be returned, with the corresponding dims as  $[[[N], [N]], [[N], [N]]]$ . If provided as a list of ints, then the dimensions is understood as the space of density matrices this superoperator is applied to: `dimensions=[2,2] dims=[[2,2],[2,2]], [[2,2],[2,2]]`.

**enforce\_tp**

[bool, default: True] If True, the trace-preserving condition of [BCSZ08] is enforced; otherwise only complete positivity is enforced.

**rank**

[int, optional] Rank of the sampled superoperator. If None, a full-rank superoperator is generated.

**seed**

[int, SeedSequence, Generator, optional] Seed to create the random number generator or a pre prepared generator. When none is supplied, a default generator is used.

**superrop**

[str, default: “super”] representation of the

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**rho**

[Qobj] A superoperator acting on vectorized  $\text{dim} \times \text{dim}$  density operators, sampled from the BCSZ distribution.

**rand\_unitary**(*dimensions, density=1, distribution='haar', \*, seed=None, dtype=None*)

Creates a random sparse unitary quantum object.

**Parameters**

**dimensions**

[(int) or (list of int) or (list of list of int)] Dimension of Hilbert space. If provided as a list of ints, then the dimension is the product over this list, but the `dims` property of the new Qobj are set to this list. This can produce either *oper* or *super* depending on the passed *dimensions*.

**density**

[float, default: 1] Density between [0,1] of output unitary operator.

**distribution**

[str {“haar”, “exp”}, default: “haar”] Method used to obtain the unitary matrices.

- haar : Haar random unitary matrix using the algorithm of [Mez07].
- exp : Uses  $\exp(-iH)$ , where H is a randomly generated Hermitian operator.

**seed**

[int, SeedSequence, Generator, optional] Seed to create the random number generator or a pre prepared generator. When none is supplied, a default generator is used.

**dtype**

[type or str, optional] Storage representation. Any data-layer known to `qutip.data.to` is accepted.

**Returns**

**oper**

[qobj] Unitary quantum operator.

## Superoperators and Liouvillians

**lindblad\_dissipator**(*a*, *b=None*, *data\_only=False*, *chi=None*)

Lindblad dissipator (generalized) for a single pair of collapse operators (*a*, *b*), or for a single collapse operator (*a*) when *b* is not specified:

$$\mathcal{D}[a, b]\rho = a\rho b^\dagger - \frac{1}{2}a^\dagger b\rho - \frac{1}{2}\rho a^\dagger b$$

### Parameters

**a**

[Qobj or QobjEvo] Left part of collapse operator.

**b**

[Qobj or QobjEvo, optional] Right part of collapse operator. If not specified, *b* defaults to *a*.

**chi**

[float, optional] In some systems it is possible to determine the statistical moments (mean, variance, etc) of the probability distribution of the occupation numbers of states by numerically evaluating the derivatives of the steady state occupation probability as a function of an artificial phase parameter *chi* which multiplies the  $a^\dagger$  term of the dissipator by  $e^{i\chi}$ . The factor  $e^{i\chi}$  is introduced via the generating function of the statistical moments. For examples of the technique, see [Full counting statistics of nano-electromechanical systems](#) and [Photon-mediated electron transport in hybrid circuit-QED](#). This parameter is deprecated and may be removed in QuTiP 5.

**data\_only**

[bool, default: False] Return the data object instead of a Qobj

### Returns

**D**

[qobj, QobjEvo] Lindblad dissipator superoperator.

**liouvillian**(*H=None*, *c\_ops=None*, *data\_only=False*, *chi=None*)

Assembles the Liouvillian superoperator from a Hamiltonian and a list of collapse operators.

### Parameters

**H**

[Qobj or QobjEvo, optional] System Hamiltonian or Hamiltonian component of a Liouvillian. Considered 0 if not given.

**c\_ops**

[array\_like of Qobj or QobjEvo, optional] A list or array of collapse operators.

**data\_only**

[bool, default: False] Return the data object instead of a Qobj

**chi**

[array\_like of float, optional] In some systems it is possible to determine the statistical moments (mean, variance, etc) of the probability distributions of occupation of various states by numerically evaluating the derivatives of the steady state occupation probability as a function of artificial phase parameters *chi* which are included in the [lindblad\\_dissipator](#) for each collapse operator. See the documentation of [lindblad\\_dissipator](#) for references and further details. This parameter is deprecated and may be removed in QuTiP 5.

### Returns

**L**

[Qobj or QobjEvo] Liouvillian superoperator.

### **operator\_to\_vector(*op*)**

Create a vector representation given a quantum operator in matrix form. The passed object should have a `Qobj.type` of 'oper' or 'super'; this function is not designed for general-purpose matrix reshaping.

#### **Parameters**

**op**  
[Qobj or QobjEvo] Quantum operator in matrix form. This must have a type of 'oper' or 'super'.

#### **Returns**

##### **Qobj or QobjEvo**

The same object, but re-cast into a column-stacked-vector form of type 'operator-ket'. The output is the same type as the passed object.

### **spost(*A*)**

Superoperator formed from post-multiplication by operator *A*

#### **Parameters**

**A**  
[Qobj or QobjEvo] Quantum operator for post multiplication.

#### **Returns**

**super**  
[Qobj or QobjEvo] Superoperator formed from input quantum object.

### **spre(*A*)**

Superoperator formed from pre-multiplication by operator *A*.

#### **Parameters**

**A**  
[Qobj or QobjEvo] Quantum operator for pre-multiplication.

#### **Returns**

**super :Qobj or QobjEvo**  
Superoperator formed from input quantum object.

### **sprepost(*A*, *B*)**

Superoperator formed from pre-multiplication by *A* and post-multiplication by *B*.

#### **Parameters**

**A**  
[Qobj or QobjEvo] Quantum operator for pre-multiplication.

**B**  
[Qobj or QobjEvo] Quantum operator for post-multiplication.

#### **Returns**

**super**  
[Qobj or QobjEvo] Superoperator formed from input quantum objects.

### **vector\_to\_operator(*op*)**

Create a matrix representation given a quantum operator in vector form. The passed object should have a `Qobj.type` of 'operator-ket'; this function is not designed for general-purpose matrix reshaping.

#### **Parameters**

**op**  
[Qobj or QobjEvo] Quantum operator in column-stacked-vector form. This must have a type of 'operator-ket'.

#### **Returns**



### Qobj or QobjEvo

The same object, but re-cast into “standard” operator form. The output is the same type as the passed object.

## Superoperator Representations

This module implements transformations between superoperator representations, including supermatrix, Kraus, Choi and Chi (process) matrix formalisms.

### **kraus\_to\_choi**(*kraus\_ops*)

Convert a list of Kraus operators into Choi representation of the channel.

Essentially, kraus operators are a decomposition of a Choi matrix, and its reconstruction from them should go as  $E = \sum_i |K_i\rangle\rangle\langle\langle K_i|$ , where we use vector representation of Kraus operators.

#### Parameters

##### **kraus\_ops**

[list[Qobj]] The list of Kraus operators to be converted to Choi representation.

#### Returns

##### **choi**

[Qobj] A quantum object representing the same map as *kraus\_ops*, such that *choi*.  
superrep == "choi".

### **kraus\_to\_super**(*kraus\_list*)

Convert a list of Kraus operators to a superoperator.

#### Parameters

##### **kraus\_list**

[list of Qobj] The list of Kraus super operators to convert.

### **to\_chi**(*q\_oper*)

Converts a Qobj representing a quantum map to a representation as a chi (process) matrix in the Pauli basis, such that the trace of the returned operator is equal to the dimension of the system.

#### Parameters

##### **q\_oper**

[Qobj] Superoperator to be converted to Chi representation. If *q\_oper* is type="oper", then it is taken to act by conjugation, such that *to\_chi*(A) == *to\_chi*(sprepost(A, A.dag())).

#### Returns

##### **chi**

[Qobj] A quantum object representing the same map as *q\_oper*, such that *chi*.  
superrep == "chi".

#### Raises

##### **TypeError:**

If the given quantum object is not a map, or cannot be converted to Chi representation.

### **to\_choi**(*q\_oper*)

Converts a Qobj representing a quantum map to the Choi representation, such that the trace of the returned operator is equal to the dimension of the system.

#### Parameters

##### **q\_oper**

[Qobj] Superoperator to be converted to Choi representation. If *q\_oper* is type="oper", then it is taken to act by conjugation, such that *to\_choi*(A) == *to\_choi*(sprepost(A, A.dag())).

### Returns

#### choi

[Qobj] A quantum object representing the same map as `q_oper`, such that `choi.superrep == "choi"`.

### Raises

#### TypeError:

If the given quantum object is not a map, or cannot be converted to Choi representation.

**to\_kraus**(*q\_oper*, *tol*=1e-09)

Converts a Qobj representing a quantum map to a list of quantum objects, each representing an operator in the Kraus decomposition of the given map.

### Parameters

#### q\_oper

[Qobj] Superoperator to be converted to Kraus representation. If `q_oper` is `type="oper"`, then it is taken to act by conjugation, such that `to_kraus(A) == to_kraus(sprepost(A, A.dag())) == [A]`.

#### tol

[Float, default: 1e-9] Optional threshold parameter for eigenvalues/Kraus ops to be discarded.

### Returns

#### kraus\_ops

[list of Qobj] A list of quantum objects, each representing a Kraus operator in the decomposition of `q_oper`.

### Raises

**TypeError: if the given quantum object is not a map, or cannot be decomposed into Kraus operators.**

**to\_stinespring**(*q\_oper*, *threshold*=1e-10)

Converts a Qobj representing a quantum map  $\Lambda$  to a pair of partial isometries  $A$  and  $B$  such that  $\Lambda(X) = \text{Tr}_2(AXB^\dagger)$  for all inputs  $X$ , where the partial trace is taken over a new index on the output dimensions of  $A$  and  $B$ .

For completely positive inputs,  $A$  will always equal  $B$  up to precision errors.

### Parameters

#### q\_oper

[Qobj] Superoperator to be converted to a Stinespring pair.

#### threshold

[float, default: 1e-10] Threshold parameter for eigenvalues/Kraus ops to be discarded.

### Returns

#### A, B

[Qobj] Quantum objects representing each of the Stinespring matrices for the input Qobj.

**to\_super**(*q\_oper*)

Converts a Qobj representing a quantum map to the supermatrix (Liouville) representation.

### Parameters

#### q\_oper

[Qobj] Superoperator to be converted to supermatrix representation. If `q_oper` is `type="oper"`, then it is taken to act by conjugation, such that `to_super(A) == sprepost(A, A.dag())`.

### Returns

### **superop**

[Qobj] A quantum object representing the same map as `q_oper`, such that `superop.superrep == "super"`.

### **Raises**

#### **TypeError**

If the given quantum object is not a map, or cannot be converted to supermatrix representation.

## **Operators and Superoperator Dimensions**

Internal use module for manipulating dims specifications.

**from\_tensor\_rep**(*tensorrep, dims*)

Reverse operator of [to\\_tensor\\_rep](#). Create a Qobj From a N-dimensions numpy array and dimensions with N indices.

### **Parameters**

**tensorrep: ndarray**

Numpy array with one dimension for each index in dims.

**dims: list of list, Dimensions**

Dimensions of the Qobj.

### **Returns**

**Qobj**

Re constructed Qobj

**to\_tensor\_rep**(*q\_oper*)

Transform a Qobj to a numpy array whose shape is the flattened dimensions.

### **Parameters**

**q\_oper: Qobj**

Object to reshape

### **Returns**

**ndarray:**

Numpy array with one dimension for each index in dims.

## **Examples**

```
>>> ket.dims
[[2, 3], [1]]
>>> to_tensor_rep(ket).shape
(2, 3, 1)
```

```
>>> oper.dims
[[2, 3], [2, 3]]
>>> to_tensor_rep(oper).shape
(2, 3, 2, 3)
```

```
>>> super_oper.dims
[[[2, 3], [2, 3]], [[2, 3], [2, 3]]]
>>> to_tensor_rep(super_oper).shape
(2, 3, 2, 3, 2, 3, 2, 3)
```

## 5.2.2 Functions acting on states and operators

### Expectation Values

**expect**(*oper*, *state*)

Calculate the expectation value for operator(s) and state(s). The expectation of state *k* on operator *A* is defined as  $\text{k.dag}() @ A @ \text{k}$ , and for density matrix *R* on operator *A* it is  $\text{trace}(A @ R)$ .

#### Parameters

**oper**

[qobj/array-like] A single or a *list* of operators for expectation value.

**state**

[qobj/array-like] A single or a *list* of quantum states or density matrices.

#### Returns

**expt**

[float/complex/array-like] Expectation value. *real* if *oper* is Hermitian, *complex* otherwise. A (nested) array of expectation values if *state* or *oper* are arrays.

### Examples

```
>>> expect(num(4), basis(4, 3)) == 3
True
```

**variance**(*oper*, *state*)

Variance of an operator for the given state vector or density matrix.

#### Parameters

**oper**

[qobj] Operator for expectation value.

**state**

[qobj/list] A single or *list* of quantum states or density matrices..

#### Returns

**var**

[float] Variance of operator ‘oper’ for given state.

### Tensor

Module for the creation of composite quantum objects via the tensor product.

**composite**(\*args)

Given two or more operators, kets or bras, returns the Qobj corresponding to a composite system over each argument. For ordinary operators and vectors, this is the tensor product, while for superoperators and vectorized operators, this is the column-reshuffled tensor product.

If a mix of Qobjs supported on Hilbert and Liouville spaces are passed in, the former are promoted. Ordinary operators are assumed to be unitaries, and are promoted using `to_super`, while kets and bras are promoted by taking their projectors and using `operator_to_vector(ket2dm(arg))`.

**super\_tensor**(\*args)

Calculate the tensor product of input superoperators, by tensoring together the underlying Hilbert spaces on which each vectorized operator acts.

#### Parameters

**args**

[array\_like] list or array of quantum objects with type="super".

**Returns**

**obj**

[qobj] A composite quantum object.

**tensor(\*args)**

Calculates the tensor product of input operators.

**Parameters**

**args**

[array\_like] list or array of quantum objects for tensor product.

**Returns**

**obj**

[qobj] A composite quantum object.

## Examples

```
>>> tensor([sigmax(), sigmax()])
Quantum object: dims = [[2, 2], [2, 2]], shape = [4, 4], type = oper, isHerm = True
Qobj data =
[[ 0.+0.j  0.+0.j  0.+0.j  1.+0.j]
 [ 0.+0.j  0.+0.j  1.+0.j  0.+0.j]
 [ 0.+0.j  1.+0.j  0.+0.j  0.+0.j]
 [ 1.+0.j  0.+0.j  0.+0.j  0.+0.j]]
```

**tensor\_contract(qobj, \*pairs)**

Contracts a qobj along one or more index pairs. Note that this uses dense representations and thus should *not* be used for very large Qobjs.

**Parameters**

**qobj: Qobj**

Operator to contract subspaces on.

**pairs**

[tuple] One or more tuples (i, j) indicating that the i and j dimensions of the original qobj should be contracted.

**Returns**

**cqobj**

[Qobj] The original Qobj with all named index pairs contracted away.

## Partial Transpose

**partial\_transpose(rho, mask, method='dense')**

Return the partial transpose of a Qobj instance *rho*, where *mask* is an array/list with length that equals the number of components of *rho* (that is, the length of *rho.dims[0]*), and the values in *mask* indicates whether or not the corresponding subsystem is to be transposed. The elements in *mask* can be boolean or integers 0 or 1, where *True/1* indicates that the corresponding subsystem should be transposed.

**Parameters**

**rho**

[Qobj] A density matrix.

**mask**

[list / array] A mask that selects which subsystems should be transposed.

**method**

[str {"dense", "sparse"}, default: "dense"] Choice of method. The "sparse" implementation can be faster for large and sparse systems (hundreds of quantum states).

**Returns**

**rho\_pr:** *Qobj*

A density matrix with the selected subsystems transposed.

## Entropy Functions

### **concurrence**(rho)

Calculate the concurrence entanglement measure for a two-qubit state.

**Parameters**

**state**

[qobj] Ket, bra, or density matrix for a two-qubit state.

**Returns**

**concur**

[float] Concurrence

## References

[1]

### **entropy\_conditional**(rho, selB, base=2.718281828459045, sparse=False)

Calculates the conditional entropy  $S(A|B) = S(A, B) - S(B)$  of a selected density matrix component.

**Parameters**

**rho**

[qobj] Density matrix of composite object

**selB**

[int/list] Selected components for density matrix B

**base**

[{e, 2}, default: e] Base of logarithm.

**sparse**

[bool, default: False] Use sparse eigensolver.

**Returns**

**ent\_cond**

[float] Value of conditional entropy

### **entropy\_linear**(rho)

Linear entropy of a density matrix.

**Parameters**

**rho**

[qobj] density matrix or ket/bra vector.

**Returns**

**entropy**

[float] Linear entropy of rho.

## Examples

```
>>> rho=0.5*fock_dm(2,0)+0.5*fock_dm(2,1)
>>> entropy_linear(rho)
0.5
```

**entropy\_mutual**(rho, selA, selB, base=2.718281828459045, sparse=False)

Calculates the mutual information  $S(A:B)$  between selection components of a system density matrix.

### Parameters

**rho**

[qobj] Density matrix for composite quantum systems

**selA**

[int/list] *int* or *list* of first selected density matrix components.

**selB**

[int/list] *int* or *list* of second selected density matrix components.

**base**

[{e, 2}, default: e] Base of logarithm.

**sparse**

[bool, default: False] Use sparse eigensolver.

### Returns

**ent\_mut**

[float] Mutual information between selected components.

**entropy\_relative**(rho, sigma, base=2.718281828459045, sparse=False, tol=1e-12)

Calculates the relative entropy  $S(\rho||\sigma)$  between two density matrices.

### Parameters

**rho**

[Qobj] First density matrix (or ket which will be converted to a density matrix).

**sigma**

[Qobj] Second density matrix (or ket which will be converted to a density matrix).

**base**

[{e, 2}, default: e] Base of logarithm. Defaults to e.

**sparse**

[bool, default: False] Flag to use sparse solver when determining the eigenvectors of the density matrices. Defaults to False.

**tol**

[float, default: 1e-12] Tolerance to use to detect 0 eigenvalues or dot product between eigenvectors. Defaults to 1e-12.

### Returns

**rel\_ent**

[float] Value of relative entropy. Guaranteed to be greater than zero and should equal zero only when rho and sigma are identical.

## References

See Nielsen & Chuang, “Quantum Computation and Quantum Information”, Section 11.3.1, pg. 511 for a detailed explanation of quantum relative entropy.

## Examples

First we define two density matrices:

```
>>> rho = qutip.ket2dm(qutip.ket("00"))
>>> sigma = rho + qutip.ket2dm(qutip.ket("01"))
>>> sigma = sigma.unit()
```

Then we calculate their relative entropy using base 2 (i.e.  $\log_2$ ) and base e (i.e.  $\log$ ).

```
>>> qutip.entropy_relative(rho, sigma, base=2)
1.0
>>> qutip.entropy_relative(rho, sigma)
0.6931471805599453
```

**entropy\_vn**(rho, base=2.718281828459045, sparse=False)

Von-Neumann entropy of density matrix

### Parameters

- rho**  
[qobj] Density matrix.
- base**  
[ $\{e, 2\}$ , default: e] Base of logarithm.
- sparse**  
[bool, default: False] Use sparse eigensolver.

### Returns

- entropy**  
[float] Von-Neumann entropy of *rho*.

## Examples

```
>>> rho=0.5*fock_dm(2,0)+0.5*fock_dm(2,1)
>>> entropy_vn(rho,2)
1.0
```

## Density Matrix Metrics

This module contains a collection of functions for calculating metrics (distance measures) between states and operators.

**average\_gate\_fidelity**(oper, target=None)

Returns the average gate fidelity of a quantum channel to the target channel, or to the identity channel if no target is given.

### Parameters

- oper**  
[Qobj/list] A unitary operator, or a superoperator in supermatrix, Choi or chi-matrix form, or a list of Kraus operators



**target**

[*Qobj*] A unitary operator

**Returns**

**fid**

[float] Average gate fidelity between oper and target, or between oper and identity.

## Notes

The average gate fidelity is defined for example in: A. Gilchrist, N.K. Langford, M.A. Nielsen, Phys. Rev. A 71, 062310 (2005). The definition of state fidelity that the average gate fidelity is based on is the one from R. Jozsa, Journal of Modern Optics, 41:12, 2315 (1994). It is the square of the fidelity implemented in [qutip.core.metrics.fidelity](#) which follows Nielsen & Chuang, “Quantum Computation and Quantum Information”

**buress\_angle**(*A*, *B*)

Returns the Bures Angle between two density matrices *A* & *B*.

The Bures angle ranges from 0, for states with unit fidelity, to  $\pi/2$ .

**Parameters**

**A**

[*qobj*] Density matrix or state vector.

**B**

[*qobj*] Density matrix or state vector with same dimensions as *A*.

**Returns**

**angle**

[float] Bures angle between density matrices.

**buress\_dist**(*A*, *B*)

Returns the Bures distance between two density matrices *A* & *B*.

The Bures distance ranges from 0, for states with unit fidelity, to  $\sqrt{2}$ .

**Parameters**

**A**

[*qobj*] Density matrix or state vector.

**B**

[*qobj*] Density matrix or state vector with same dimensions as *A*.

**Returns**

**dist**

[float] Bures distance between density matrices.

**dnorm**(*A*, *B=None*, *solver='CVXOPT'*, *verbose=False*, *force\_solve=False*, *sparse=True*)

Calculates the diamond norm of the quantum map *q\_oper*, using the simplified semidefinite program of [Wat13].

The diamond norm SDP is solved by using [CVXPY](#).

**Parameters**

**A**

[*Qobj*] Quantum map to take the diamond norm of.

**B**

[*Qobj* or *None*] If provided, the diamond norm of  $A - B$  is taken instead.

**solver**

[str {"CVXOPT", "SCS"}, default: "CVXOPT"] Solver to use with CVXPY. "SCS" tends to be significantly faster, but somewhat less accurate.

**verbose**

[bool, default: False] If True, prints additional information about the solution.

**force\_solve**

[bool, default: False] If True, forces dnorm to solve the associated SDP, even if a special case is known for the argument.

**sparse**

[bool, default: True] Whether to use sparse matrices in the convex optimisation problem. Default True.

**Returns**

**dn**

[float] Diamond norm of q\_oper.

**Raises**

**ImportError**

If CVXPY cannot be imported.

**fidelity(A, B)**

Calculates the fidelity (pseudo-metric) between two density matrices.

**Parameters**

**A**

[qobj] Density matrix or state vector.

**B**

[qobj] Density matrix or state vector with same dimensions as A.

**Returns**

**fid**

[float] Fidelity pseudo-metric between A and B.

**Notes**

Uses the definition from Nielsen & Chuang, "Quantum Computation and Quantum Information". It is the square root of the fidelity defined in R. Jozsa, Journal of Modern Optics, 41:12, 2315 (1994), used in [qutip.core.metrics.process\\_fidelity](#).

**Examples**

```
>>> x = fock_dm(5,3)
>>> y = coherent_dm(5,1)
>>> np.testing.assert_almost_equal(fidelity(x,y), 0.24104350624628332)
```

**hellinger\_dist(A, B, sparse=False, tol=0)**

Calculates the quantum Hellinger distance between two density matrices.

Formula:

$$\text{hellinger\_dist}(A, B) = \sqrt{2 - 2 * \text{tr}(\sqrt{A} * \sqrt{B})}$$

See: D. Spehner, F. Illuminati, M. Orszag, and W. Roga, "Geometric measures of quantum correlations with Bures and Hellinger distances" arXiv:1611.03449

**Parameters**

**A**  
[Qobj] Density matrix or state vector.

**B**  
[Qobj] Density matrix or state vector with same dimensions as A.

**tol**  
[float, default: 0] Tolerance used by sparse eigensolver, if used. (0 = Machine precision)

**sparse**  
[bool, default: False] Use sparse eigensolver.

#### Returns

**hellinger\_dist**  
[float] Quantum Hellinger distance between A and B. Ranges from 0 to  $\sqrt{2}$ .

#### Examples

```
>>> x = fock_dm(5,3)
>>> y = coherent_dm(5,1)
>>> np.allclose(hellinger_dist(x, y), 1.3725145002591095)
True
```

#### hilbert\_dist(A, B)

Returns the Hilbert-Schmidt distance between two density matrices A & B.

##### Parameters

**A**  
[qobj] Density matrix or state vector.

**B**  
[qobj] Density matrix or state vector with same dimensions as A.

##### Returns

**dist**  
[float] Hilbert-Schmidt distance between density matrices.

#### Notes

See V. Vedral and M. B. Plenio, Phys. Rev. A 57, 1619 (1998).

#### process\_fidelity(oper, target=None)

Returns the process fidelity of a quantum channel to the target channel, or to the identity channel if no target is given. The process fidelity between two channels is defined as the state fidelity between their normalized Choi matrices.

##### Parameters

**oper**  
[Qobj/list] A unitary operator, or a superoperator in supermatrix, Choi or chi-matrix form, or a list of Kraus operators

**target**  
[Qobj/list, optional] A unitary operator, or a superoperator in supermatrix, Choi or chi-matrix form, or a list of Kraus operators

##### Returns

**fid**  
[float] Process fidelity between oper and target, or between oper and identity.

## Notes

Since Qutip 5.0, this function computes the process fidelity as defined for example in: A. Gilchrist, N.K. Langford, M.A. Nielsen, Phys. Rev. A 71, 062310 (2005). Previously, it computed a function that is now implemented as `get_fidelity` in `qutip-qtrl`.

The definition of state fidelity that the process fidelity is based on is the one from R. Jozsa, Journal of Modern Optics, 41:12, 2315 (1994). It is the square of the one implemented in [`qutip.core.metrics.fidelity`](#) which follows Nielsen & Chuang, “Quantum Computation and Quantum Information”

**tracedist**(*A*, *B*, *sparse=False*, *tol=0*)

Calculates the trace distance between two density matrices.. See: Nielsen & Chuang, “Quantum Computation and Quantum Information”

### Parameters

**A**

[qobj] Density matrix or state vector.

**B**

[qobj] Density matrix or state vector with same dimensions as A.

**tol**

[float, default: 0] Tolerance used by sparse eigensolver, if used. (0 = Machine precision)

**sparse**

[bool, default: False] Use sparse eigensolver.

### Returns

**tracedist**

[float] Trace distance between A and B.

## Examples

```
>>> x=fock_dm(5,3)
>>> y=coherent_dm(5,1)
>>> np.testing.assert_almost_equal(tracedist(x,y), 0.9705143161472971)
```

**unitarity**(*oper*)

Returns the unitarity of a quantum map, defined as the Frobenius norm of the unital block of that map’s superoperator representation.

### Parameters

**oper**

[Qobj] Quantum map under consideration.

### Returns

**u**

[float] Unitarity of *oper*.

## Continuous Variables

This module contains a collection functions for calculating continuous variable quantities from fock-basis representation of the state of multi-mode fields.

**correlation\_matrix**(*basis*, *rho=None*)

Given a basis set of operators  $\{a\}_n$ , calculate the correlation matrix:

$$C_{mn} = \langle a_m a_n \rangle$$

### Parameters

#### **basis**

[list] List of operators that defines the basis for the correlation matrix.

#### **rho**

[Qobj, optional] Density matrix for which to calculate the correlation matrix. If *rho* is *None*, then a matrix of correlation matrix operators is returned instead of expectation values of those operators.

### Returns

#### **corr\_mat**

[ndarray] A 2-dimensional *array* of correlation values or operators.

**correlation\_matrix\_field**(*a1*, *a2*, *rho=None*)

Calculates the correlation matrix for given field operators  $a_1$  and  $a_2$ . If a density matrix is given the expectation values are calculated, otherwise a matrix with operators is returned.

### Parameters

#### **a1**

[Qobj] Field operator for mode 1.

#### **a2**

[Qobj] Field operator for mode 2.

#### **rho**

[Qobj, optional] Density matrix for which to calculate the covariance matrix.

### Returns

#### **cov\_mat**

[ndarray] Array of complex numbers or Qobj's A 2-dimensional *array* of covariance values, or, if  $\rho=0$ , a matrix of operators.

**correlation\_matrix\_quadrature**(*a1*, *a2*, *rho=None*, *g=1.4142135623730951*)

Calculate the quadrature correlation matrix with given field operators  $a_1$  and  $a_2$ . If a density matrix is given the expectation values are calculated, otherwise a matrix with operators is returned.

### Parameters

#### **a1**

[Qobj] Field operator for mode 1.

#### **a2**

[Qobj] Field operator for mode 2.

#### **rho**

[Qobj, optional] Density matrix for which to calculate the covariance matrix.

#### **g**

[float, default:  $\sqrt{2}$ ] Scaling factor for  $a = 0.5 * g * (x + iy)$ , default  $g = \sqrt{2}$ . The value of  $g$  is related to the value of  $\hbar$  in the commutation relation  $[x, y] = i * \hbar$  via  $\hbar = 2/g ** 2$  giving the default value  $\hbar=1$ .

### Returns

**corr\_mat**

[ndarray] Array of complex numbers or Qobj's A 2-dimensional *array* of covariance values for the field quadratures, or, if rho=0, a matrix of operators.

**covariance\_matrix**(basis, rho, symmetrized=True)

Given a basis set of operators  $\{a\}_n$ , calculate the covariance matrix:

$$V_{mn} = \frac{1}{2} \langle a_m a_n + a_n a_m \rangle - \langle a_m \rangle \langle a_n \rangle$$

or, if of the optional argument *symmetrized=False*,

$$V_{mn} = \langle a_m a_n \rangle - \langle a_m \rangle \langle a_n \rangle$$

**Parameters**

**basis**

[list] List of operators that defines the basis for the covariance matrix.

**rho**

[Qobj] Density matrix for which to calculate the covariance matrix.

**symmetrized**

[bool, default: True] Flag indicating whether the symmetrized (default) or non-symmetrized correlation matrix is to be calculated.

**Returns**

**corr\_mat**

[ndarray] A 2-dimensional array of covariance values.

**logarithmic\_negativity**(V, g=1.4142135623730951)

Calculates the logarithmic negativity given a symmetrized covariance matrix, see [qutip.continuous\\_variables.covariance\\_matrix](#). Note that the two-mode field state that is described by V must be Gaussian for this function to be applicable.

**Parameters**

**V**

[ndarray] The covariance matrix.

**g**

[float, default: sqrt(2)] Scaling factor for  $a = 0.5 * g * (x + iy)$ , default  $g = \sqrt{2}$ . The value of g is related to the value of hbar in the commutation relation  $[x, y] = i * \hbar$  via  $\hbar = 2/g ** 2$  giving the default value  $\hbar = 1$ .

**Returns**

**N**

[float] The logarithmic negativity for the two-mode Gaussian state that is described by the the Wigner covariance matrix V.

**wigner\_covariance\_matrix**(a1=None, a2=None, R=None, rho=None, g=1.4142135623730951)

Calculates the Wigner covariance matrix  $V_{ij} = \frac{1}{2}(R_{ij} + R_{ji})$ , given the quadrature correlation matrix  $R_{ij} = \langle R_i R_j \rangle - \langle R_i \rangle \langle R_j \rangle$ , where  $R = (q_1, p_1, q_2, p_2)^T$  is the vector with quadrature operators for the two modes.

Alternatively, if  $R = \text{None}$ , and if annihilation operators a1 and a2 for the two modes are supplied instead, the quadrature correlation matrix is constructed from the annihilation operators before then the covariance matrix is calculated.

**Parameters**

**a1**

[Qobj, optional] Field operator for mode 1.

**a2**  
[Qobj, optional] Field operator for mode 2.

**R**  
[ndarray, optional] The quadrature correlation matrix.

**rho**  
[Qobj, optional] Density matrix for which to calculate the covariance matrix.

**g**  
[float, default: sqrt(2)] Scaling factor for  $a = 0.5 * g * (x + iy)$ , default  $g = \text{sqrt}(2)$ . The value of  $g$  is related to the value of  $\hbar$  in the commutation relation  $[x, y] = i * \hbar$  via  $\hbar = 2/g ** 2$  giving the default value  $\hbar=1$ .

#### Returns

**cov\_mat**  
[ndarray] A 2-dimensional array of covariance values.

## 5.2.3 Measurement

### Measurement of quantum states

Module for measuring quantum objects.

**measure**(state, ops, tol=None)

A dispatch method that provides measurement results handling both observable style measurements and projector style measurements (POVMs and PVMs).

For return signatures, please check:

- [measure\\_observable](#) for observable measurements.
- [measure\\_povm](#) for POVM measurements.

#### Parameters

**state**  
[Qobj] The ket or density matrix specifying the state to measure.

**ops**  
[Qobj or list of Qobj]  

- measurement observable (Qobj); or
- list of measurement operators  $M_i$  or kets (list of Qobj) Either:
  1. specifying a POVM s.t.  $E_i = M_i^\dagger M_i$
  2. projection operators if ops correspond to projectors (s.t.  $E_i = M_i^\dagger = M_i$ )
  3. kets (transformed to projectors)

**tol**  
[float, optional] Smallest value for the probabilities. Default is qutip's core settings' atol.

**measure\_observable**(state, op, tol=None)

Perform a measurement specified by an operator on the given state.

This function simulates the classic quantum measurement described in many introductory texts on quantum mechanics. The measurement collapses the state to one of the eigenstates of the given operator and the result of the measurement is the corresponding eigenvalue.

#### Parameters

**state**  
 [Qobj] The ket or density matrix specifying the state to measure.

**op**  
 [Qobj] The measurement operator.

**tol**  
 [float, optional] Smallest value for the probabilities. Default is qutip's core settings' atol.

#### Returns

**measured\_value**  
 [float] The result of the measurement (one of the eigenvalues of op).

**state**  
 [Qobj] The new state (a ket if a ket was given, otherwise a density matrix).

### Examples

Measure the z-component of the spin of the spin-up basis state:

```
>>> measure_observable(basis(2, 0), sigmaz())
(1.0, Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[-1.]
 [ 0.]])
```

Since the spin-up basis is an eigenstate of sigmaz, this measurement always returns 1 as the measurement result (the eigenvalue of the spin-up basis) and the original state (up to a global phase).

Measure the x-component of the spin of the spin-down basis state:

```
>>> measure_observable(basis(2, 1), sigmax())
(-1.0, Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[-0.70710678]
 [ 0.70710678]])
```

This measurement returns 1 fifty percent of the time and -1 the other fifty percent of the time. The new state returned is the corresponding eigenstate of sigmax.

One may also perform a measurement on a density matrix. Below we perform the same measurement as above, but on the density matrix representing the pure spin-down state:

```
>>> measure_observable(ket2dm(basis(2, 1)), sigmax())
(-1.0, Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper
Qobj data =
[[ 0.5 -0.5]
 [-0.5  0.5]])
```

The measurement result is the same, but the new state is returned as a density matrix.

**measure\_povm**(state, ops, tol=None)

Perform a measurement specified by list of POVMs.

This function simulates a POVM measurement. The measurement collapses the state to one of the resultant states of the measurement and returns the index of the operator corresponding to the collapsed state as well as the collapsed state.

#### Parameters



**state**

[*Qobj*] The ket or density matrix specifying the state to measure.

**ops**

[list of *Qobj*] List of measurement operators  $M_i$  or kets. Either:

1. specifying a POVM s.t.  $E_i = M_i^\dagger M_i$
2. projection operators if ops correspond to projectors (s.t.  $E_i = M_i^\dagger = M_i$ )
3. kets (transformed to projectors)

**tol**

[float, optional] Smallest value for the probabilities. Default is qutip's core settings' atol.

**Returns**

**index**

[float] The resultant index of the measurement.

**state**

[*Qobj*] The new state (a ket if a ket was given, otherwise a density matrix).

**measurement\_statistics**(*state, ops, tol=None*)

A dispatch method that provides measurement statistics handling both observable style measurements and projector style measurements(POVMs and PVMs).

For return signatures, please check:

- *measurement\_statistics\_observable* for observable measurements.
- *measurement\_statistics\_povm* for POVM measurements.

**Parameters**

**state**

[*Qobj*] The ket or density matrix specifying the state to measure.

**ops**

[*Qobj* or list of *Qobj*]

- measurement observable (:class:Qobj); or
- list of measurement operators  $M_i$  or kets (list of *Qobj*) Either:
  1. specifying a POVM s.t.  $E_i = M_i^\dagger * M_i$
  2. projection operators if ops correspond to projectors (s.t.  $E_i = M_i^\dagger = M_i$ )
  3. kets (transformed to projectors)

**tol**

[float, optional] Smallest value for the probabilities. Default is qutip's core settings' atol.

**measurement\_statistics\_observable**(*state, op, tol=None*)

Return the measurement eigenvalues, eigenstates (or projectors) and measurement probabilities for the given state and measurement operator.

**Parameters**

**state**

[*Qobj*] The ket or density matrix specifying the state to measure.

**op**

[*Qobj*] The measurement operator.

**tol**

[float, optional] Smallest value for the probabilities. Default is qutip's core settings' `atol`.

#### Returns

**eigenvalues: list of float**

The list of eigenvalues of the measurement operator.

**projectors: list of *Qobj***

Return the projectors onto the eigenstates.

**probabilities: list of float**

The probability of measuring the state as being in the corresponding eigenstate (and the measurement result being the corresponding eigenvalue).

**measurement\_statistics\_povm**(*state*, *ops*, *tol=None*)

Returns measurement statistics (resultant states and probabilities) for a measurement specified by a set of positive operator valued measurements on a specified ket or density matrix.

#### Parameters

**state**

[*Qobj*] The ket or density matrix specifying the state to measure.

**ops**

[list of *Qobj*] List of measurement operators  $M_i$  or kets. Either:

1. specifying a POVM s.t.  $E_i = M_i^\dagger M_i$
2. projection operators if ops correspond to projectors (s.t.  $E_i = M_i^\dagger = M_i$ )
3. kets (transformed to projectors)

**tol**

[float, optional] Smallest value for the probabilities. Smaller probabilities will be rounded to 0. Default is qutip's core settings' `atol`.

#### Returns

**collapsed\_states**

[list of *Qobj*] The collapsed states obtained after measuring the qubits and obtaining the qubit specified by the target in the state specified by the index.

**probabilities**

[list of floats] The probability of measuring a state in the state specified by the index.

## 5.2.4 Dynamics and Time-Evolution

### Schrödinger Equation

This module provides solvers for the unitary Schrodinger equation.

**sesolve**(*H*, *psi0*, *tlist*, *e\_ops=None*, *args=None*, *options=None*, *\*\*kwargs*)

Schrodinger equation evolution of a state vector or unitary matrix for a given Hamiltonian.

Evolve the state vector (*psi0*) using a given Hamiltonian (*H*), by integrating the set of ordinary differential equations that define the system. Alternatively evolve a unitary matrix in solving the Schrodinger operator equation.

The output is either the state vector or unitary matrix at arbitrary points in time (*tlist*), or the expectation values of the supplied operators (*e\_ops*). If *e\_ops* is a callback function, it is invoked for each time in *tlist* with time and the state as arguments, and the function does not use any return values. *e\_ops* cannot be used in conjunction with solving the Schrodinger operator equation

#### Time-dependent operators

For time-dependent problems, `H` and `c_ops` can be a [QobjEvo](#) or object that can be interpreted as [QobjEvo](#) such as a list of ([Qobj](#), Coefficient) pairs or a function.

### Parameters

#### `H`

[[Qobj](#), [QobjEvo](#), [QobjEvo](#) compatible format.] System Hamiltonian as a [Qobj](#) or [QobjEvo](#) for time-dependent Hamiltonians. List of [[Qobj](#), Coefficient] or callable that can be made into [QobjEvo](#) are also accepted.

#### `psi0`

[[Qobj](#)] initial state vector (ket) or initial unitary operator  $\psi_0 = U$

#### `tlist`

[list / array] list of times for  $t$ .

#### `e_ops`

[[Qobj](#), callable, or list, optional] Single operator or list of operators for which to evaluate expectation values or callable or list of callable. Callable signature must be,  $f(t: \text{float}, \text{state}: \text{Qobj})$ . See [expect](#) for more detail of operator expectation.

#### `args`

[dict, optional] dictionary of parameters for time-dependent Hamiltonians

#### `options`

[dict, optional] Dictionary of options for the solver.

- `store_final_state` : bool  
Whether or not to store the final state of the evolution in the result class.
- `store_states` : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- `normalize_output` : bool  
Normalize output state to hide ODE numerical errors.
- `progress_bar` : str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- `progress_kwargs` : dict  
kwargs to pass to the progress\_bar. Qutip's bars use *chunk\_size*.
- `method` : str ["adams", "bdf", "lsoda", "dop853", "vern9", etc.]  
Which differential equation integration method to use.
- `atol`, `rtol` : float  
Absolute and relative tolerance of the ODE integrator.
- `nsteps` : int  
Maximum number of (internally defined) steps allowed in one `tlist` step.
- `max_step` : float  
Maximum length of one internal step. When using pulses, it should be less than half the width of the thinnest pulse.

Other options could be supported depending on the integration method, see [Integrator](#).

### Returns

#### result: [Result](#)

An instance of the class [Result](#), which contains a list of array `result.expect` of expectation values for the times specified by `tlist`, and/or a list `result.states` of state vectors or density matrices corresponding to the times in `tlist` [if `e_ops` is an empty list of `store_states=True` in options].

## Master Equation

This module provides solvers for the Lindblad master equation and von Neumann equation.

**mesolve**(*H*, *rho0*, *tlist*, *c\_ops*=None, *e\_ops*=None, *args*=None, *options*=None, *\*\*kwargs*)

Master equation evolution of a density matrix for a given Hamiltonian and set of collapse operators, or a Liouvillian.

Evolve the state vector or density matrix (*rho0*) using a given Hamiltonian or Liouvillian (*H*) and an optional set of collapse operators (*c\_ops*), by integrating the set of ordinary differential equations that define the system. In the absence of collapse operators the system is evolved according to the unitary evolution of the Hamiltonian.

The output is either the state vector at arbitrary points in time (*tlist*), or the expectation values of the supplied operators (*e\_ops*). If *e\_ops* is a callback function, it is invoked for each time in *tlist* with time and the state as arguments, and the function does not use any return values.

If either *H* or the Qobj elements in *c\_ops* are superoperators, they will be treated as direct contributions to the total system Liouvillian. This allows the solution of master equations that are not in standard Lindblad form.

### Time-dependent operators

For time-dependent problems, *H* and *c\_ops* can be a [QobjEvo](#) or object that can be interpreted as [QobjEvo](#) such as a list of (Qobj, Coefficient) pairs or a function.

### Additional options

Additional options to *mesolve* can be set via the *options* argument. Many ODE integration options can be set this way, and the *store\_states* and *store\_final\_state* options can be used to store states even though expectation values are requested via the *e\_ops* argument.

### Parameters

#### **H**

[[Qobj](#), [QobjEvo](#), [QobjEvo](#) compatible format.] Possibly time-dependent system Liouvillian or Hamiltonian as a Qobj or QobjEvo. List of [[Qobj](#), Coefficient] or callable that can be made into [QobjEvo](#) are also accepted.

#### **rho0**

[[Qobj](#)] initial density matrix or state vector (ket).

#### **tlist**

[list / array] list of times for *t*.

#### **c\_ops**

[list of ([QobjEvo](#), [QobjEvo](#) compatible format)] Single collapse operator, or list of collapse operators, or a list of Liouvillian superoperators. None is equivalent to an empty list.

#### **e\_ops**

[list of [Qobj](#) / callback function, optional] Single operator or list of operators for which to evaluate expectation values or callable or list of callable. Callable signature must be, *f(t: float, state: Qobj)*. See *expect* for more detail of operator expectation.

#### **args**

[dict, optional] dictionary of parameters for time-dependent Hamiltonians and collapse operators.

#### **options**

[dict, optional] Dictionary of options for the solver.

- *store\_final\_state* : bool  
Whether or not to store the final state of the evolution in the result class.
- *store\_states* : bool, None

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

- `normalize_output` : bool  
Normalize output state to hide ODE numerical errors.
- `progress_bar` : str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- `progress_kwargs` : dict  
kwargs to pass to the `progress_bar`. Qutip's bars use *chunk\_size*.
- `method` : str ["adams", "bdf", "lsoda", "dop853", "vern9", etc.]  
Which differential equation integration method to use.
- `atol`, `rtol` : float  
Absolute and relative tolerance of the ODE integrator.
- `nsteps` : int  
Maximum number of (internally defined) steps allowed in one `tlist` step.
- `max_step` : float  
Maximum length of one internal step. When using pulses, it should be less than half the width of the thinnest pulse.

Other options could be supported depending on the integration method, see [Integrator](#).

## Returns

**result:** [Result](#)

An instance of the class [Result](#), which contains a *list of array* `result.expect` of expectation values for the times specified by `tlist`, and/or a *list* `result.states` of state vectors or density matrices corresponding to the times in `tlist` [if `e_ops` is an empty list of `store_states=True` in options].

## Notes

When no collapse operator are given and the  $H$  is not a superoperator, it will defer to `sesolve`.

## Monte Carlo Evolution

**`mcsolve`**( $H$ , *state*, *tlist*, *c\_ops*=(), *e\_ops*=None, *ntraj*=500, \*, *args*=None, *options*=None, *seeds*=None, *target\_tol*=None, *timeout*=None, *\*\*kwargs*)

Monte Carlo evolution of a state vector  $|\psi\rangle$  for a given Hamiltonian and sets of collapse operators. Options for the underlying ODE solver are given by the Options class.

### Parameters

**$H$**

[[Qobj](#), [QobjEvo](#), list, callable.] System Hamiltonian as a [Qobj](#), [QobjEvo](#). It can also be any input type that [QobjEvo](#) accepts (see [QobjEvo](#)'s documentation).  $H$  can also be a superoperator (liouvillian) if some collapse operators are to be treated deterministically.

***state***

[[Qobj](#)] Initial state vector.

***tlist***

[array\_like] Times at which results are recorded.

***c\_ops***

[list] A list of collapse operators in any input type that [QobjEvo](#) accepts (see

*QobjEvo*'s documentation). They must be operators even if  $H$  is a superoperator. If none are given, the solver will defer to *sesolve* or *mesolve*.

#### **e\_ops**

[list, optional] A list of operator as *Qobj*, *QobjEvo* or callable with signature of (t, state: *Qobj*) for calculating expectation values. When no *e\_ops* are given, the solver will default to save the states.

#### **ntraj**

[int, default: 500] Maximum number of trajectories to run. Can be cut short if a time limit is passed with the *timeout* keyword or if the target tolerance is reached, see *target\_tol*.

#### **args**

[dict, optional] Arguments for time-dependent Hamiltonian and collapse operator terms.

#### **options**

[dict, optional] Dictionary of options for the solver.

- *store\_final\_state* : bool  
Whether or not to store the final state of the evolution in the result class.
- *store\_states* : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- *progress\_bar* : str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- *progress\_kwargs* : dict  
kwargs to pass to the *progress\_bar*. Qutip's bars use *chunk\_size*.
- *method* : str ["adams", "bdf", "lsoda", "dop853", "vern9", etc.]  
Which differential equation integration method to use.
- *atol*, *rtol* : float  
Absolute and relative tolerance of the ODE integrator.
- *nsteps* : int  
Maximum number of (internally defined) steps allowed in one *tlist* step.
- *max\_step* : float  
Maximum length of one internal step. When using pulses, it should be less than half the width of the thinnest pulse.
- *keep\_runs\_results* : bool, [False]  
Whether to store results from all trajectories or just store the averages.
- *map* : str {"serial", "parallel", "loky", "mpi"}  
How to run the trajectories. "parallel" uses the multiprocessing module to run in parallel while "loky" and "mpi" use the "loky" and "mpi4py" modules to do so.
- *num\_cpus* : int  
Number of cpus to use when running in parallel. None detect the number of available cpus.
- *norm\_t\_tol*, *norm\_tol*, *norm\_steps* : float, float, int  
Parameters used to find the collapse location. *norm\_t\_tol* and *norm\_tol* are the tolerance in time and norm respectively. An error will be raised if the collapse could not be found within *norm\_steps* tries.
- *mc\_corr\_eps* : float  
Small number used to detect non-physical collapse caused by numerical imprecision.

- `improved_sampling` : Bool

Whether to use the improved sampling algorithm from Abdelhafez et al. PRA (2019)

Additional options are listed under [options](#). More options may be available depending on the selected differential equation integration method, see [Integrator](#).

#### seeds

[int, SeedSequence, list, optional] Seed for the random number generator. It can be a single seed used to spawn seeds for each trajectory or a list of seeds, one for each trajectory. Seeds are saved in the result and they can be reused with:

```
seeds=prev_result.seeds
```

#### target\_tol

[float, tuple, list, optional] Target tolerance of the evolution. The evolution will compute trajectories until the error on the expectation values is lower than this tolerance. The maximum number of trajectories employed is given by `ntraj`. The error is computed using jackknife resampling. `target_tol` can be an absolute tolerance or a pair of absolute and relative tolerance, in that order. Lastly, it can be a list of pairs of (atol, rtol) for each `e_ops`.

#### timeout

[float, optional] Maximum time for the evolution in second. When reached, no more trajectories will be computed.

### Returns

#### results

[[McResult](#)] Object storing all results from the simulation. Which results is saved depends on the presence of `e_ops` and the options used. `collapse` and `photocurrent` is available to Monte Carlo simulation results.

### Notes

The simulation will end when the first end condition is reached between `ntraj`, `timeout` and `target_tol`.

**nm\_mcsolve**(*H*, *state*, *tlist*, *ops\_and\_rates*=(), *e\_ops*=None, *ntraj*=500, \*, *args*=None, *options*=None, *seeds*=None, *target\_tol*=None, *timeout*=None)

Monte-Carlo evolution corresponding to a Lindblad equation with “rates” that may be negative. Usage of this function is analogous to `mcsolve`, but the `c_ops` parameter is replaced by an `ops_and_rates` parameter to allow for negative rates. Options for the underlying ODE solver are given by the `Options` class.

### Parameters

#### H

[[Qobj](#), [QobjEvo](#), list, callable.] System Hamiltonian as a [Qobj](#), [QobjEvo](#). It can also be any input type that [QobjEvo](#) accepts (see [QobjEvo](#)’s documentation). `H` can also be a superoperator (liouvillian) if some collapse operators are to be treated deterministically.

#### state

[[Qobj](#)] Initial state vector.

#### tlist

[array\_like] Times at which results are recorded.

#### ops\_and\_rates

[list] A list of tuples (`L`, `Gamma`), where the Lindblad operator `L` is a [Qobj](#) and `Gamma` represents the corresponding rate, which is allowed to be negative. The Lindblad operators must be operators even if `H` is a superoperator. If none are given, the solver will defer to `sesolve` or `mesolve`. Each rate `Gamma` may be just a number (in the case of a constant rate) or, otherwise, specified using any format accepted by [coefficient](#).

#### **e\_ops**

[list, optional] A list of operator as Qobj, QobjEvo or callable with signature of (t, state: Qobj) for calculating expectation values. When no e\_ops are given, the solver will default to save the states.

#### **ntraj**

[int, default: 500] Maximum number of trajectories to run. Can be cut short if a time limit is passed with the `timeout` keyword or if the target tolerance is reached, see `target_tol`.

#### **args**

[dict, optional] Arguments for time-dependent Hamiltonian and collapse operator terms.

#### **options**

[dict, optional] Dictionary of options for the solver.

- `store_final_state` : bool  
Whether or not to store the final state of the evolution in the result class.
- `store_states` : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- `progress_bar` : str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- `progress_kwarg` : dict  
kwargs to pass to the progress\_bar. Qutip's bars use *chunk\_size*.
- `method` : str ["adams", "bdf", "lsoda", "dop853", "vern9", etc.]  
Which differential equation integration method to use.
- `atol`, `rtol` : float  
Absolute and relative tolerance of the ODE integrator.
- `nsteps` : int  
Maximum number of (internally defined) steps allowed in one `tlist` step.
- `max_step` : float  
Maximum length of one internal step. When using pulses, it should be less than half the width of the thinnest pulse.
- `keep_runs_results` : bool, [False]  
Whether to store results from all trajectories or just store the averages.
- `map` : str {"serial", "parallel", "loky", "mpi"}  
How to run the trajectories. "parallel" uses the multiprocessing module to run in parallel while "loky" and "mpi" use the "loky" and "mpi4py" modules to do so.
- `num_cpus` : int  
Number of cpus to use when running in parallel. None detect the number of available cpus.
- `norm_t_tol`, `norm_tol`, `norm_steps` : float, float, int  
Parameters used to find the collapse location. `norm_t_tol` and `norm_tol` are the tolerance in time and norm respectively. An error will be raised if the collapse could not be found within `norm_steps` tries.
- `mc_corr_eps` : float  
Small number used to detect non-physical collapse caused by numerical imprecision.
- `completeness_rtol`, `completeness_atol` : float, float



Parameters used in determining whether the given Lindblad operators satisfy a certain completeness relation. If they do not, an additional Lindblad operator is added automatically (with zero rate).

- `martingale_quad_limit` : float or int  
An upper bound on the number of subintervals used in the adaptive integration of the martingale.

Note that the ‘`improved_sampling`’ option is not currently supported. Additional options are listed under [options](#). More options may be available depending on the selected differential equation integration method, see [Integrator](#).

#### seeds

[int, SeedSequence, list, optional] Seed for the random number generator. It can be a single seed used to spawn seeds for each trajectory or a list of seeds, one for each trajectory. Seeds are saved in the result and they can be reused with:

```
seeds=prev_result.seeds
```

#### target\_tol

[float, tuple, list, optional] Target tolerance of the evolution. The evolution will compute trajectories until the error on the expectation values is lower than this tolerance. The maximum number of trajectories employed is given by `ntraj`. The error is computed using jackknife resampling. `target_tol` can be an absolute tolerance or a pair of absolute and relative tolerance, in that order. Lastly, it can be a list of pairs of (atol, rtol) for each `e_ops`.

#### timeout

[float, optional] Maximum time for the evolution in seconds. When reached, no more trajectories will be computed.

### Returns

#### results

[[NnmcmcResult](#)] Object storing all results from the simulation. Compared to a result returned by `mcsolve`, this result contains the additional field `trace` (and `runs_trace` if `store_final_state` is set). Note that the states on the individual trajectories are not normalized. This field contains the average of their trace, which will converge to one in the limit of sufficiently many trajectories.

## Krylov Subspace Solver

**krylovsolve**(*H*, *psi0*, *tlist*, *krylov\_dim*, *e\_ops*=None, *args*=None, *options*=None)

Schrodinger equation evolution of a state vector for time independent Hamiltonians using Krylov method.

Evolve the state vector (“psi0”) finding an approximation for the time evolution operator of Hamiltonian (“H”) by obtaining the projection of the time evolution operator on a set of small dimensional Krylov subspaces ( $m \ll \dim(H)$ ).

The output is either the state vector or unitary matrix at arbitrary points in time (*tlist*), or the expectation values of the supplied operators (*e\_ops*). If *e\_ops* is a callback function, it is invoked for each time in *tlist* with time and the state as arguments, and the function does not use any return values. *e\_ops* cannot be used in conjunction with solving the Schrodinger operator equation

#### Parameters

##### H

[[Qobj](#), [QobjEvo](#), [QobjEvo](#) compatible format.] System Hamiltonian as a [Qobj](#) or [QobjEvo](#) for time-dependent Hamiltonians. List of [[Qobj](#), Coefficient] or callable that can be made into [QobjEvo](#) are also accepted.

##### psi0

[[Qobj](#)] Initial state vector (ket)

**tlist**

[*list* / *array*] list of times for  $t$ .

**krylov\_dim: int**

Dimension of Krylov approximation subspaces used for the time evolution approximation.

**e\_ops**

[*Qobj*, callable, or list, optional] Single operator or list of operators for which to evaluate expectation values or callable or list of callable. Callable signature must be,  $f(t: \text{float}, \text{state}: \text{Qobj})$ . See [expect](#) for more detail of operator expectation.

**args**

[dict, optional] dictionary of parameters for time-dependent Hamiltonians

**options**

[dict, optional] Dictionary of options for the solver.

- **store\_final\_state** : bool  
Whether or not to store the final state of the evolution in the result class.
- **store\_states** : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- **normalize\_output** : bool  
Normalize output state to hide ODE numerical errors.
- **progress\_bar** : str { 'text', 'enhanced', 'tqdm', '' }  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- **progress\_kwargs** : dict  
kwargs to pass to the progress\_bar. Qutip's bars use *chunk\_size*.
- **atol**: float  
Absolute tolerance of the ODE integrator.
- **nsteps** : int  
Maximum number of (internally defined) steps allowed in one **tlist** step.
- **min\_step, max\_step** : float  
Minimum and maximum length of one internal step.
- **always\_compute\_step**: bool  
If True, the step length is computed each time a new Krylov subspace is computed. Otherwise it is computed only once when creating the integrator.
- **sub\_system\_tol**: float  
Tolerance to detect an happy breakdown. An happy breakdown happens when the initial ket is in a subspace of the Hamiltonian smaller than **krylov\_dim**.

**Returns**

**result: [Result](#)**

An instance of the class [Result](#), which contains a *list of array* **result.expect** of expectation values for the times specified by **tlist**, and/or a *list* **result.states** of state vectors or density matrices corresponding to the times in **tlist** [if **e\_ops** is an empty list of **store\_states=True** in options].

## Bloch-Redfield Master Equation

This module provides solvers for the Lindblad master equation and von Neumann equation.

**brmesolve**(*H*, *psi0*, *tlist*, *a\_ops*=(), *e\_ops*=(), *c\_ops*=(), *args*=None, *sec\_cutoff*=0.1, *options*=None, *\*\*kwargs*)

Solves for the dynamics of a system using the Bloch-Redfield master equation, given an input Hamiltonian, Hermitian bath-coupling terms and their associated spectral functions, as well as possible Lindblad collapse operators.

### Parameters

#### **H**

[*Qobj*, *QobjEvo*] Possibly time-dependent system Liouvillian or Hamiltonian as a *Qobj* or *QobjEvo*. list of [*Qobj*, Coefficient] or callable that can be made into *QobjEvo* are also accepted.

#### **psi0: Qobj**

Initial density matrix or state vector (ket).

#### **tlist**

[array\_like] List of times for evaluating evolution

#### **a\_ops**

[list of (a\_op, spectra)] Nested list of system operators that couple to the environment, and the corresponding bath spectra.

#### **a\_op**

[*Qobj*, *QobjEvo*] The operator coupling to the environment. Must be hermitian.

#### **spectra**

[Coefficient, str, func] The corresponding bath spectral response. Can be a *Coefficient* using an 'w' args, a function of the frequency or a string. Coefficient build from a numpy array are understood as a function of w instead of t. Function are expected to be of the signature f(w) or f(t, w, \*\*args).

The spectra function can depend on t if the corresponding a\_op is a *QobjEvo*.

Example:

```
a_ops = [
    (a+a.dag(), ('w>0', args={"w": 0})),
    (QobjEvo(a+a.dag()), 'w > exp(-t)'),
    (QobjEvo([b+b.dag(), lambda t: ...]), lambda w: ...),
    (c+c.dag(), SpectraCoefficient(coefficient(array, tlist=ws))),
]
```

#### **e\_ops**

[list of *Qobj* / callback function, optional] Single operator or list of operators for which to evaluate expectation values or callable or list of callable. Callable signature must be, f(t: float, state: *Qobj*). See `expect` for more detail of operator expectation

#### **c\_ops**

[list of (*QobjEvo*, *QobjEvo* compatible format), optional] List of collapse operators.

#### **args**

[dict, optional] Dictionary of parameters for time-dependent Hamiltonians and collapse operators. The key w is reserved for the spectra function.

#### **sec\_cutoff**

[float, default: 0.1] Cutoff for secular approximation. Use -1 if secular approximation is not used when evaluating bath-coupling terms.

#### **options**

[dict, optional] Dictionary of options for the solver.

- `store_final_state` : bool  
Whether or not to store the final state of the evolution in the result class.
  - `store_states` : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
  - `normalize_output` : bool  
Normalize output state to hide ODE numerical errors.
  - `progress_bar` : str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
  - `progress_kwargs` : dict  
kwargs to pass to the progress\_bar. Qutip's bars use *chunk\_size*.
  - `tensor_type` : str ['sparse', 'dense', 'data']  
Which data type to use when computing the brtensor. With a cutoff 'sparse' is usually the most efficient.
  - `sparse_eigsolver` : bool {False} Whether to use the sparse eigensolver
  - `method` : str ["adams", "bdf", "lsoda", "dop853", "vern9", etc.] Which differential equation integration method to use.
  - `atol`, `rtol` : float  
Absolute and relative tolerance of the ODE integrator.
  - `nsteps` : int  
Maximum number of (internally defined) steps allowed in one `tlist` step.
  - `max_step` : float, 0  
Maximum length of one internal step. When using pulses, it should be less than half the width of the thinnest pulse.
- Other options could be supported depending on the integration method, see [Integrator](#).

### Returns

**result:** [Result](#)

An instance of the class `qutip.solver.Result`, which contains either an array of expectation values, for operators given in `e_ops`, or a list of states for the times specified by `tlist`.

## Floquet States and Floquet-Markov Master Equation

**floquet\_tensor**(*H*, *c\_ops*, *spectra\_cb*, *T=0*, *w\_th=0.0*, *kmax=5*, *nT=100*)

Construct a tensor that represents the master equation in the floquet basis.

Simplest RWA approximation [Grifoni et al, Phys.Rep. 304 229 (1998)]

### Parameters

**H**

[[QobjEvo](#), [FloquetBasis](#)] Periodic Hamiltonian a floquet basis system.

**T**

[float, optional] The period of the time-dependence of the hamiltonian. Optional if H is a [FloquetBasis](#) object.

**c\_ops**

[list of [Qobj](#)] list of collapse operators.

**spectra\_cb**

[list callback functions] List of callback functions that compute the noise power spectrum as a function of frequency for the collapse operators in *c\_ops*.

**w\_th**

[float, default: 0.0] The temperature in units of frequency.

**kmax**

[int, default: 5] The truncation of the number of sidebands (default 5).

**nT**

[int, default: 100] The number of integration steps (for calculating *X*) within one period.

**Returns**

**output**

[array] The Floquet-Markov master equation tensor *R*.

**fmmesolve**(*H*, *rho0*, *tlist*, *c\_ops*=None, *e\_ops*=None, *spectra\_cb*=None, *T*=0, *w\_th*=0.0, *args*=None, *options*=None)

Solve the dynamics for the system using the Floquet-Markov master equation.

**Parameters**

**H**

[*Qobj*, *QobjEvo*, *QobjEvo* compatible format.] Periodic system Hamiltonian as *QobjEvo*. List of [*Qobj*, Coefficient] or callable that can be made into *QobjEvo* are also accepted.

**rho0 / psi0**

[*Qobj*] Initial density matrix or state vector (ket).

**tlist**

[list / array] List of times for *t*.

**c\_ops**

[list of *Qobj*, optional] List of collapse operators. Time dependent collapse operators are not supported. Fall back on *fsesolve* if not provided.

**e\_ops**

[list of *Qobj* / callback function, optional] List of operators for which to evaluate expectation values. The states are reverted to the lab basis before applying the

**spectra\_cb**

[list callback functions, default: lambda w: (w > 0)] List of callback functions that compute the noise power spectrum as a function of frequency for the collapse operators in *c\_ops*.

**T**

[float, default=tlist[-1]] The period of the time-dependence of the hamiltonian. The default value 0 indicates that the 'tlist' spans a single period of the driving.

**w\_th**

[float, default: 0.0] The temperature of the environment in units of frequency. For example, if the Hamiltonian written in units of 2pi GHz, and the temperature is given in K, use the following conversion:

temperature = 25e-3 # unit K  
h = 6.626e-34 kB = 1.38e-23  
args['w\_th'] = temperature \* (kB / h) \* 2 \* pi \* 1e-9

**args**

[dict, optional] Dictionary of parameters for time-dependent Hamiltonian

**options**

[dict, optional] Dictionary of options for the solver.

- store\_final\_state : bool

Whether or not to store the final state of the evolution in the result class.

- `store_states` : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- `store_floquet_states` : bool  
Whether or not to store the density matrices in the floquet basis in `result.floquet_states`.
- `normalize_output` : bool  
Normalize output state to hide ODE numerical errors.
- `progress_bar` : str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- `progress_kwargs` : dict  
kwargs to pass to the `progress_bar`. Qutip's bars use *chunk\_size*.
- `method` : str ["adams", "bdf", "lsoda", "dop853", "vern9", etc.]  
Which differential equation integration method to use.
- `atol`, `rtol` : float  
Absolute and relative tolerance of the ODE integrator.
- `nsteps` : int  
Maximum number of (internally defined) steps allowed in one `tlist` step.
- `max_step` : float  
Maximum length of one internal step. When using pulses, it should be less than half the width of the thinnest pulse.

Other options could be supported depending on the integration method, see [Integrator](#).

## Returns

**result:** [Result](#)

An instance of the class [Result](#), which contains the expectation values for the times specified by `tlist`, and/or the state density matrices corresponding to the times.

**fsesolve**(*H*, *psi0*, *tlist*, *e\_ops*=None, *T*=0.0, *args*=None, *options*=None)

Solve the Schrodinger equation using the Floquet formalism.

## Parameters

**H**

[[Qobj](#), [QobjEvo](#), [QobjEvo](#) compatible format.] Periodic system Hamiltonian as [QobjEvo](#). List of [[Qobj](#), [Coefficient](#)] or callable that can be made into [QobjEvo](#) are also accepted.

**psi0**

[[Qobj](#)] Initial state vector (ket). If an operator is provided,

**tlist**

[list / array] List of times for *t*.

**e\_ops**

[list of [Qobj](#) / callback function, optional] List of operators for which to evaluate expectation values. If this list is empty, the state vectors for each time in *tlist* will be returned instead of expectation values.

**T**

[float, default=tlist[-1]] The period of the time-dependence of the hamiltonian.

**args**

[dictionary, optional] Dictionary with variables required to evaluate H.

### options

[dict, optional] Options for the results.

- `store_final_state` : bool  
Whether or not to store the final state of the evolution in the result class.
- `store_states` : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- `normalize_output` : bool  
Normalize output state to hide ODE numerical errors.

### Returns

#### output

[[Result](#)] An instance of the class [Result](#), which contains either an *array* of expectation values or an array of state vectors, for the times specified by *tlist*.

## Stochastic Schrödinger Equation and Master Equation

**smesolve**(*H*, *rho0*, *tlist*, *c\_ops*=(), *sc\_ops*=(), *heterodyne*=False, \*, *e\_ops*=(), *args*={}, *ntraj*=500, *options*=None, *seeds*=None, *target\_tol*=None, *timeout*=None, *\*\*kwargs*)

Solve stochastic master equation.

### Parameters

#### H

[[Qobj](#), [QobjEvo](#), [QobjEvo](#) compatible format.] System Hamiltonian as a [Qobj](#) or [QobjEvo](#) for time-dependent Hamiltonians. List of [[Qobj](#), [Coefficient](#)] or callable that can be made into [QobjEvo](#) are also accepted.

#### rho0

[[Qobj](#)] Initial density matrix or state vector (ket).

#### tlist

[list / array] List of times for *t*.

#### c\_ops

[list of ([QobjEvo](#), [QobjEvo](#) compatible format), optional] Deterministic collapse operator which will contribute with a standard Lindblad type of dissipation.

#### sc\_ops

[list of ([QobjEvo](#), [QobjEvo](#) compatible format)] List of stochastic collapse operators.

#### e\_ops

[*: qobj*, callable, or list, optional] Single operator or list of operators for which to evaluate expectation values or callable or list of callable. Callable signature must be, *f(t: float, state: Qobj)*. See [expect](#) for more detail of operator expectation.

#### args

[dict, optional] Dictionary of parameters for time-dependent Hamiltonians and collapse operators.

#### ntraj

[int, default: 500] Number of trajectories to compute.

#### heterodyne

[bool, default: False] Whether to use heterodyne or homodyne detection.

#### seeds

[int, [SeedSequence](#), list, optional] Seed for the random number generator. It can be a single seed used to spawn seeds for each trajectory or a list of seeds, one for each trajectory. Seeds are saved in the result and they can be reused with:

```
seeds=prev_result.seeds
```

When using a parallel map, the trajectories can be re-ordered.

### target\_tol

[float, tuple, list], optional] Target tolerance of the evolution. The evolution will compute trajectories until the error on the expectation values is lower than this tolerance. The maximum number of trajectories employed is given by `ntraj`. The error is computed using jackknife resampling. `target_tol` can be an absolute tolerance or a pair of absolute and relative tolerance, in that order. Lastly, it can be a list of pairs of (`atol`, `rtol`) for each `e_ops`.

### timeout

[float, optional] Maximum time for the evolution in second. When reached, no more trajectories will be computed. Overwrite the option of the same name.

### options

[dict, optional] Dictionary of options for the solver.

- `store_final_state` : bool  
Whether or not to store the final state of the evolution in the result class.
- `store_states` : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- `store_measurement`: bool  
Whether to store the measurement and wiener process for each trajectories.
- `keep_runs_results` : bool  
Whether to store results from all trajectories or just store the averages.
- `normalize_output` : bool  
Normalize output state to hide ODE numerical errors.
- `progress_bar` : str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- `progress_kwargs` : dict  
kwargs to pass to the `progress_bar`. Qutip's bars use *chunk\_size*.
- `method` : str  
Which stochastic differential equation integration method to use. Main ones are {'euler', 'rouchon', 'platen', 'taylor1.5\_imp'}
- `map` : str {'serial', 'parallel', 'loky', 'mpi'}  
How to run the trajectories. 'parallel' uses the multiprocessing module to run in parallel while 'loky' and 'mpi' use the 'loky' and 'mpi4py' modules to do so.
- `num_cpus` : NoneType, int  
Number of cpus to use when running in parallel. None detect the number of available cpus.
- `dt` : float  
The finite steps lenght for the Stochastic integration method. Default change depending on the integrator.

Additional options are listed under [options](#). More options may be available depending on the selected differential equation integration method, see [SIntegrator](#).

### Returns



**output:** *Result*

An instance of the class *Result*.

**ssesolve**(*H*, *psi0*, *tlist*, *sc\_ops*=(), *heterodyne*=False, \*, *e\_ops*=(), *args*={}, *ntraj*=500, *options*=None, *seeds*=None, *target\_tol*=None, *timeout*=None, \*\**kwargs*)

Solve stochastic Schrodinger equation.

**Parameters**

**H**

[*Qobj*, *QobjEvo*, *QobjEvo* compatible format.] System Hamiltonian as a *Qobj* or *QobjEvo* for time-dependent Hamiltonians. List of [*Qobj*, *Coefficient*] or callable that can be made into *QobjEvo* are also accepted.

**psi0**

[*Qobj*] Initial state vector (ket).

**tlist**

[*list* / *array*] List of times for *t*.

**sc\_ops**

[list of (*QobjEvo*, *QobjEvo* compatible format)] List of stochastic collapse operators.

**e\_ops**

[*qobj*, callable, or list, optional] Single operator or list of operators for which to evaluate expectation values or callable or list of callable. Callable signature must be, *f(t: float, state: Qobj)*. See **expect** for more detail of operator expectation.

**args**

[dict, optional] Dictionary of parameters for time-dependent Hamiltonians and collapse operators.

**ntraj**

[int, default: 500] Number of trajectories to compute.

**heterodyne**

[bool, default: False] Whether to use heterodyne or homodyne detection.

**seeds**

[int, *SeedSequence*, list, optional] Seed for the random number generator. It can be a single seed used to spawn seeds for each trajectory or a list of seeds, one for each trajectory. Seeds are saved in the result and they can be reused with:

```
seeds=prev_result.seeds
```

**target\_tol**

[{float, tuple, list}, optional] Target tolerance of the evolution. The evolution will compute trajectories until the error on the expectation values is lower than this tolerance. The maximum number of trajectories employed is given by *ntraj*. The error is computed using jackknife resampling. *target\_tol* can be an absolute tolerance or a pair of absolute and relative tolerance, in that order. Lastly, it can be a list of pairs of (atol, rtol) for each *e\_ops*.

**timeout**

[float, optional] Maximum time for the evolution in second. When reached, no more trajectories will be computed. Overwrite the option of the same name.

**options**

[dict, optional] Dictionary of options for the solver.

- *store\_final\_state* : bool  
Whether or not to store the final state of the evolution in the result class.
- *store\_states* : bool, None

Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.

- `store_measurement`: bool Whether to store the measurement and wiener process, or brownian noise for each trajectories.
- `keep_runs_results`: bool  
Whether to store results from all trajectories or just store the averages.
- `normalize_output`: bool  
Normalize output state to hide ODE numerical errors.
- `progress_bar`: str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- `progress_kwargs`: dict  
kwargs to pass to the `progress_bar`. Qutip's bars use *chunk\_size*.
- `method`: str  
Which stochastic differential equation integration method to use. Main ones are {'euler', 'rouchon', 'platen', 'taylor1.5\_imp'}
- `map`: str {"serial", "parallel", "loky", "mpi"}  
How to run the trajectories. "parallel" uses the multiprocessing module to run in parallel while "loky" and "mpi" use the "loky" and "mpi4py" modules to do so.
- `num_cpus`: NoneType, int  
Number of cpus to use when running in parallel. None detect the number of available cpus.
- `dt`: float  
The finite steps lenght for the Stochastic integration method. Default change depending on the integrator.

Additional options are listed under [options](#). More options may be available depending on the selected differential equation integration method, see [SIntegrator](#).

## Returns

**output:** [Result](#)

An instance of the class [Result](#).

## Constructing time dependent systems

`coefficient`(*base*, \*, *tlist=None*, *args={}*, *args\_ctypes={}*, *order=3*, *compile\_opt=None*, *function\_style=None*, *boundary\_conditions=None*, \*\**kwargs*)

Build Coefficient for time dependent systems:

```
` QobjEvo = Qobj + Qobj * Coefficient + Qobj * Coefficient + ... `
```

The coefficients can be a function, a string or a numpy array. Other packages may add support for other kind of coefficients.

For function based coefficients, the function signature must be either:

- `f(t, ...)` where the other arguments are supplied as ordinary "pythonic" arguments (e.g. `f(t, w, a=5)`)
- `f(t, args)` where the arguments are supplied in a "dict" named `args`

By default the signature style is controlled by the `qutip.settings.core["function_coefficient_style"]` setting, but it may be overridden here by specifying either `function_style="pythonic"` or `function_style="dict"`.

*Examples:*

- pythonic style function signature:

```
def f1_t(t, w):
    return np.exp(-1j * t * w)

coeff1 = coefficient(f1_t, args={"w": 1.})
```

- dict style function signature:

```
def f2_t(t, args):
    return np.exp(-1j * t * args["w"])

coeff2 = coefficient(f2_t, args={"w": 1.})
```

For string based coefficients, the string must be a compilable python code resulting in a complex. The following symbols are defined:

sin, cos, tan, asin, acos, atan, pi, sinh, cosh, tanh, asinh, acosh, atanh, exp, log, log10, erf, zorf, sqrt, real, imag, conj, abs, norm, arg, proj, numpy as np, scipy.special as spe (python interface) and cython\_special (scipy cython interface)

*Examples:*

```
coeff = coefficient('exp(-1j*w1*t)', args={"w1":1.})
```

‘args’ is needed for string coefficient at compilation. It is a dict of (name:object). The keys must be a valid variables string.

Compilation options can be passed as “compile\_opt=CompilationOptions(...)”.

For numpy array format, the array must be an 1d of dtype float or complex. A list of times (float64) at which the coefficients must be given (tlist). The coefficients array must have the same len as the tlist. The time of the tlist do not need to be equidistant, but must be sorted. By default, a cubic spline interpolation will be used to compute the coefficient at time t. The keyword `order` sets the order of the interpolation. When `order = 0`, the interpolation is step function that evaluates to the most recent value.

*Examples:*

```
tlist = np.logspace(-5,0,100)
H = QobjEvo(np.exp(-1j*tlist), tlist=tlist)
```

scipy.interpolate’s CubicSpline, PPoly and Bspline are also converted to interpolated coefficients (the same kind of coefficient created from ndarray). Other interpolation methods from scipy are converted to a function-based coefficient (the same kind of coefficient created from callables).

### Parameters

#### base

[object] Base object to make into a Coefficient.

#### args

[dict, optional] Dictionary of arguments to pass to the function or string coefficient.

#### order

[int, default=3] Order of the spline for array based coefficient.

#### tlist

[iterable, optional] Times for each element of an array based coefficient.

#### function\_style

[str {"dict", "pythonic", None}, optional] Function signature of function based coefficients.

**args\_ctypes**

[dict, optional] C type for the args when compiling array based coefficients.

**compile\_opt**

[CompilationOptions, optional] Sets of options for the compilation of string based coefficients.

**boundary\_conditions: 2-tupule, str or None, optional**

Specify boundary conditions for spline interpolation.

**\*\*kwargs**

Extra arguments to pass the the coefficients.

## Hierarchical Equations of Motion

This module provides solvers for system-bath evolution using the HEOM (hierarchy equations of motion).

See [https://en.wikipedia.org/wiki/Hierarchical\\_equations\\_of\\_motion](https://en.wikipedia.org/wiki/Hierarchical_equations_of_motion) for a very basic introduction to the technique.

The implementation is derived from the BoFiN library (see <https://github.com/tehrunn/bofin>) which was itself derived from an earlier implementation in QuTiP itself.

For backwards compatibility with QuTiP 4.6 and below, a new version of HSolverDL (the Drude-Lorentz specific HEOM solver) is provided. It is implemented on top of the new HEOMSolver but should largely be a drop-in replacement for the old HSolverDL.

**heomsolve**(*H, bath, max\_depth, state0, tlist, \*, e\_ops=None, args=None, options=None*)

Hierarchical Equations of Motion (HEOM) solver that supports multiple baths.

The baths must be all either bosonic or fermionic baths.

If you need to run many evolutions of the same system and bath, consider using *HEOMSolver* directly to avoid having to continually reconstruct the equation hierarchy for every evolution.

### Parameters

**H**

[*Qobj*, *QobjEvo*] Possibly time-dependent system Liouvillian or Hamiltonian as a *Qobj* or *QobjEvo*. list of [*Qobj*, Coefficient] or callable that can be made into *QobjEvo* are also accepted.

**bath**

[Bath or list of Bath] A *Bath* containing the exponents of the expansion of the bath correlation function and their associated coefficients and coupling operators, or a list of baths.

If multiple baths are given, they must all be either fermionic or bosonic baths.

**max\_depth**

[int] The maximum depth of the heirarchy (i.e. the maximum number of bath exponent “excitations” to retain).

**state0**

[*Qobj* or *HierarchyADOsState* or array-like] If *rho0* is a *Qobj* the it is the initial state of the system (i.e. a *Qobj* density matrix).

If it is a *HierarchyADOsState* or array-like, then *rho0* gives the initial state of all ADOs.

Usually the state of the ADOs would be determine from a previous call to *.run(...)* with the solver results option *store\_ados* set to True. For example, *result = solver.run(...)* could be followed by *solver.run(result.ado\_states[-1], tlist)*.

If a numpy array-like is passed its shape must be `(number_of_ados, n, n)` where `(n, n)` is the system shape (i.e. shape of the system density matrix) and the ADOs must be in the same order as in `.ados.labels`.

#### **tlist**

[list] An ordered list of times at which to return the value of the state.

#### **e\_ops**

[Qobj / QobjEvo / callable / list / dict / None, optional] A list or dictionary of operators as *Qobj*, *QobjEvo* and/or callable functions (they can be mixed) or a single operator or callable function. For an operator *op*, the result will be computed using `(state * op).tr()` and the state at each time *t*. For callable functions, *f*, the result is computed using `f(t, ado_state)`. The values are stored in the `expect` and `e_data` attributes of the result (see the return section below).

#### **args**

[dict, optional] Change the args of the RHS for the evolution.

#### **options**

[dict, optional] Generic solver options.

- `store_final_state` : bool  
Whether or not to store the final state of the evolution in the result class.
- `store_states` : bool, None  
Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- `store_ados` : bool  
Whether or not to store the HEOM ADOs.
- `normalize_output` : bool  
Normalize output state to hide ODE numerical errors.
- `progress_bar` : str {'text', 'enhanced', 'tqdm', ''}  
How to present the solver progress. 'tqdm' uses the python module of the same name and raise an error if not installed. Empty string or False will disable the bar.
- `progress_kwargs` : dict  
kwargs to pass to the progress\_bar. Qutip's bars use *chunk\_size*.
- `state_data_type`: str {'dense', 'CSR', 'Dia', }  
Name of the data type of the state used during the ODE evolution. Use an empty string to keep the input state type. Many integrator can only work with *Dense*.
- `method` : str ["adams", "bdf", "lsoda", "dop853", "vern9", etc.]  
Which differential equation integration method to use.
- `atol, rtol` : float  
Absolute and relative tolerance of the ODE integrator.
- `nsteps` : int  
Maximum number of (internally defined) steps allowed in one `tlist` step.
- `max_step` : float,  
Maximum lenght of one internal step. When using pulses, it should be less than half the width of the thinnest pulse.

#### **Returns**

##### *HEOMResult*

The results of the simulation run, with the following important attributes:

- `times`: the times *t* (i.e. the `tlist`).

- **states**: the system state at each time  $t$  (only available if **e\_ops** was `None` or if the solver option **store\_states** was set to `True`).
- **ado\_states**: the full ADO state at each time (only available if the results option **ado\_return** was set to `True`). Each element is an instance of [HierarchyADOsState](#). The state of a particular ADO may be extracted from `result.ado_states[i]` by calling `extract`.
- **expect**: a list containing the values of each **e\_ops** at time  $t$ .
- **e\_data**: a dictionary containing the values of each **e\_ops** at time  $t$ . The keys are those given by **e\_ops** if it was a dict, otherwise they are the indexes of the supplied **e\_ops**.

See [HEOMResult](#) and [Result](#) for the complete list of attributes.

## Correlation Functions

**coherence\_function\_g1**(*H, state0, taulist, c\_ops, a\_op, solver='me', args=None, options=None*)

Calculate the normalized first-order quantum coherence function:

$$g^{(1)}(\tau) = \frac{\langle A^\dagger(\tau)A(0) \rangle}{\sqrt{\langle A^\dagger(\tau)A(\tau) \rangle \langle A^\dagger(0)A(0) \rangle}}$$

using the quantum regression theorem and the evolution solver indicated by the *solver* parameter.

### Parameters

**H**

[[Qobj](#), [QobjEvo](#)] System Hamiltonian, may be time-dependent for solver choice of *me*.

**state0**

[[Qobj](#)] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ . If 'state0' is 'None', then the steady state will be used as the initial state. The 'steady-state' is only implemented if **c\_ops** are provided and the Hamiltonian is constant.

**taulist**

[array\_like] List of times for  $\tau$ . **taulist** must be positive and contain the element 0.

**c\_ops**

[list of [[Qobj](#), [QobjEvo](#)]] List of collapse operators

**a\_op**

[[Qobj](#), [QobjEvo](#)] Operator A.

**solver**

[str {'me', 'es'}, default: 'me'] Choice of solver, *me* for master-equation, and *es* for exponential series. *es* is equivalent to *me* with `options={"method": "diag"}`.

**args**

[dict, optional] dictionary of parameters for time-dependent Hamiltonians

**options**

[dict, optional] Options for the solver.

### Returns

**g1, G1**

[tuple] The normalized and unnormalized second-order coherence function.

**coherence\_function\_g2**(*H, state0, taulist, c\_ops, a\_op, solver='me', args=None, options=None*)

Calculate the normalized second-order quantum coherence function:

$$g^{(2)}(\tau) = \frac{\langle A^\dagger(0)A^\dagger(\tau)A(\tau)A(0) \rangle}{\langle A^\dagger(\tau)A(\tau) \rangle \langle A^\dagger(0)A(0) \rangle}$$

using the quantum regression theorem and the evolution solver indicated by the *solver* parameter.

## Parameters

### H

[*Qobj*, *QobjEvo*] System Hamiltonian, may be time-dependent for solver choice of *me*.

### state0

[*Qobj*] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ . If 'state0' is 'None', then the steady state will be used as the initial state. The 'steady-state' is only implemented if *c\_ops* are provided and the Hamiltonian is constant.

### taulist

[array\_like] List of times for  $\tau$ . *taulist* must be positive and contain the element 0.

### c\_ops

[list] List of collapse operators, may be time-dependent for solver choice of *me*.

### a\_op

[*Qobj*] Operator A.

### args

[dict, optional] Dictionary of arguments to be passed to solver.

### solver

[str {'me', 'es'}, default: 'me'] Choice of solver, *me* for master-equation, and *es* for exponential series. *es* is equivalent to *me* with `options={"method": "diag"}`.

### options

[dict, optional] Options for the solver.

## Returns

### g2, G2

[tuple] The normalized and unnormalized second-order coherence function.

**correlation\_2op\_1t**(*H*, *state0*, *taulist*, *c\_ops*, *a\_op*, *b\_op*, *solver*='me', *reverse*=False, *args*=None, *options*=None)

Calculate the two-operator one-time correlation function:  $\langle A(\tau)B(0) \rangle$  along one time axis using the quantum regression theorem and the evolution solver indicated by the *solver* parameter.

## Parameters

### H

[*Qobj*, *QobjEvo*] System Hamiltonian, may be time-dependent for solver choice of *me*.

### state0

[*Qobj*] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ . If 'state0' is 'None', then the steady state will be used as the initial state. The 'steady-state' is only implemented if *c\_ops* are provided and the Hamiltonian is constant.

### taulist

[array\_like] List of times for  $\tau$ . *taulist* must be positive and contain the element 0.

### c\_ops

[list of {*Qobj*, *QobjEvo*}] List of collapse operators

### a\_op

[*Qobj*, *QobjEvo*] Operator A.

### b\_op

[*Qobj*, *QobjEvo*] Operator B.

### reverse

[bool, default: False] If True, calculate  $\langle A(t)B(t + \tau) \rangle$  instead of  $\langle A(t + \tau)B(t) \rangle$ .

### solver

[str {'me', 'es'}, default: 'me'] Choice of solver, *me* for master-equation, and *es* for exponential series. *es* is equivalent to *me* with `options={"method": "diag"}`.

**options**

[dict, optional] Options for the solver.

**Returns**

**corr\_vec**

[ndarray] An array of correlation values for the times specified by `taulist`.

See also:

[\*correlation\\_3op\*](#)

Similar function supporting various solver types.

**References**

See, Gardiner, Quantum Noise, Section 5.2.

**correlation\_2op\_2t**(*H, state0, tlist, taulist, c\_ops, a\_op, b\_op, solver='me', reverse=False, args=None, options=None*)

Calculate the two-operator two-time correlation function:  $\langle A(t + \tau)B(t) \rangle$  along two time axes using the quantum regression theorem and the evolution solver indicated by the `solver` parameter.

**Parameters**

**H**

[*Qobj*, *QobjEvo*] System Hamiltonian, may be time-dependent for solver choice of *me*.

**state0**

[*Qobj*] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ . If 'state0' is 'None', then the steady state will be used as the initial state. The 'steady-state' is only implemented if `c_ops` are provided and the Hamiltonian is constant.

**tlist**

[array\_like] List of times for  $t$ . `tlist` must be positive and contain the element 0. When taking steady-steady correlations only one `tlist` value is necessary, i.e. when  $t \rightarrow \infty$ . If `tlist` is None, `tlist=[0]` is assumed.

**taulist**

[array\_like] List of times for  $\tau$ . `taulist` must be positive and contain the element 0.

**c\_ops**

[list of [*Qobj*, *QobjEvo*]] List of collapse operators

**a\_op**

[*Qobj*, *QobjEvo*] Operator A.

**b\_op**

[*Qobj*, *QobjEvo*] Operator B.

**reverse**

[bool, default: False] If True, calculate  $\langle A(t)B(t + \tau) \rangle$  instead of  $\langle A(t + \tau)B(t) \rangle$ .

**solver**

[str {'me', 'es'}, default: 'me'] Choice of solver, *me* for master-equation, and *es* for exponential series. *es* is equivalent to *me* with `options={"method": "diag"}`.

**options**

[dict, optional] Options for the solver.

**Returns**

**corr\_mat**

[ndarray] An 2-dimensional array (matrix) of correlation values for the times specified by `tlist` (first index) and `taulist` (second index).

See also:



### **correlation\_3op**

Similar function supporting various solver types.

### **References**

See, Gardiner, Quantum Noise, Section 5.2.

**correlation\_3op**(*solver*, *state0*, *tlist*, *taulist*, *A=None*, *B=None*, *C=None*)

Calculate the three-operator two-time correlation function:

$$\langle A(t)B(t+\tau)C(t) \rangle.$$

from a open system *Solver*.

Note: it is not possible to calculate a physically meaningful correlation where  $\tau < 0$ .

#### **Parameters**

**solver**

[*MESolver*, *BRSolver*] Qutip solver for an open system.

**state0**

[*Qobj*] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ .

**tlist**

[array\_like] List of times for  $t$ . tlist must be positive and contain the element 0.

**taulist**

[array\_like] List of times for  $\tau$ . taulist must be positive and contain the element 0.

**A, B, C**

[*Qobj*, *QobjEvo*, optional, default=None] Operators A, B, C from the equation  $\langle A(t)B(t+\tau)C(t) \rangle$  in the Schrodinger picture. They do not need to be all provided. For example, if A is not provided,  $\langle B(t+\tau)C(t) \rangle$  is computed.

#### **Returns**

**corr\_mat**

[array] An 2-dimensional array (matrix) of correlation values for the times specified by *tlist* (first index) and *taulist* (second index). If *tlist* is None, then a 1-dimensional array of correlation values is returned instead.

**correlation\_3op\_1t**(*H*, *state0*, *taulist*, *c\_ops*, *a\_op*, *b\_op*, *c\_op*, *solver='me'*, *args=None*, *options=None*)

Calculate the three-operator two-time correlation function:  $\langle A(0)B(\tau)C(0) \rangle$  along one time axis using the quantum regression theorem and the evolution solver indicated by the *solver* parameter.

Note: it is not possible to calculate a physically meaningful correlation of this form where  $\tau < 0$ .

#### **Parameters**

**H**

[*Qobj*, *QobjEvo*] System Hamiltonian, may be time-dependent for solver choice of *me*.

**state0**

[*Qobj*] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ . If 'state0' is 'None', then the steady state will be used as the initial state. The 'steady-state' is only implemented if *c\_ops* are provided and the Hamiltonian is constant.

**taulist**

[array\_like] List of times for  $\tau$ . taulist must be positive and contain the element 0.

**c\_ops**

[list of [*Qobj*, *QobjEvo*]] List of collapse operators

**a\_op**

[*Qobj*, *QobjEvo*] Operator A.

**b\_op**

[*Qobj*, *QobjEvo*] Operator B.

**c\_op**

[*Qobj*, *QobjEvo*] Operator C.

**solver**

[str {'me', 'es'}, default: 'me'] Choice of solver, me for master-equation, and es for exponential series. es is equivalent to me with options={"method": "diag"}.

**options**

[dict, optional] Options for the solver.

## Returns

**corr\_vec**

[array] An array of correlation values for the times specified by **taulist**.

See also:

[\*correlation\\_3op\*](#)

Similar function supporting various solver types.

## References

See, Gardiner, Quantum Noise, Section 5.2.

**correlation\_3op\_2t**(*H*, *state0*, *tlist*, *taulist*, *c\_ops*, *a\_op*, *b\_op*, *c\_op*, *solver*='me', *args*=None, *options*=None)

Calculate the three-operator two-time correlation function:  $\langle A(t)B(t+\tau)C(t) \rangle$  along two time axes using the quantum regression theorem and the evolution solver indicated by the *solver* parameter.

Note: it is not possible to calculate a physically meaningful correlation of this form where  $\tau < 0$ .

## Parameters

**H**

[*Qobj*, *QobjEvo*] System Hamiltonian, may be time-dependent for solver choice of me.

**state0**

[*Qobj*] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ . If 'state0' is 'None', then the steady state will be used as the initial state. The 'steady-state' is only implemented if *c\_ops* are provided and the Hamiltonian is constant.

**tlist**

[array\_like] List of times for *t*. tlist must be positive and contain the element 0. When taking steady-steady correlations only one tlist value is necessary, i.e. when  $t \rightarrow \infty$ . If tlist is None, tlist=[0] is assumed.

**taulist**

[array\_like] List of times for  $\tau$ . taulist must be positive and contain the element 0.

**c\_ops**

[list of {*Qobj*, *QobjEvo*}] List of collapse operators

**a\_op**

[*Qobj*, *QobjEvo*] Operator A.

**b\_op**

[*Qobj*, *QobjEvo*] Operator B.

**c\_op**

[*Qobj*, *QobjEvo*] Operator C.

**solver**

[str {'me', 'es'}, default: 'me'] Choice of solver, me for master-equation, and es for exponential series. es is equivalent to me with options={"method": "diag"}.

**options**

[dict, optional] Options for the solver. Only used with me solver.

**Returns**

**corr\_mat**

[array] An 2-dimensional array (matrix) of correlation values for the times specified by tlist (first index) and taulist (second index).

See also:

[\*correlation\\_3op\*](#)

Similar function supporting various solver types.

**References**

See, Gardiner, Quantum Noise, Section 5.2.

**spectrum**(*H*, *wlist*, *c\_ops*, *a\_op*, *b\_op*, *solver*='es')

Calculate the spectrum of the correlation function  $\lim_{t \rightarrow \infty} \langle A(t + \tau) B(t) \rangle$ , i.e., the Fourier transform of the correlation function:

$$S(\omega) = \int_{-\infty}^{\infty} \lim_{t \rightarrow \infty} \langle A(t + \tau) B(t) \rangle e^{-i\omega\tau} d\tau.$$

using the solver indicated by the **solver** parameter. Note: this spectrum is only defined for stationary statistics (uses steady state rho0)

**Parameters**

**H**

[qobj] system Hamiltonian.

**wlist**

[array\_like] List of frequencies for  $\omega$ .

**c\_ops**

[list] List of collapse operators.

**a\_op**

[Qobj] Operator A.

**b\_op**

[Qobj] Operator B.

**solver**

[str, {'es', 'pi', 'solve'}, default: 'es'] Choice of solver, es for exponential series and pi for psuedo-inverse, solve for generic solver.

**Returns**

**spectrum**

[array] An array with spectrum  $S(\omega)$  for the frequencies specified in *wlist*.

**spectrum\_correlation\_fft**(*tlist*, *y*, *inverse*=False)

Calculate the power spectrum corresponding to a two-time correlation function using FFT.

**Parameters**

**tlist**

[array\_like] list/array of times *t* which the correlation function is given.

**y**  
[array\_like] list/array of correlations corresponding to time delays  $t$ .

**inverse: bool, default: False**

boolean parameter for using a positive exponent in the Fourier Transform instead. Default is False.

### Returns

**w, S**  
[tuple] Returns an array of angular frequencies 'w' and the corresponding two-sided power spectrum 'S(w)'.

## Steady-state Solvers

**pseudo\_inverse**(*L*, *rhoss=None*, *w=None*, *method='splu'*, *\**, *use\_rcm=False*, *\*\*kwargs*)

Compute the pseudo inverse for a Liouvillian superoperator, optionally given its steady state density matrix (which will be computed if not given).

### Parameters

**L**  
[Qobj] A Liouvillian superoperator for which to compute the pseudo inverse.

**rhoss**  
[Qobj, optional] A steadystate density matrix as Qobj instance, for the Liouvillian superoperator L.

**w**  
[double, optional] frequency at which to evaluate pseudo-inverse. Can be zero for dense systems and large sparse systems. Small sparse systems can fail for zero frequencies.

**sparse**  
[bool, optional] Flag that indicate whether to use sparse or dense matrix methods when computing the pseudo inverse.

**method**  
[str, optional] Method used to compute matrix inverse. Choice are 'pinv' to use scipy's function of the same name, or a linear system solver. Default supported solver are:

- "solve", "lstsq" dense solver from numpy.linalg
- "spsolve", "gmres", "lgmres", "bicgstab", "splu" sparse solver from scipy.sparse.linalg
- "mkl\_spsolve", sparse solver by mkl.

Extension to qutip, such as qutip-tensorflow, can use come with their own solver. When L use these data backends, see the corresponding libraries `linalg` for available solver.

**use\_rcm**  
[bool, default: False] Use reverse Cuthill-Mckee reordering to minimize fill-in in the LU factorization of the Liouvillian.

**kwargs**  
[dictionary] Additional keyword arguments for setting parameters for solver methods.

### Returns

**R**  
[Qobj] Returns a Qobj instance representing the pseudo inverse of L.

## Notes

In general the inverse of a sparse matrix will be dense. If you are applying the inverse to a density matrix then it is better to cast the problem as an  $Ax=b$  type problem where the explicit calculation of the inverse is not required. See page 67 of “Electrons in nanostructures” C. Flindt, PhD Thesis available online: <https://orbit.dtu.dk/en/publications/electrons-in-nanostructures-coherent-manipulation-and-counting-st>

Note also that the definition of the pseudo-inverse herein is different from `numpy.linalg.pinv()` alone, as it includes pre and post projection onto the subspace defined by the projector  $Q$ .

**steadystate**( $A$ ,  $c\_ops=[]$ ,  $*$ ,  $method='direct'$ ,  $solver=None$ ,  $**kwargs$ )

Calculates the steady state for quantum evolution subject to the supplied Hamiltonian or Liouvillian operator and (if given a Hamiltonian) a list of collapse operators.

If the user passes a Hamiltonian then it, along with the list of collapse operators, will be converted into a Liouvillian operator in Lindblad form.

### Parameters

**A**

[*Qobj*] A Hamiltonian or Liouvillian operator.

**c\_op\_list**

[list] A list of collapse operators.

**method**

[str, {“direct”, “eigen”, “svd”, “power”}], default: “direct”] The allowed methods are composed of 2 parts, the steadystate method: - “direct”: Solving  $L(\rho_{ss}) = 0$  - “eigen”: Eigenvalue problem - “svd”: Singular value decomposition - “power”: Inverse-power method

**solver**

[str, optional] ‘direct’ and ‘power’ methods only. Solver to use when solving the  $L(\rho_{ss}) = 0$  equation. Default supported solver are:

- “solve”, “lstsq” dense solver from `numpy.linalg`
- “spsolve”, “gmres”, “lgmres”, “bicgstab” sparse solver from `scipy.sparse.linalg`
- “mkl\_spsolve” sparse solver by mkl.

Extension to qutip, such as qutip-tensorflow, can use come with their own solver. When **A** and **c\_ops** use these data backends, see the corresponding libraries `linalg` for available solver.

Extra options for these solver can be passed in **\*\*kw**.

**use\_rcm**

[bool, default: False] Use reverse Cuthill-Mckee reordering to minimize fill-in in the LU factorization of the Liouvillian. Used with ‘direct’ or ‘power’ method.

**use\_wbm**

[bool, default: False] Use Weighted Bipartite Matching reordering to make the Liouvillian diagonally dominant. This is useful for iterative preconditioners only. Used with ‘direct’ or ‘power’ method.

**weight**

[float, optional] Sets the size of the elements used for adding the unity trace condition to the linear solvers. This is set to the average abs value of the Liouvillian elements if not specified by the user. Used with ‘direct’ method.

**power\_tol**

[float, default: 1e-12] Tolerance for the solution when using the ‘power’ method.

**power\_maxiter**

[int, default: 10] Maximum number of iteration to use when looking for a solution when using the ‘power’ method.

**power\_eps: double, default: 1e-15**

Small weight used in the “power” method.

**sparse: bool, default: True**

Whether to use the sparse eigen solver with the “eigen” method (default sparse). With “direct” and “power” method, when the solver is not specified, it is used to set whether “solve” or “spsolve” is used as default solver.

**\*\*kwargs**

Extra options to pass to the linear system solver. See the documentation of the used solver in `numpy.linalg` or `scipy.sparse.linalg` to see what extra arguments are supported.

## Returns

**dm**

[qobj] Steady state density matrix.

**info**

[dict, optional] Dictionary containing solver-specific information about the solution.

## Notes

The SVD method works only for dense operators (i.e. small systems).

**steadystate\_floquet**(*H\_0*, *c\_ops*, *Op\_t*, *w\_d*=1.0, *n\_it*=3, *sparse*=False, *solver*=None, **\*\*kwargs**)

**Calculates the effective steady state for a driven**

system with a time-dependent sinusoidal term:

$$\hat{\mathcal{H}}(t) = \hat{H}_0 + \hat{O} \cos(\omega_d t)$$

## Parameters

**H\_0**

[Qobj] A Hamiltonian or Liouvillian operator.

**c\_ops**

[list] A list of collapse operators.

**Op\_t**

[Qobj] The interaction operator which is multiplied by the cosine

**w\_d**

[float, default: 1.0] The frequency of the drive

**n\_it**

[int, default: 3] The number of iterations for the solver

**sparse**

[bool, default: False] Solve for the steady state using sparse algorithms.

**solver**

[str, optional] Solver to use when solving the linear system. Default supported solver are:

- “solve”, “lstsq” dense solver from `numpy.linalg`
- “spsolve”, “gmres”, “lgmres”, “bicgstab” sparse solver from `scipy.sparse.linalg`
- “mkl\_spsolve” sparse solver by mkl.

Extensions to qutip, such as qutip-tensorflow, may provide their own solvers. When **H\_0** and **c\_ops** use these data backends, see their documentation for the names and details of additional solvers they may provide.

**\*\*kwargs:**

Extra options to pass to the linear system solver. See the documentation of the used solver in `numpy.linalg` or `scipy.sparse.linalg` to see what extra arguments are supported.

**Returns**

**dm**

[qobj] Steady state density matrix.

**Notes**

See: Sze Meng Tan, <https://copilot.caltech.edu/documents/16743/qousersguide.pdf>, Section (10.16)

**Propagators**

**propagator**(*H*, *t*, *c\_ops*=(), *args*=None, *options*=None, **\*\*kwargs**)

Calculate the propagator  $U(t)$  for the density matrix or wave function such that  $\psi(t) = U(t)\psi(0)$  or  $\rho_{vec}(t) = U(t)\rho_{vec}(0)$  where  $\rho_{vec}$  is the vector representation of the density matrix.

**Parameters**

**H**

[Qobj, QobjEvo, QobjEvo compatible format] Possibly time-dependent system Liou-villian or Hamiltonian as a Qobj or QobjEvo. list of [Qobj, Coefficient] or callable that can be made into QobjEvo are also accepted.

**t**

[float or array-like] Time or list of times for which to evaluate the propagator.

**c\_ops**

[list, optional] List of Qobj or QobjEvo collapse operators.

**args**

[dictionary, optional] Parameters to callback functions for time-dependent Hamiltonians and collapse operators.

**options**

[dict, optional] Options for the solver.

**\*\*kwargs**

Extra parameters to use when creating the QobjEvo from a list format H.

**Returns**

**U**

[Qobj, list] Instance representing the propagator(s)  $U(t)$ . Return a single Qobj when *t* is a number or a list when *t* is a list.

**propagator\_steadystate**(*U*)

Find the steady state for successive applications of the propagator *U*.

**Parameters**

**U**

[Qobj] Operator representing the propagator.

**Returns**

**a**

[Qobj] Instance representing the steady-state density matrix.

## Scattering in Quantum Optical Systems

Photon scattering in quantum optical systems

This module includes a collection of functions for numerically computing photon scattering in driven arbitrary systems coupled to some configuration of output waveguides. The implementation of these functions closely follows the mathematical treatment given in K.A. Fischer, et. al., Scattering of Coherent Pulses from Quantum Optical Systems (2017, arXiv:1710.02875).

**scattering\_probability**(*H*, *psi0*, *n\_emissions*, *c\_ops*, *tlist*, *system\_zero\_state*=None, *construct\_effective\_hamiltonian*=True)

Compute the integrated probability of scattering *n* photons in an arbitrary system. This function accepts a nonlinearly spaced array of times.

### Parameters

#### **H**

[*Qobj* or list] System-waveguide(s) Hamiltonian or effective Hamiltonian in *Qobj* or list-callback format. If *construct\_effective\_hamiltonian* is not specified, an effective Hamiltonian is constructed from *H* and *c\_ops*.

#### **psi0**

[*Qobj*] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ .

#### **n\_emissions**

[int] Number of photons emitted by the system (into any combination of waveguides).

#### **c\_ops**

[list] List of collapse operators for each waveguide; these are assumed to include spontaneous decay rates, e.g.  $\sigma = \sqrt{\gamma} \cdot a$ .

#### **tlist**

[array\_like] List of times for  $\tau_i$ . *tlist* should contain 0 and exceed the pulse duration / temporal region of interest; *tlist* need not be linearly spaced.

#### **system\_zero\_state**

[*Qobj*, optional] State representing zero excitations in the system. Defaults to *basis(systemDims, 0)*.

#### **construct\_effective\_hamiltonian**

[bool, default: True] Whether an effective Hamiltonian should be constructed from *H* and *c\_ops*:  $H_{eff} = H - \frac{i}{2} \sum_n \sigma_n^\dagger \sigma_n$  Default: True.

### Returns

#### **scattering\_prob**

[float] The probability of scattering *n* photons from the system over the time range specified.

**temporal\_basis\_vector**(*waveguide\_emission\_indices*, *n\_time\_bins*)

Generate a temporal basis vector for emissions at specified time bins into specified waveguides.

### Parameters

#### **waveguide\_emission\_indices**

[list or tuple] List of indices where photon emission occurs for each waveguide, e.g. [[t1\_wg1], [t1\_wg2, t2\_wg2], [], [t1\_wg4, t2\_wg4, t3\_wg4]].

#### **n\_time\_bins**

[int] Number of time bins; the range over which each index can vary.

### Returns

#### **temporal\_basis\_vector**

[*Qobj*] A basis vector representing photon scattering at the specified indices. If there are *W* waveguides, *T* times, and *N* photon emissions, then the basis vector has dimensionality  $(W \cdot T)^N$ .



**temporal\_scattered\_state**(*H*, *psi0*, *n\_emissions*, *c\_ops*, *tlist*, *system\_zero\_state*=None, *construct\_effective\_hamiltonian*=True)

Compute the scattered n-photon state projected onto the temporal basis.

#### Parameters

##### **H**

[*Qobj* or list] System-waveguide(s) Hamiltonian or effective Hamiltonian in *Qobj* or list-callback format. If *construct\_effective\_hamiltonian* is not specified, an effective Hamiltonian is constructed from *H* and *c\_ops*.

##### **psi0**

[*Qobj*] Initial state density matrix  $\rho(t_0)$  or state vector  $\psi(t_0)$ .

##### **n\_emissions**

[int] Number of photon emissions to calculate.

##### **c\_ops**

[list] List of collapse operators for each waveguide; these are assumed to include spontaneous decay rates, e.g.  $\sigma = \sqrt{\gamma} \cdot a$

##### **tlist**

[array\_like] List of times for  $\tau_i$ . *tlist* should contain 0 and exceed the pulse duration / temporal region of interest.

##### **system\_zero\_state**

[*Qobj*, optional] State representing zero excitations in the system. Defaults to  $\psi(t_0)$

##### **construct\_effective\_hamiltonian**

[bool, default: True] Whether an effective Hamiltonian should be constructed from *H* and *c\_ops*:  $H_{eff} = H - \frac{i}{2} \sum_n \sigma_n^\dagger \sigma_n$  Default: True.

#### Returns

##### **phi\_n**

[*Qobj*] The scattered bath state projected onto the temporal basis given by *tlist*. If there are *W* waveguides, *T* times, and *N* photon emissions, then the state is a tensor product state with dimensionality  $T^{(W*N)}$ .

## Permutational Invariance

Permutational Invariant Quantum Solver (PIQS)

This module calculates the Liouvillian for the dynamics of ensembles of identical two-level systems (TLS) in the presence of local and collective processes by exploiting permutational symmetry and using the Dicke basis. It also allows to characterize nonlinear functions of the density matrix.

**am**(*j*, *m*)

Calculate the operator *am* used later.

The action of *ap* is given by:  $J_-|j, m\rangle = A_-(jm)|j, m-1\rangle$

#### Parameters

##### **j: float**

The value for *j*.

##### **m: float**

The value for *m*.

#### Returns

##### **a\_minus: float**

The value of  $a_-$ .

**ap**( $j, m$ )

Calculate the coefficient  $a_p$  by applying  $J_+|j, m\rangle$ .

The action of  $a_p$  is given by:  $J_+|j, m\rangle = A_+(j, m)|j, m+1\rangle$

**Parameters**

**j, m: float**

The value for  $j$  and  $m$  in the Dicke basis  $|j, m\rangle$ .

**Returns**

**a\_plus: float**

The value of  $a_+$ .

**block\_matrix**( $N$ , *elements='ones'*)

Construct the block-diagonal matrix for the Dicke basis.

**Parameters**

**N**

[int] Number of two-level systems.

**elements**

[str {'ones', 'degeneracy'}, default: 'ones']

**Returns**

**block\_matr**

[ndarray] A 2D block-diagonal matrix with dimension (nds,nds), where nds is the number of Dicke states for  $N$  two-level systems. Filled with ones or the value of degeneracy at each matrix element.

**collapse\_uncoupled**( $N$ , *emission=0.0, dephasing=0.0, pumping=0.0, collective\_emission=0.0, collective\_dephasing=0.0, collective\_pumping=0.0*)

Create the collapse operators ( $c_{ops}$ ) of the Lindbladian in the uncoupled basis

These operators are in the uncoupled basis of the two-level system (TLS)  $SU(2)$  Pauli matrices.

**Parameters**

**N: int**

The number of two-level systems.

**emission: float, default: 0.0**

Incoherent emission coefficient (also nonradiative emission).

**dephasing: float, default: 0.0**

Local dephasing coefficient.

**pumping: float, default: 0.0**

Incoherent pumping coefficient.

**collective\_emission: float, default: 0.0**

Collective (superradiant) emission coefficient.

**collective\_pumping: float, default: 0.0**

Collective pumping coefficient.

**collective\_dephasing: float, default: 0.0**

Collective dephasing coefficient.

**Returns**

**c\_ops: list**

The list of collapse operators as [Qobj](#) for the system.

## Notes

The collapse operator list can be given to *qutip.mesolve*. Notice that the operators are placed in a Hilbert space of dimension  $2^N$ . Thus the method is suitable only for small N (of the order of 10).

**css**(*N*, *x*=0.7071067811865475, *y*=0.7071067811865475, *basis*='dicke', *coordinates*='cartesian')

Generate the density matrix of the Coherent Spin State (CSS).

It can be defined as,  $|CSS\rangle = \prod_i^N (a|1\rangle_i + b|0\rangle_i)$  with  $a = \sin(\frac{\theta}{2})$ ,  $b = e^{i\phi} \cos(\frac{\theta}{2})$ . The default basis is that of Dicke space  $|j, m\rangle\langle j, m'|$ . The default state is the symmetric CSS,  $|CSS\rangle = |+\rangle$ .

### Parameters

**N: int**

The number of two-level systems.

**x, y: float, default: sqrt(1/2)**

The coefficients of the CSS state.

**basis: str {"dicke", "uncoupled"}, default: "dicke"**

The basis to use.

**coordinates: str {"cartesian", "polar"}, default: "cartesian"**

If polar then the coefficients are constructed as  $\sin(x/2), \cos(x/2)e^{iy}$ .

### Returns

**rho: Qobj**

The CSS state density matrix.

**dicke**(*N*, *j*, *m*)

Generate a Dicke state as a pure density matrix in the Dicke basis.

For instance, the superradiant state given by  $|j, m\rangle = |1, 0\rangle$  for  $N=2$ , and the state is represented as a density matrix of size (nds, nds) or (4, 4), with the (1, 1) element set to 1.

### Parameters

**N: int**

The number of two-level systems.

**j: float**

The eigenvalue j of the Dicke state (j, m).

**m: float**

The eigenvalue m of the Dicke state (j, m).

### Returns

**rho: Qobj**

The density matrix.

**dicke\_basis**(*N*, *jmm1*)

Initialize the density matrix of a Dicke state for several (j, m, m1).

This function can be used to build arbitrary states in the Dicke basis  $|j, m\rangle\langle j, m'|$ . We create coefficients for each (j, m, m1) value in the dictionary *jmm1*. The mapping for the (i, k) index of the density matrix to the  $|j, m\rangle$  values is given by the cythonized function *jmm1\_dictionary*. A density matrix is created from the given dictionary of coefficients for each (j, m, m1).

### Parameters

**N: int**

The number of two-level systems.

**jmm1: dict**

A dictionary of {(j, m, m1): p} that gives a density p for the (j, m, m1) matrix element.

### Returns

**rho:** *Qobj*

The density matrix in the Dicke basis.

**dicke\_blocks**(*rho*)

Create the list of blocks for block-diagonal density matrix in the Dicke basis.

**Parameters**

**rho**

[*Qobj*] A 2D block-diagonal matrix of ones with dimension (nds,nds), where nds is the number of Dicke states for N two-level systems.

**Returns**

**square\_blocks:** list of np.ndarray

Give back the blocks list.

**dicke\_blocks\_full**(*rho*)

Give the full ( $2^N$ -dimensional) list of blocks for a Dicke-basis matrix.

**Parameters**

**rho**

[*Qobj*] A 2D block-diagonal matrix of ones with dimension (nds,nds), where nds is the number of Dicke states for N two-level systems.

**Returns**

**full\_blocks**

[list] The list of blocks expanded in the  $2^N$  space for N qubits.

**dicke\_function\_trace**(*f*, *rho*)

Calculate the trace of a function on a Dicke density matrix. :param f: A Taylor-expandable function of *rho*.

:type f: function :param rho: A density matrix in the Dicke basis. :type rho: *Qobj*

**Returns**

**res**

[float] Trace of a nonlinear function on *rho*.

**energy\_degeneracy**(*N*, *m*)

Calculate the number of Dicke states with same energy.

The use of the `Decimals` class allows to explore  $N > 1000$ , unlike the built-in function `scipy.special.binom`.

**Parameters**

**N:** int

The number of two-level systems.

**m:** float

Total spin z-axis projection eigenvalue. This is proportional to the total energy.

**Returns**

**degeneracy:** int

The energy degeneracy

**entropy\_vn\_dicke**(*rho*)

Von Neumann Entropy of a Dicke-basis density matrix.

**Parameters**

**rho**

[*Qobj*] A 2D block-diagonal matrix of ones with dimension (nds, nds), where nds is the number of Dicke states for N two-level systems.

**Returns**

**entropy\_dm: float**

Entropy. Use degeneracy to multiply each block.

**excited**(*N*, *basis*='dicke')

Generate the density matrix for the excited state.

This state is given by (N/2, N/2) in the default Dicke basis. If the argument *basis* is “uncoupled” then it generates the state in a  $2^N$  dimensional Hilbert space.

**Parameters**

**N: int**

The number of two-level systems.

**basis: str, {“dicke”, “uncoupled”}, default: “dicke”**

The basis to use.

**Returns**

**state: *Qobj***

The excited state density matrix in the requested basis.

**ghz**(*N*, *basis*='dicke')

Generate the density matrix of the GHZ state.

If the argument *basis* is “uncoupled” then it generates the state in a  $2^N$ -dimensional Hilbert space.

**Parameters**

**N: int**

The number of two-level systems.

**basis: str, {“dicke”, “uncoupled”}, default: “dicke”**

The basis to use.

**Returns**

**state: *Qobj***

The GHZ state density matrix in the requested basis.

**ground**(*N*, *basis*='dicke')

Generate the density matrix of the ground state.

This state is given by (N/2, -N/2) in the Dicke basis. If the argument *basis* is “uncoupled” then it generates the state in a  $2^N$ -dimensional Hilbert space.

**Parameters**

**N: int**

The number of two-level systems.

**basis: str, {“dicke”, “uncoupled”}, default: “dicke”**

The basis to use.

**Returns**

**state: *Qobj***

The ground state density matrix in the requested basis.

**identity\_uncoupled**(*N*)

Generate the identity in a  $2^N$ -dimensional Hilbert space.

The identity matrix is formed from the tensor product of N TLSs.

**Parameters**

**N: int**

The number of two-level systems.

**Returns**

**identity:** *Qobj*

The identity matrix.

**isdiagonal**(*mat*)

Check if the input matrix is diagonal.

**Parameters**

**mat:** ndarray/Qobj

A 2D numpy array

**Returns**

**diag:** bool

True/False depending on whether the input matrix is diagonal.

**jspin**(*N, op=None, basis='dicke'*)

Calculate the list of collective operators of the total algebra.

The Dicke basis  $|j, m\rangle\langle j, m'|$  is used by default. Otherwise with “uncoupled” the operators are in a  $2^N$  space.

**Parameters**

**N:** int

Number of two-level systems.

**op:** str {'x', 'y', 'z', '+', '-'}, optional

The operator to return 'x','y','z','+','-'. If no operator given, then output is the list of operators for ['x','y','z'].

**basis:** str {"dicke", "uncoupled"}, default: “dicke”

The basis of the operators.

**Returns**

**j\_alg:** list or *Qobj*

A list of *qutip.Qobj* representing all the operators in the “dicke” or “uncoupled” basis or a single operator requested.

**m\_degeneracy**(*N, m*)

Calculate the number of Dicke states  $|j, m\rangle$  with same energy.

**Parameters**

**N:** int

The number of two-level systems.

**m:** float

Total spin z-axis projection eigenvalue (proportional to the total energy).

**Returns**

**degeneracy:** int

The m-degeneracy.

**num\_dicke\_ladders**(*N*)

Calculate the total number of ladders in the Dicke space.

For a collection of N two-level systems it counts how many different “j” exist or the number of blocks in the block-diagonal matrix.

**Parameters**

**N:** int

The number of two-level systems.

**Returns**

**Nj: int**

The number of Dicke ladders.

**num\_dicke\_states**(*N*)

Calculate the number of Dicke states.

**Parameters**

**N: int**

The number of two-level systems.

**Returns**

**nds: int**

The number of Dicke states.

**num\_tls**(*nds*)

Calculate the number of two-level systems.

**Parameters**

**nds: int**

The number of Dicke states.

**Returns**

**N: int**

The number of two-level systems.

**purity\_dicke**(*rho*)

Calculate purity of a density matrix in the Dicke basis. It accounts for the degenerate blocks in the density matrix.

**Parameters**

**rho**

[*Qobj*] Density matrix in the Dicke basis of `qutip.piqs.jspin(N)`, for *N* spins.

**Returns**

**purity**

[float] The purity of the quantum state. It's 1 for pure states,  $0 \leq \text{purity} < 1$  for mixed states.

**spin\_algebra**(*N*, *op=None*)

Create the list [*sx*, *sy*, *sz*] with the spin operators.

The operators are constructed for a collection of *N* two-level systems (TLSs). Each element of the list, i.e., *sx*, is a vector of *qutip.Qobj* objects (spin matrices), as it contains the list of the SU(2) Pauli matrices for the *N* TLSs. Each TLS operator *sx*[*i*], with *i* = 0, ..., (*N*-1), is placed in a  $2^N$ -dimensional Hilbert space.

**Parameters**

**N: int**

The number of two-level systems.

**Returns**

**spin\_operators: list or *Qobj***

A list of *qutip.Qobj* operators - [*sx*, *sy*, *sz*] or the requested operator.

## Notes

$sx[i]$  is  $\frac{\sigma_x}{2}$  in the composite Hilbert space.

### **state\_degeneracy**( $N, j$ )

Calculate the degeneracy of the Dicke state.

Each state  $|j, m\rangle$  includes  $D(N, j)$  irreducible representations  $|j, m, \alpha\rangle$ .

Uses Decimals to calculate higher numerator and denominators numbers.

#### Parameters

**N: int**

The number of two-level systems.

**j: float**

Total spin eigenvalue (cooperativity).

#### Returns

**degeneracy: int**

The state degeneracy.

### **superradiant**( $N, basis='dicke'$ )

Generate the density matrix of the superradiant state.

This state is given by  $(N/2, 0)$  or  $(N/2, 0.5)$  in the Dicke basis. If the argument *basis* is “uncoupled” then it generates the state in a  $2^{*N}$  dim Hilbert space.

#### Parameters

**N: int**

The number of two-level systems.

**basis: str, {“dicke”, “uncoupled”}, default: “dicke”**

The basis to use.

#### Returns

**state: Qobj**

The superradiant state density matrix in the requested basis.

### **tau\_column**( $\tau, k, j$ )

Determine the column index for the non-zero elements of the matrix for a particular row  $k$  and the value of  $j$  from the Dicke space.

#### Parameters

**tau: str**

The tau function to check for this  $k$  and  $j$ .

**k: int**

The row of the matrix  $M$  for which the non zero elements have to be calculated.

**j: float**

The value of  $j$  for this row.



## 5.2.5 Visualization

### Pseudoprobability Functions

**qfunc**(state: Qobj, xvec, yvec, g: float = 1.4142135623730951, precompute\_memory: float = 1024)

Husimi-Q function of a given state vector or density matrix at phase-space points  $0.5 * g * (xvec + i*yvec)$ .

#### Parameters

##### state

[Qobj] A state vector or density matrix. This cannot have tensor-product structure.

##### xvec, yvec

[array\_like] x- and y-coordinates at which to calculate the Husimi-Q function.

##### g

[float, default: sqrt(2)] Scaling factor for  $a = 0.5 * g * (x + iy)$ . The value of  $g$  is related to the value of  $\hbar$  in the commutation relation  $[x, y] = i\hbar$  via  $\hbar = 2/g^2$ , so the default corresponds to  $\hbar = 1$ .

##### precompute\_memory

[real, default: 1024] Size in MB that may be used during calculations as working space when dealing with density-matrix inputs. This is ignored for state-vector inputs. The bound is not quite exact due to other, order-of-magnitude smaller, intermediaries being necessary, but is a good approximation. If you want to use the same iterative algorithm for density matrices that is used for single kets, set `precompute_memory=None`.

#### Returns

##### ndarray

Values representing the Husimi-Q function calculated over the specified range [xvec, yvec].

#### See also:

##### QFunc

a class-based version, more efficient if you want to calculate the Husimi-Q function for several states over the same coordinates.

**spin\_q\_function**(rho, theta, phi)

The Husimi Q function for spins is defined as  $Q(\theta, \phi) = \text{SCS.dag}() * \rho * \text{SCS}$  for the spin coherent state  $\text{SCS} = \text{spin\_coherent}(j, \theta, \phi)$  where  $j$  is the spin length. The implementation here is more efficient as it doesn't generate all of the SCS at  $\theta$  and  $\phi$  (see references).

The spin Q function is normal when integrated over the surface of the sphere

$$\frac{4\pi}{2j+1} \int_{\phi} \int_{\theta} Q(\theta, \phi) \sin(\theta) d\theta d\phi = 1$$

#### Parameters

##### state

[qobj] A state vector or density matrix for a spin-j quantum system.

##### theta

[array\_like] Polar (colatitude) angle at which to calculate the Husimi-Q function.

##### phi

[array\_like] Azimuthal angle at which to calculate the Husimi-Q function.

#### Returns

##### Q, THETA, PHI

[2d-array] Values representing the spin Husimi Q function at the values specified by THETA and PHI.

## References

- [1] Lee Loh, Y., & Kim, M. (2015). American J. of Phys., 83(1), 30–35. <https://doi.org/10.1119/1.4898595>

**spin\_wigner**(*rho*, *theta*, *phi*)

Wigner function for a spin-j system.

The spin W function is normal when integrated over the surface of the sphere

$$\sqrt{\frac{4\pi}{2j+1}} \int_{\phi} \int_{\theta} W(\theta, \phi) \sin(\theta) d\theta d\phi = 1$$

## Parameters

**state**

[qobj] A state vector or density matrix for a spin-j quantum system.

**theta**

[array\_like] Polar (colatitude) angle at which to calculate the W function.

**phi**

[array\_like] Azimuthal angle at which to calculate the W function.

## Returns

**W, THETA, PHI**

[2d-array] Values representing the spin Wigner function at the values specified by THETA and PHI.

## References

- [1] Agarwal, G. S. (1981). Phys. Rev. A, 24(6), 2889–2896. <https://doi.org/10.1103/PhysRevA.24.2889>
- [2] Dowling, J. P., Agarwal, G. S., & Schleich, W. P. (1994). Phys. Rev. A, 49(5), 4101–4109. <https://doi.org/10.1103/PhysRevA.49.4101>
- [3] Conversion between Wigner 3-j symbol and Clebsch-Gordan coefficients taken from Wikipedia ([https://en.wikipedia.org/wiki/3-j\\_symbol](https://en.wikipedia.org/wiki/3-j_symbol))

**wigner**(*psi*, *xvec*, *yvec*=None, *method*='clenshaw', *g*=1.4142135623730951, *sparse*=False, *parfor*=False)

Wigner function for a state vector or density matrix at points *xvec* + *i* \* *yvec*.

## Parameters

**state**

[qobj] A state vector or density matrix.

**xvec**

[array\_like] x-coordinates at which to calculate the Wigner function.

**yvec**

[array\_like] y-coordinates at which to calculate the Wigner function. Does not apply to the 'fft' method.

**g**

[float, default: sqrt(2)] Scaling factor for  $a = 0.5 * g * (x + iy)$ , default  $g = \sqrt{2}$ . The value of  $g$  is related to the value of  $\hbar$  in the commutation relation  $[x, y] = i * \hbar$  via  $\hbar = 2/g^2$  giving the default value  $\hbar = 1$ .

**method**

[string {'clenshaw', 'iterative', 'laguerre', 'fft'}, default: 'clenshaw'] Select method 'clenshaw', 'iterative', 'laguerre', or 'fft', where 'clenshaw' and 'iterative' use an iterative method to evaluate the Wigner functions for density matrices  $|m\rangle\langle n|$ , while 'laguerre' uses the Laguerre polynomials in scipy for the same task. The 'fft' method evaluates the Fourier transform of the density matrix. The 'iterative' method is default,

and in general recommended, but the ‘laguerre’ method is more efficient for very sparse density matrices (e.g., superpositions of Fock states in a large Hilbert space). The ‘clenshaw’ method is the preferred method for dealing with density matrices that have a large number of excitations ( $> \sim 50$ ). ‘clenshaw’ is a fast and numerically stable method.

**sparse**

[bool, optional] Tells the default solver whether or not to keep the input density matrix in sparse format. As the dimensions of the density matrix grow, setting this flag can result in increased performance.

**parfor**

[bool, optional] Flag for calculating the Laguerre polynomial based Wigner function method=‘laguerre’ in parallel using the parfor function.

**Returns**

**W**

[array] Values representing the Wigner function calculated over the specified range [xvec,yvec].

**yvec**

[array] FFT ONLY. Returns the y-coordinate values calculated via the Fourier transform.

**Notes**

The ‘fft’ method accepts only an xvec input for the x-coordinate. The y-coordinates are calculated internally.

**References**

Ulf Leonhardt, Measuring the Quantum State of Light, (Cambridge University Press, 1997)

**Graphs and Visualization**

Functions for visualizing results of quantum dynamics simulations, visualizations of quantum states and processes.

**hinton**(rho, x\_basis=None, y\_basis=None, color\_style='scaled', label\_top=True, \*, cmap=None, colorbar=True, fig=None, ax=None)

Draws a Hinton diagram to visualize a density matrix or superoperator.

**Parameters**

**rho**

[qobj] Input density matrix or superoperator.

---

**Note:** Hinton plots of superoperators are currently only supported for qubits.

---

**x\_basis**

[list of strings, optional] list of x ticklabels to represent x basis of the input.

**y\_basis**

[list of strings, optional] list of y ticklabels to represent y basis of the input.

**color\_style**

[str, {"scaled", "threshold", "phase"}], default: “scaled”] Determines how colors are assigned to each square:

- If set to "scaled" (default), each color is chosen by passing the absolute value of the corresponding matrix element into *cmap* with the sign of the real part.

- If set to "threshold", each square is plotted as the maximum of *cmap* for the positive real part and as the minimum for the negative part of the matrix element; note that this generalizes "threshold" to complex numbers.
- If set to "phase", each color is chosen according to the angle of the corresponding matrix element.

**label\_top**

[bool, default: True] If True, x ticklabels will be placed on top, otherwise they will appear below the plot.

**cmap**

[a matplotlib colormap instance, optional] Color map to use when plotting.

**colorbar**

[bool, default: True] Whether (True) or not (False) a colorbar should be attached.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The ax context in which the plot will be drawn.

**Returns**

**fig, output**

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

**Raises**

**ValueError**

Input argument is not a quantum object.

## Examples

```
>>> import qutip
```

```
>>> dm = qutip.rand_dm(4)
>>> fig, ax = qutip.hinton(dm)
>>> fig.show()
```

```
>>> qutip.settings.colorblind_safe = True
>>> fig, ax = qutip.hinton(dm, color_style="threshold")
>>> fig.show()
>>> qutip.settings.colorblind_safe = False
```

```
>>> fig, ax = qutip.hinton(dm, color_style="phase")
>>> fig.show()
```

**matrix\_histogram**(*M*, *x\_basis*=None, *y\_basis*=None, *limits*=None, *bar\_style*='real', *color\_limits*=None, *color\_style*='real', *options*=None, \*, *cmap*=None, *colorbar*=True, *fig*=None, *ax*=None)

Draw a histogram for the matrix *M*, with the given *x* and *y* labels and title.

**Parameters**

**M**

[Matrix of Qobj] The matrix to visualize

**x\_basis**

[list of strings, optional] list of x ticklabels

**y\_basis**

[list of strings, optional] list of y ticklabels

**limits**

[list/array with two float numbers, optional] The z-axis limits [min, max]

**bar\_style**

[str, {"real", "img", "abs", "phase"}, default: "real"]

- If set to "real" (default), each bar is plotted as the real part of the corresponding matrix element
- If set to "img", each bar is plotted as the imaginary part of the corresponding matrix element
- If set to "abs", each bar is plotted as the absolute value of the corresponding matrix element
- If set to "phase" (default), each bar is plotted as the angle of the corresponding matrix element

**color\_limits**

[list/array with two float numbers, optional] The limits of colorbar [min, max]

**color\_style**

[str, {"real", "img", "abs", "phase"}, default: "real"] Determines how colors are assigned to each square:

- If set to "real" (default), each color is chosen according to the real part of the corresponding matrix element.
- If set to "img", each color is chosen according to the imaginary part of the corresponding matrix element.
- If set to "abs", each color is chosen according to the absolute value of the corresponding matrix element.
- If set to "phase", each color is chosen according to the angle of the corresponding matrix element.

**cmap**

[a matplotlib colormap instance, optional] Color map to use when plotting.

**colorbar**

[bool, default: True] show colorbar

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

**options**

[dict, optional] A dictionary containing extra options for the plot. The names (keys) and values of the options are described below:

**'zticks'**

[list of numbers, optional] A list of z-axis tick locations.

**'bars\_spacing'**

[float, default: 0.1] spacing between bars.

**'bars\_alpha'**

[float, default: 1.] transparency of bars, should be in range 0 - 1

**'bars\_lw'**

[float, default: 0.5] linewidth of bars' edges.

**‘bars\_edgecolor’**

[color, default: ‘k’] The colors of the bars’ edges. Examples: ‘k’, (0.1, 0.2, 0.5) or ‘#0f0f0f80’.

**‘shade’**

[bool, default: True] Whether to shade the dark sides of the bars (True) or not (False). The shading is relative to plot’s source of light.

**‘azim’**

[float, default: -35] The azimuthal viewing angle.

**‘elev’**

[float, default: 35] The elevation viewing angle.

**‘stick’**

[bool, default: False] Changes xlim and ylim in such a way that bars next to XZ and YZ planes will stick to those planes. This option has no effect if `ax` is passed as a parameter.

**‘cbar\_pad’**

[float, default: 0.04] The fraction of the original axes between the colorbar and the new image axes. (i.e. the padding between the 3D figure and the colorbar).

**‘cbar\_to\_z’**

[bool, default: False] Whether to set the color of maximum and minimum z-values to the maximum and minimum colors in the colorbar (True) or not (False).

**‘threshold’: float, optional**

Threshold for when bars of smaller height should be transparent. If not set, all bars are colored according to the color map.

**Returns**

**fig, output**

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

**Raises**

**ValueError**

Input argument is not valid.

**plot\_energy\_levels**(*H\_list*, *h\_labels=None*, *energy\_levels=None*, *N=0*, *\**, *fig=None*, *ax=None*)

Plot the energy level diagrams for a list of Hamiltonians. Include up to *N* energy levels. For each element in *H\_list*, the energy levels diagram for the cumulative Hamiltonian  $\text{sum}(H\_list[0:n])$  is plotted, where *n* is the index of an element in *H\_list*.

**Parameters**

**H\_list**

[List of Qobj] A list of Hamiltonians.

**h\_labels**

[List of string, optional] A list of xticklabels for each Hamiltonian

**energy\_levels**

[List of string, optional] A list of yticklabels to the left of energy levels of the initial Hamiltonian.

**N**

[int, default: 0] The number of energy levels to plot

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

#### Returns

**fig, ax**

[tuple] A tuple of the matplotlib figure and axes instances used to produce the figure.

#### Raises

**ValueError**

Input argument is not valid.

**plot\_expectation\_values**(*results*, *ylabels=None*, \*, *fig=None*, *axes=None*)

Visualize the results (expectation values) for an evolution solver. *results* is assumed to be an instance of `Result`, or a list of `Result` instances.

#### Parameters

**results**

[(list of) [Result](#)] List of results objects returned by any of the QuTiP evolution solvers.

**ylabels**

[list of strings, optional] The y-axis labels. List should be of the same length as *results*.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**axes**

[(list of) axes instances, optional] The axes context in which the plot will be drawn.

#### Returns

**fig, axes**

[tuple] A tuple of the matplotlib figure and array of axes instances used to produce the figure.

**plot\_fock\_distribution**(*rho*, *fock\_numbers=None*, *color='green'*, *unit\_y\_range=True*, \*, *fig=None*, *ax=None*)

Plot the Fock distribution for a density matrix (or ket) that describes an oscillator mode.

#### Parameters

**rho**

[[Qobj](#)] The density matrix (or ket) of the state to visualize.

**fock\_numbers**

[list of strings, optional] list of x ticklabels to represent fock numbers

**color**

[color or list of colors, default: "green"] The colors of the bar faces.

**unit\_y\_range**

[bool, default: True] Set y-axis limits [0, 1] or not

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

#### Returns

**fig, output**

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

**plot\_qubism**(ket, theme='light', how='pairs', grid\_iteration=1, legend\_iteration=0, \*, fig=None, ax=None)

Qubism plot for pure states of many qudits. Works best for spin chains, especially with even number of particles of the same dimension. Allows to see entanglement between first 2k particles and the rest.

---

**Note:** colorblind\_safe does not apply because of its unique colormap

---

### Parameters

#### ket

[Qobj] Pure state for plotting.

#### theme

[str { 'light', 'dark' }, default: 'light'] Set coloring theme for mapping complex values into colors. See: complex\_array\_to\_rgb.

#### how

[str { 'pairs', 'pairs\_skewed' or 'before\_after' }, default: 'pairs'] Type of Qubism plotting. Options:

- 'pairs' - typical coordinates,
- 'pairs\_skewed' - for ferromagnetic/antriferromagnetic plots,
- 'before\_after' - related to Schmidt plot (see also: plot\_schmidt).

#### grid\_iteration

[int, default: 1] Helper lines to be drawn on plot. Show tiles for 2\*grid\_iteration particles vs all others.

#### legend\_iteration

[int or 'grid\_iteration' or 'all', default: 0] Show labels for first 2\*legend\_iteration particles. Option 'grid\_iteration' sets the same number of particles as for grid\_iteration. Option 'all' makes label for all particles. Typically it should be 0, 1, 2 or perhaps 3.

#### fig

[a matplotlib figure instance, optional] The figure canvas on which the plot will be drawn.

#### ax

[a matplotlib axis instance, optional] The axis context in which the plot will be drawn.

### Returns

#### fig, output

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

### Notes

See also [1].

### References

[1]

**plot\_schmidt**(ket, theme='light', splitting=None, labels\_iteration=(3, 2), \*, fig=None, ax=None)

Plotting scheme related to Schmidt decomposition. Converts a state into a matrix ( $A_{ij} \rightarrow A_i^j$ ), where rows are first particles and columns - last.

See also: plot\_qubism with how='before\_after' for a similar plot.



---

**Note:** `colorblind_safe` does not apply because of its unique colormap

---

### Parameters

#### **ket**

[Qobj] Pure state for plotting.

#### **theme**

[str {'light', 'dark'}, default: 'light'] Set coloring theme for mapping complex values into colors. See: `complex_array_to_rgb`.

#### **splitting**

[int, optional] Plot for a number of first particles versus the rest. If not given, it is (number of particles + 1) // 2.

#### **labels\_iteration**

[int or pair of ints, default: (3, 2)] Number of particles to be shown as tick labels, for first (vertical) and last (horizontal) particles, respectively.

#### **fig**

[a matplotlib figure instance, optional] The figure canvas on which the plot will be drawn.

#### **ax**

[a matplotlib axis instance, optional] The axis context in which the plot will be drawn.

### Returns

#### **fig, output**

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

**plot\_spin\_distribution**(*P*, *THETA*, *PHI*, *projection='2d'*, *\**, *cmap=None*, *colorbar=False*, *fig=None*, *ax=None*)

Plots a spin distribution (given as meshgrid data).

### Parameters

#### **P**

[matrix] Distribution values as a meshgrid matrix.

#### **THETA**

[matrix] Meshgrid matrix for the theta coordinate. Its range is between 0 and pi

#### **PHI**

[matrix] Meshgrid matrix for the phi coordinate. Its range is between 0 and 2\*pi

#### **projection: str {'2d', '3d'}, default: '2d'**

Specify whether the spin distribution function is to be plotted as a 2D projection where the surface of the unit sphere is mapped on the unit disk ('2d') or surface plot ('3d').

#### **cmap**

[a matplotlib cmap instance, optional] The colormap.

#### **colorbar**

[bool, default: False] Whether (True) or not (False) a colorbar should be attached to the Wigner function graph.

#### **fig**

[a matplotlib figure instance, optional] The figure canvas on which the plot will be drawn.

#### **ax**

[a matplotlib axis instance, optional] The axis context in which the plot will be drawn.

### Returns

**fig, output**

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

**plot\_wigner**(rho, xvec=None, yvec=None, method='clenshaw', projection='2d', g=1.4142135623730951, sparse=False, parfor=False, \*, cmap=None, colorbar=False, fig=None, ax=None)

Plot the the Wigner function for a density matrix (or ket) that describes an oscillator mode.

**Parameters**

**rho**

[*Qobj*] The density matrix (or ket) of the state to visualize.

**xvec**

[array\_like, optional] x-coordinates at which to calculate the Wigner function.

**yvec**

[array\_like, optional] y-coordinates at which to calculate the Wigner function. Does not apply to the 'fft' method.

**method**

[str {'clenshaw', 'iterative', 'laguerre', 'fft'}, default: 'clenshaw'] The method used for calculating the wigner function. See the documentation for qutip.wigner for details.

**projection: str {'2d', '3d'}, default: '2d'**

Specify whether the Wigner function is to be plotted as a contour graph ('2d') or surface plot ('3d').

**g**

[float] Scaling factor for  $a = 0.5 * g * (x + iy)$ , default  $g = \sqrt{2}$ . See the documentation for qutip.wigner for details.

**sparse**

[bool {False, True}] Flag for sparse format. See the documentation for qutip.wigner for details.

**parfor**

[bool {False, True}] Flag for parallel calculation. See the documentation for qutip.wigner for details.

**cmap**

[a matplotlib cmap instance, optional] The colormap.

**colorbar**

[bool, default: False] Whether (True) or not (False) a colorbar should be attached to the Wigner function graph.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

**Returns**

**fig, output**

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

**plot\_wigner\_sphere**(wigner, reflections=False, \*, cmap=None, colorbar=True, fig=None, ax=None)

Plots a coloured Bloch sphere.

**Parameters**

**wigner**

[a wigner transformation] The wigner transformation at *steps* different theta and phi.

**reflections**

[bool, default: False] If the reflections of the sphere should be plotted as well.

**cmap**

[a matplotlib colormap instance, optional] Color map to use when plotting.

**colorbar**

[bool, default: True] Whether (True) or not (False) a colorbar should be attached.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The ax context in which the plot will be drawn.

**Returns**

**fig, output**

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

**Notes**

Special thanks to Russell P Rundle for writing this function.

**sphereplot**(*values, theta, phi, \*, cmap=None, colorbar=True, fig=None, ax=None*)

Plots a matrix of values on a sphere

**Parameters**

**values**

[array] Data set to be plotted

**theta**

[float] Angle with respect to z-axis. Its range is between 0 and pi

**phi**

[float] Angle in x-y plane. Its range is between 0 and 2\*pi

**cmap**

[a matplotlib colormap instance, optional] Color map to use when plotting.

**colorbar**

[bool, default: True] Whether (True) or not (False) a colorbar should be attached.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

**Returns**

**fig, output**

[tuple] A tuple of the matplotlib figure and the axes instance or animation instance used to produce the figure.

Functions to animate results of quantum dynamics simulations,

**anim\_fock\_distribution**(*rhos, fock\_numbers=None, color='green', unit\_y\_range=True, \*, fig=None, ax=None*)

Animation of the Fock distribution for a density matrix (or ket) that describes an oscillator mode.

**Parameters**

**rhos**

[*Result* or list of *Qobj*] The density matrix (or ket) of the state to visualize.

**fock\_numbers**

[list of strings, optional] list of x ticklabels to represent fock numbers

**color**

[color or list of colors, default: “green”] The colors of the bar faces.

**unit\_y\_range**

[bool, default: True] Set y-axis limits [0, 1] or not

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

### Returns

**fig, ani**

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

**anim\_hinton**(*rhos*, *x\_basis=None*, *y\_basis=None*, *color\_style='scaled'*, *label\_top=True*, \*, *cmap=None*, *colorbar=True*, *fig=None*, *ax=None*)

Draws an animation of Hinton diagram.

### Parameters

**rhos**

[*Result* or list of *Qobj*] Input density matrix or superoperator.

---

**Note:** Hinton plots of superoperators are currently only supported for qubits.

---

**x\_basis**

[list of strings, optional] list of x ticklabels to represent x basis of the input.

**y\_basis**

[list of strings, optional] list of y ticklabels to represent y basis of the input.

**color\_style**

[str, {“scaled”, “threshold”, “phase”}, default: “scaled”] Determines how colors are assigned to each square:

- If set to “scaled” (default), each color is chosen by passing the absolute value of the corresponding matrix element into *cmap* with the sign of the real part.
- If set to “threshold”, each square is plotted as the maximum of *cmap* for the positive real part and as the minimum for the negative part of the matrix element; note that this generalizes “threshold” to complex numbers.
- If set to “phase”, each color is chosen according to the angle of the corresponding matrix element.

**label\_top**

[bool, default: True] If True, x ticklabels will be placed on top, otherwise they will appear below the plot.

**cmap**

[a matplotlib colormap instance, optional] Color map to use when plotting.

**colorbar**

[bool, default: True] Whether (True) or not (False) a colorbar should be attached.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The ax context in which the plot will be drawn.

## Returns

**fig, ani**

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

## Raises

**ValueError**

Input argument is not a quantum object.

**anim\_matrix\_histogram**(*Ms*, *x\_basis=None*, *y\_basis=None*, *limits=None*, *bar\_style='real'*, *color\_limits=None*, *color\_style='real'*, *options=None*, \*, *cmap=None*, *colorbar=True*, *fig=None*, *ax=None*)

Draw an animation of a histogram for the matrix *M*, with the given *x* and *y* labels.

## Parameters

**Ms**

[list of matrices or [Result](#)] The matrix to visualize

**x\_basis**

[list of strings, optional] list of *x* ticklabels

**y\_basis**

[list of strings, optional] list of *y* ticklabels

**limits**

[list/array with two float numbers, optional] The *z*-axis limits [min, max]

**bar\_style**

[str, {"real", "img", "abs", "phase"}, default: "real"]

- If set to "real" (default), each bar is plotted as the real part of the corresponding matrix element
- If set to "img", each bar is plotted as the imaginary part of the corresponding matrix element
- If set to "abs", each bar is plotted as the absolute value of the corresponding matrix element
- If set to "phase" (default), each bar is plotted as the angle of the corresponding matrix element

**color\_limits**

[list/array with two float numbers, optional] The limits of colorbar [min, max]

**color\_style**

[str, {"real", "img", "abs", "phase"}, default: "real"] Determines how colors are assigned to each square:

- If set to "real" (default), each color is chosen according to the real part of the corresponding matrix element.
- If set to "img", each color is chosen according to the imaginary part of the corresponding matrix element.
- If set to "abs", each color is chosen according to the absolute value of the corresponding matrix element.

- If set to "phase", each color is chosen according to the angle of the corresponding matrix element.

**cmap**

[a matplotlib colormap instance, optional] Color map to use when plotting.

**colorbar**

[bool, default: True] show colorbar

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

**options**

[dict, optional] A dictionary containing extra options for the plot. The names (keys) and values of the options are described below:

**‘zticks’**

[list of numbers, optional] A list of z-axis tick locations.

**‘bars\_spacing’**

[float, default: 0.1] spacing between bars.

**‘bars\_alpha’**

[float, default: 1.] transparency of bars, should be in range 0 - 1

**‘bars\_lw’**

[float, default: 0.5] linewidth of bars’ edges.

**‘bars\_edgecolor’**

[color, default: ‘k’] The colors of the bars’ edges. Examples: ‘k’, (0.1, 0.2, 0.5) or ‘#0f0f0f80’.

**‘shade’**

[bool, default: True] Whether to shade the dark sides of the bars (True) or not (False). The shading is relative to plot’s source of light.

**‘azim’**

[float, default: -35] The azimuthal viewing angle.

**‘elev’**

[float, default: 35] The elevation viewing angle.

**‘stick’**

[bool, default: False] Changes xlim and ylim in such a way that bars next to XZ and YZ planes will stick to those planes. This option has no effect if ax is passed as a parameter.

**‘cbar\_pad’**

[float, default: 0.04] The fraction of the original axes between the colorbar and the new image axes. (i.e. the padding between the 3D figure and the colorbar).

**‘cbar\_to\_z’**

[bool, default: False] Whether to set the color of maximum and minimum z-values to the maximum and minimum colors in the colorbar (True) or not (False).

**‘threshold’: float, optional**

Threshold for when bars of smaller height should be transparent. If not set, all bars are colored according to the color map.

**Returns**

**fig, ani**

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

## Raises

### ValueError

Input argument is not valid.

**anim\_qubism**(*kets*, *theme*='light', *how*='pairs', *grid\_iteration*=1, *legend\_iteration*=0, \*, *fig*=None, *ax*=None)

Animation of Qubism plot for pure states of many qudits. Works best for spin chains, especially with even number of particles of the same dimension. Allows to see entanglement between first 2k particles and the rest.

---

**Note:** colorblind\_safe does not apply because of its unique colormap

---

## Parameters

### kets

[*Result* or list of *Qobj*] Pure states for animation.

### theme

[str {'light', 'dark'}, default: 'light'] Set coloring theme for mapping complex values into colors. See: `complex_array_to_rgb`.

### how

[str {'pairs', 'pairs\_skewed', 'before\_after'}, default: 'pairs'] Type of Qubism plotting. Options:

- 'pairs' - typical coordinates,
- 'pairs\_skewed' - for ferromagnetic/antriferromagnetic plots,
- 'before\_after' - related to Schmidt plot (see also: `plot_schmidt`).

### grid\_iteration

[int, default: 1] Helper lines to be drawn on plot. Show tiles for 2\*grid\_iteration particles vs all others.

### legend\_iteration

[int or 'grid\_iteration' or 'all', default: 0] Show labels for first 2\*legend\_iteration particles. Option 'grid\_iteration' sets the same number of particles as for grid\_iteration. Option 'all' makes label for all particles. Typically it should be 0, 1, 2 or perhaps 3.

### fig

[a matplotlib figure instance, optional] The figure canvas on which the plot will be drawn.

### ax

[a matplotlib axis instance, optional] The axis context in which the plot will be drawn.

## Returns

### fig, ani

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

## Notes

See also [1].

## References

[1]

**anim\_schmidt**(*kets*, *theme*='light', *splitting*=None, *labels\_iteration*=(3, 2), \*, *fig*=None, *ax*=None)

Animation of Schmidt decomposition. Converts a state into a matrix ( $A_{ij} \rightarrow A_i^j$ ), where rows are first particles and columns - last.

See also: `plot_qubism` with `how='before_after'` for a similar plot.

---

**Note:** `colorblind_safe` does not apply because of its unique colormap

---

## Parameters

### ket

[*Result* or list of *Qobj*] Pure states for animation.

### theme

[str { 'light', 'dark' }, default: 'light'] Set coloring theme for mapping complex values into colors. See: `complex_array_to_rgb`.

### splitting

[int, optional] Plot for a number of first particles versus the rest. If not given, it is (number of particles + 1) // 2.

### labels\_iteration

[int or pair of ints, default: (3, 2)] Number of particles to be shown as tick labels, for first (vertical) and last (horizontal) particles, respectively.

### fig

[a matplotlib figure instance, optional] The figure canvas on which the plot will be drawn.

### ax

[a matplotlib axis instance, optional] The axis context in which the plot will be drawn.

## Returns

### fig, ani

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

**anim\_sphereplot**(*V*, *theta*, *phi*, \*, *cmap*=None, *colorbar*=True, *fig*=None, *ax*=None)

animation of a matrices of values on a sphere

## Parameters

### V

[list of array instances] Data set to be plotted

### theta

[float] Angle with respect to z-axis. Its range is between 0 and pi

### phi

[float] Angle in x-y plane. Its range is between 0 and 2\*pi

### cmap

[a matplotlib colormap instance, optional] Color map to use when plotting.



**colorbar**

[bool, default: True] Whether (True) or not (False) a colorbar should be attached.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

**Returns**

**fig, ani**

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

**anim\_spin\_distribution**(*Ps, THETA, PHI, projection='2d', \*, cmap=None, colorbar=False, fig=None, ax=None*)

Animation of a spin distribution (given as meshgrid data).

**Parameters**

**Ps**

[list of matrices] Distribution values as a meshgrid matrix.

**THETA**

[matrix] Meshgrid matrix for the theta coordinate. Its range is between 0 and pi

**PHI**

[matrix] Meshgrid matrix for the phi coordinate. Its range is between 0 and 2\*pi

**projection: str {'2d', '3d'}, default: '2d'**

Specify whether the spin distribution function is to be plotted as a 2D projection where the surface of the unit sphere is mapped on the unit disk ('2d') or surface plot ('3d').

**cmap**

[a matplotlib cmap instance, optional] The colormap.

**colorbar**

[bool, default: False] Whether (True) or not (False) a colorbar should be attached to the Wigner function graph.

**fig**

[a matplotlib figure instance, optional] The figure canvas on which the plot will be drawn.

**ax**

[a matplotlib axis instance, optional] The axis context in which the plot will be drawn.

**Returns**

**fig, ani**

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

**anim\_wigner**(*rhos, xvec=None, yvec=None, method='clenshaw', projection='2d', g=1.4142135623730951, sparse=False, parfor=False, \*, cmap=None, colorbar=False, fig=None, ax=None*)

Animation of the Wigner function for a density matrix (or ket) that describes an oscillator mode.

**Parameters**

**rhos**

[[Result](#) or list of [Qobj](#)] The density matrix (or ket) of the state to visualize.

**xvec**

[array\_like, optional] x-coordinates at which to calculate the Wigner function.

**yvec**

[array\_like, optional] y-coordinates at which to calculate the Wigner function. Does not apply to the 'fft' method.

**method**

[str {'clenshaw', 'iterative', 'laguerre', 'fft'}, default: 'clenshaw'] The method used for calculating the wigner function. See the documentation for qutip.wigner for details.

**projection: str {'2d', '3d'}, default: '2d'**

Specify whether the Wigner function is to be plotted as a contour graph ('2d') or surface plot ('3d').

**g**

[float] Scaling factor for  $a = 0.5 * g * (x + iy)$ , default  $g = \sqrt{2}$ . See the documentation for qutip.wigner for details.

**sparse**

[bool {False, True}] Flag for sparse format. See the documentation for qutip.wigner for details.

**parfor**

[bool {False, True}] Flag for parallel calculation. See the documentation for qutip.wigner for details.

**cmap**

[a matplotlib cmap instance, optional] The colormap.

**colorbar**

[bool, default: False] Whether (True) or not (False) a colorbar should be attached to the Wigner function graph.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The axes context in which the plot will be drawn.

**Returns**

**fig, ani**

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

**anim\_wigner\_sphere**(*wigners, reflections=False, \*, cmap=None, colorbar=True, fig=None, ax=None*)

Animate a coloured Bloch sphere.

**Parameters**

**wigners**

[list of transformations] The wigner transformation at *steps* different theta and phi.

**reflections**

[bool, default: False] If the reflections of the sphere should be plotted as well.

**cmap**

[a matplotlib colormap instance, optional] Color map to use when plotting.

**colorbar**

[bool, default: True] Whether (True) or not (False) a colorbar should be attached.

**fig**

[a matplotlib Figure instance, optional] The Figure canvas in which the plot will be drawn.

**ax**

[a matplotlib axes instance, optional] The ax context in which the plot will be drawn.

## Returns

### **fig, ani**

[tuple] A tuple of the matplotlib figure and the animation instance used to produce the figure.

## Notes

Special thanks to Russell P Rundle for writing this function.

This module contains utility functions that enhance Matplotlib in one way or another.

### **complex\_phase\_cmap()**

Create a cyclic colormap for representing the phase of complex variables

## Returns

### **cmap**

A matplotlib linear segmented colormap.

**wigner\_cmap**(*W, levels=1024, shift=0, max\_color='#09224F', mid\_color='#FFFFFF', min\_color='#530017', neg\_color='#FF97D4', invert=False*)

A custom colormap that emphasizes negative values by creating a nonlinear colormap.

## Parameters

### **W**

[array] Wigner function array, or any array.

### **levels**

[int, default: 1024] Number of color levels to create.

### **shift**

[float, default: 0] Shifts the value at which Wigner elements are emphasized. This parameter should typically be negative and small (i.e -1e-5).

### **max\_color**

[str, default: '#09224F'] String for color corresponding to maximum value of data. Accepts any string format compatible with the Matplotlib.colors.ColorConverter.

### **mid\_color**

[str, default: '#FFFFFF'] Color corresponding to zero values. Accepts any string format compatible with the Matplotlib.colors.ColorConverter.

### **min\_color**

[str, default: '#530017'] Color corresponding to minimum data values. Accepts any string format compatible with the Matplotlib.colors.ColorConverter.

### **neg\_color**

[str, default: '#FF97D4'] Color that starts highlighting negative values. Accepts any string format compatible with the Matplotlib.colors.ColorConverter.

### **invert**

[bool, default: False] Invert the color scheme for negative values so that smaller negative values have darker color.

## Returns

Returns a Matplotlib colormap instance for use in plotting.

## Notes

The ‘shift’ parameter allows you to vary where the colormap begins to highlight negative colors. This is beneficial in cases where there are small negative Wigner elements due to numerical round-off and/or truncation.

## Quantum Process Tomography

### **qpt**(*U*, *op\_basis\_list*)

Calculate the quantum process tomography chi matrix for a given (possibly nonunitary) transformation matrix *U*, which transforms a density matrix in vector form according to:

$$\text{vec}(\rho) = U * \text{vec}(\rho_0)$$

or

$$\rho = \text{unstack\_columns}(U * \text{stack\_columns}(\rho_0))$$

*U* can be calculated for an open quantum system using the QuTiP propagator function.

#### Parameters

**U**

[Qobj] Transformation operator. Can be calculated using QuTiP propagator function.

**op\_basis\_list**

[list] A list of Qobj’s representing the basis states.

#### Returns

**chi**

[array] QPT chi matrix

### **qpt\_plot**(*chi*, *lbls\_list*, *title=None*, *fig=None*, *axes=None*)

Visualize the quantum process tomography chi matrix. Plot the real and imaginary parts separately.

#### Parameters

**chi**

[array] Input QPT chi matrix.

**lbls\_list**

[list] List of labels for QPT plot axes.

**title**

[str, optional] Plot title.

**fig**

[figure instance, optional] User defined figure instance used for generating QPT plot.

**axes**

[list of figure axis instance, optional] User defined figure axis instance (list of two axes) used for generating QPT plot.

#### Returns

**fig, ax**

[tuple] A tuple of the matplotlib figure and axes instances used to produce the figure.

### **qpt\_plot\_combined**(*chi*, *lbls\_list*, *title=None*, *fig=None*, *ax=None*, *figsize=(8, 6)*, *threshold=None*)

Visualize the quantum process tomography chi matrix. Plot bars with height and color corresponding to the absolute value and phase, respectively.

#### Parameters

**chi**

[array] Input QPT chi matrix.

**lbls\_list**

[list] List of labels for QPT plot axes.

**title**

[str, optional] Plot title.

**fig**

[figure instance, optional] User defined figure instance used for generating QPT plot.

**figsize**

[(int, int), default: (8, 6)] Size of the figure when the `fig` is not provided.

**ax**

[figure axis instance, optional] User defined figure axis instance used for generating QPT plot (alternative to the `fig` argument).

**threshold: float, optional**

Threshold for when bars of smaller height should be transparent. If not set, all bars are colored according to the color map.

**Returns**

**fig, ax**

[tuple] A tuple of the matplotlib figure and axes instances used to produce the figure.

## 5.2.6 Non-Markovian Solvers

This module contains an implementation of the non-Markovian transfer tensor method (TTM), introduced in [1].

[1] Javier Cerrillo and Jianshu Cao, Phys. Rev. Lett 112, 110401 (2014)

**ttmsolve**(*dynmaps*, *state0*, *times*, *e\_ops*=(), *num\_learning*=0, *options*=None)

Expand time-evolution using the Transfer Tensor Method [1], based on a set of precomputed dynamical maps.

**Parameters**

**dynmaps**

[list of *Qobj*, callable] List of precomputed dynamical maps (superoperators) for the first times of *times* or a callable function that returns the superoperator at a given time.

**state0**

[*Qobj*] Initial density matrix or state vector (ket).

**times**

[array\_like] List of times  $t_n$  at which to compute results. Must be uniformly spaced.

**e\_ops**

[*Qobj*, callable, or list, optional] Single operator or list of operators for which to evaluate expectation values or callable or list of callable. Callable signature must be,  $f(t: \text{float}, \text{state}: \text{Qobj})$ . See `expect` for more detail of operator expectation.

**num\_learning**

[int, default: 0] Number of times used to construct the `dynmaps` operators when `dynmaps` is a callable.

**options**

[dictionary, optional] Dictionary of options for the solver.

- `store_final_state` : bool Whether or not to store the final state of the evolution in the result class.
- `store_states` : bool, None Whether or not to store the state vectors or density matrices. On *None* the states will be saved if no expectation operators are given.
- `normalize_output` : bool Normalize output state to hide ODE numerical errors.

- **threshold** : float Threshold for halting. Halts if  $||T_n - T_{n-1}||$  is below threshold.

#### Returns

**output:** *Result*

An instance of the class *Result*.

## 5.2.7 Utility Functions

### Utility Functions

This module contains utility functions that are commonly needed in other qutip modules.

**clebsch**(*j1, j2, j3, m1, m2, m3*)

Calculates the Clebsch-Gordon coefficient for coupling (*j1,m1*) and (*j2,m2*) to give (*j3,m3*).

#### Parameters

**j1**

[float] Total angular momentum 1.

**j2**

[float] Total angular momentum 2.

**j3**

[float] Total angular momentum 3.

**m1**

[float] z-component of angular momentum 1.

**m2**

[float] z-component of angular momentum 2.

**m3**

[float] z-component of angular momentum 3.

#### Returns

**cg\_coeff**

[float] Requested Clebsch-Gordan coefficient.

**convert\_unit**(*value, orig='meV', to='GHz'*)

Convert an energy from unit *orig* to unit *to*.

#### Parameters

**value**

[float / array] The energy in the old unit.

**orig**

[str, {"J", "eV", "meV", "GHz", "mK"}], default: "meV"] The name of the original unit.

**to**

[str, {"J", "eV", "meV", "GHz", "mK"}], default: "GHz"] The name of the new unit.

#### Returns

**value\_new\_unit**

[float / array] The energy in the new unit.

**n\_thermal**(*w, w\_th*)

Return the number of photons in thermal equilibrium for an harmonic oscillator mode with frequency 'w', at the temperature described by 'w\_th' where  $\omega_{th} = k_B T / \hbar$ .

#### Parameters

**w**  
[float or ndarray] Frequency of the oscillator.

**w\_th**  
[float] The temperature in units of frequency (or the same units as *w*).

#### Returns

**n\_avg**  
[float or array] Return the number of average photons in thermal equilibrium for a an oscillator with the given frequency and temperature.

### File I/O Functions

**file\_data\_read**(*filename*, *sep=None*)

Retrieves an array of data from the requested file.

#### Parameters

**filename**  
[str or pathlib.Path] Name of file containing requested data.

**sep**  
[str, optional] Seperator used to store data.

#### Returns

**data**  
[array\_like] Data from selected file.

**file\_data\_store**(*filename*, *data*, *numtype='complex'*, *numformat='decimal'*, *sep=','*)

Stores a matrix of data to a file to be read by an external program.

#### Parameters

**filename**  
[str or pathlib.Path] Name of data file to be stored, including extension.

**data: array\_like**  
Data to be written to file.

**numtype**  
[str { 'complex', 'real' }, default: 'complex'] Type of numerical data.

**numformat**  
[str { 'decimal', 'exp' }, default: 'decimal'] Format for written data.

**sep**  
[str, default: ','] Single-character field separator. Usually a tab, space, comma, or semi-colon.

**qload**(*filename*)

Loads data file from file *filename* in current directory.

#### Parameters

**filename**  
[str or pathlib.Path] Name of data file to be loaded.

#### Returns

**qobject**  
[instance / array\_like] Object retrieved from requested file.

**qsave**(*data*, *name*='qutip\_data')

Saves given data to file named 'filename.qu' in current directory.

#### Parameters

##### **data**

[instance/array\_like] Input Python object to be stored.

##### **filename**

[str or pathlib.Path, default: "qutip\_data"] Name of output data file.

## Parallelization

This module provides functions for parallel execution of loops and function mappings, using the builtin Python module multiprocessing or the loky parallel execution library.

**loky\_pmap**(*task*, *values*, *task\_args*=None, *task\_kwargs*=None, *reduce\_func*=None, *map\_kw*=None, *progress\_bar*=None, *progress\_bar\_kwargs*={})

Parallel execution of a mapping of *values* to the function *task*. This is functionally equivalent to:

```
result = [task(value, *task_args, **task_kwargs) for value in values]
```

Use the loky module instead of multiprocessing.

#### Parameters

##### **task**

[a Python function] The function that is to be called for each value in *task\_vec*.

##### **values**

[array / list] The list or array of values for which the *task* function is to be evaluated.

##### **task\_args**

[list, optional] The optional additional arguments to the *task* function.

##### **task\_kwargs**

[dictionary, optional] The optional additional keyword arguments to the *task* function.

##### **reduce\_func**

[func, optional] If provided, it will be called with the output of each task instead of storing them in a list. Note that the order in which results are passed to *reduce\_func* is not defined. It should return None or a number. When returning a number, it represents the estimation of the number of tasks left. On a return <= 0, the map will end early.

##### **progress\_bar**

[str, optional] Progress bar options's string for showing progress.

##### **progress\_bar\_kwargs**

[dict, optional] Options for the progress bar.

##### **map\_kw: dict, optional**

Dictionary containing entry for: - *timeout*: float, Maximum time (sec) for the whole map. - *num\_cpus*: int, Number of jobs to run at once. - *fail\_fast*: bool, Abort at the first error.

#### Returns

##### **result**

[list] The result list contains the value of *task*(*value*, *\*task\_args*, *\*\*task\_kwargs*) for each value in *values*. If a *reduce\_func* is provided, and empty list will be returned.

**mpi\_pmap**(*task*, *values*, *task\_args*=None, *task\_kwargs*=None, *reduce\_func*=None, *map\_kw*=None, *progress\_bar*=None, *progress\_bar\_kwargs*={})

Parallel execution of a mapping of *values* to the function *task*. This is functionally equivalent to:



```
result = [task(value, *task_args, **task_kwargs) for value in values]
```

Uses the `mpi4py` module to execute the tasks asynchronously with MPI processes. For more information, consult the documentation of `mpi4py` and the `mpi4py.MPIPoolExecutor` class.

Note: in keeping consistent with the API of `parallel_map`, the parameter determining the number of requested worker processes is called `num_cpus`. The value of `map_kw['num_cpus']` is passed to the `MPIPoolExecutor` as its `max_workers` argument. If this parameter is not provided, the environment variable `QUTIP_NUM_PROCESSES` is used instead. If this environment variable is not set either, QuTiP will use default values that might be unsuitable for MPI applications.

### Parameters

#### **task**

[a Python function] The function that is to be called for each value in `task_vec`.

#### **values**

[array / list] The list or array of values for which the `task` function is to be evaluated.

#### **task\_args**

[list, optional] The optional additional arguments to the `task` function.

#### **task\_kwargs**

[dictionary, optional] The optional additional keyword arguments to the `task` function.

#### **reduce\_func**

[func, optional] If provided, it will be called with the output of each task instead of storing them in a list. Note that the order in which results are passed to `reduce_func` is not defined. It should return `None` or a number. When returning a number, it represents the estimation of the number of tasks left. On a return `<= 0`, the map will end early.

#### **progress\_bar**

[str, optional] Progress bar options's string for showing progress.

#### **progress\_bar\_kwargs**

[dict, optional] Options for the progress bar.

#### **map\_kw: dict, optional**

Dictionary containing entry for: - `timeout`: float, Maximum time (sec) for the whole map. - `num_cpus`: int, Number of jobs to run at once. - `fail_fast`: bool, Abort at the first error. All remaining entries of `map_kw` will be passed to the `mpi4py.MPIPoolExecutor` constructor.

### Returns

#### **result**

[list] The result list contains the value of `task(value, *task_args, **task_kwargs)` for each value in `values`. If a `reduce_func` is provided, and empty list will be returned.

**parallel\_map**(*task, values, task\_args=None, task\_kwargs=None, reduce\_func=None, map\_kw=None, progress\_bar=None, progress\_bar\_kwargs={}*)

Parallel execution of a mapping of `values` to the function `task`. This is functionally equivalent to:

```
result = [task(value, *task_args, **task_kwargs) for value in values]
```

### Parameters

#### **task**

[a Python function] The function that is to be called for each value in `task_vec`.

#### **values**

[array / list] The list or array of values for which the `task` function is to be evaluated.

**task\_args**

[list, optional] The optional additional arguments to the `task` function.

**task\_kwargs**

[dictionary, optional] The optional additional keyword arguments to the `task` function.

**reduce\_func**

[func, optional] If provided, it will be called with the output of each task instead of storing them in a list. Note that the order in which results are passed to `reduce_func` is not defined. It should return `None` or a number. When returning a number, it represents the estimation of the number of tasks left. On a return  $\leq 0$ , the map will end early.

**progress\_bar**

[str, optional] Progress bar options's string for showing progress.

**progress\_bar\_kwargs**

[dict, optional] Options for the progress bar.

**map\_kw: dict, optional**

Dictionary containing entry for: - `timeout`: float, Maximum time (sec) for the whole map. - `num_cpus`: int, Number of jobs to run at once. - `fail_fast`: bool, Abort at the first error.

**Returns**

**result**

[list] The result list contains the value of `task(value, *task_args, **task_kwargs)` for each value in `values`. If a `reduce_func` is provided, and empty list will be returned.

**serial\_map**(*task, values, task\_args=None, task\_kwargs=None, reduce\_func=None, map\_kw=None, progress\_bar=None, progress\_bar\_kwargs={}*)

Serial mapping function with the same call signature as `parallel_map`, for easy switching between serial and parallel execution. This is functionally equivalent to:

```
result = [task(value, *task_args, **task_kwargs) for value in values]
```

This function work as a drop-in replacement of `parallel_map`.

**Parameters**

**task**

[a Python function] The function that is to be called for each value in `task_vec`.

**values**

[array / list] The list or array of values for which the `task` function is to be evaluated.

**task\_args**

[list, optional] The optional additional argument to the `task` function.

**task\_kwargs**

[dictionary, optional] The optional additional keyword argument to the `task` function.

**reduce\_func**

[func, optional] If provided, it will be called with the output of each tasks instead of storing a them in a list. It should return `None` or a number. When returning a number, it represent the estimation of the number of task left. On a return  $\leq 0$ , the map will end early.

**progress\_bar**

[str, optional] Progress bar options's string for showing progress.

**progress\_bar\_kwargs**

[dict, optional] Options for the progress bar.

**map\_kw: dict, optional**

Dictionary containing: - timeout: float, Maximum time (sec) for the whole map. - fail\_fast: bool, Raise an error at the first.

**Returns**

**result**

[list] The result list contains the value of `task(value, *task_args, **task_kwargs)` for each value in `values`. If a `reduce_func` is provided, and empty list will be returned.

## IPython Notebook Tools

This module contains utility functions for using QuTiP with IPython notebooks.

**version\_table(verbose=False)**

Print an HTML-formatted table with version numbers for QuTiP and its dependencies. Use it in a IPython notebook to show which versions of different packages that were used to run the notebook. This should make it possible to reproduce the environment and the calculation later on.

**Parameters**

**verbose**

[bool, default: False] Add extra information about install location.

**Returns**

**version\_table: str**

Return an HTML-formatted string containing version information for QuTiP dependencies.

## Miscellaneous

**about()**

About box for QuTiP. Gives version numbers for QuTiP, NumPy, SciPy, Cython, and Matplotlib.

**simdiag(*ops*, *evals*: bool = True, \*, *tol*: float = 1e-14, *safe\_mode*: bool = True)**

Simultaneous diagonalization of commuting Hermitian matrices.

**Parameters**

**ops**

[list, array] list or array of qobjs representing commuting Hermitian operators.

**evals**

[bool, default: True] Whether to return the eigenvalues for each ops and eigenvectors or just the eigenvectors.

**tol**

[float, default: 1e-14] Tolerance for detecting degenerate eigenstates.

**safe\_mode**

[bool, default: True] Whether to check that all ops are Hermitian and commuting. If set to False and operators are not commuting, the eigenvectors returned will often be eigenvectors of only the first operator.

**Returns**

**eigs**

[tuple] Tuple of arrays representing eigvecs and eigvals of quantum objects corresponding to simultaneous eigenvectors and eigenvalues for each operator.



# Chapter 6

## Change Log

### 6.1 QuTiP 5.0.0 (2024-03-26)

QuTiP 5 is a redesign of many of the core components of QuTiP (`Qobj`, `QobjEvo`, solvers) to make them more consistent and more flexible.

`Qobj` may now be stored in either sparse or dense representations, and the two may be mixed sensibly as needed. `QobjEvo` is now used consistently throughout QuTiP, and the implementation has been substantially cleaned up. A new `Coefficient` class is used to represent the time-dependent factors inside `QobjEvo`.

The solvers have been rewritten to work well with the new data layer and the concept of `Integrators` which solve ODEs has been introduced. In future, new data layers may provide their own `Integrators` specialized to their representation of the underlying data.

Much of the user-facing API of QuTiP remains familiar, but there have had to be many small breaking changes. If we can make changes to easy migrating code from QuTiP 4 to QuTiP 5, please let us know.

An extensive list of changes follows.

#### 6.1.1 Contributors

QuTiP 5 has been a large effort by many people over the last three years.

In particular:

- Jake Lishman led the implementation of the new data layer and coefficients.
- Eric Giguère led the implementation of the new `QobjEvo` interface and solvers.
- Boxi Li led the updating of QuTiP's QIP support and the creation of `qutip_qip`.

Other members of the QuTiP Admin team have been heavily involved in reviewing, testing and designing QuTiP 5:

- Alexander Pitchford
- Asier Galicia
- Nathan Shammah
- Shahnawaz Ahmed
- Neill Lambert
- Simon Cross
- Paul Menczel

Two Google Summer of Code contributors updated the tutorials and benchmarks to QuTiP 5:

- Christian Staufenbiel updated many of the tutorials (<https://github.com/qutip/qutip-tutorials/>).
- Xavier Sproken update the benchmarks (<https://github.com/qutip/qutip-benchmark/>).

During an internship at RIKEN, Patrick Hopf created a new quantum control method and improved the existing methods interface:

- Patrick Hopf created new quantum control package (<https://github.com/qutip/qutip-qoc/>).

Four experimental data layers backends were written either as part of Google Summer of Code or as separate projects. While these are still alpha quality, they helped significantly to test the data layer API:

- `qutip-tensorflow`: a TensorFlow backend by Asier Galicia (<https://github.com/qutip/qutip-tensorflow>)
- `qutip-cupy`: a CuPy GPU backend by Felipe Bivort Haiek (<https://github.com/qutip/qutip-cupy/>)
- `qutip-tensornetwork`: a TensorNetwork backend by Asier Galicia (<https://github.com/qutip/qutip-tensornetwork>)
- `qutip-jax`: a JAX backend by Eric Giguère (<https://github.com/qutip/qutip-jax/>)

Finally, Yuji Tamakoshi updated the visualization function and added animation functions as part of Google Summer of Code project.

We have also had many other contributors, whose specific contributions are detailed below:

- Pieter Eendebak (updated the required SciPy to 1.5+, #1982 <https://github.com/qutip/qutip/pull/1982>).
- Pieter Eendebak (reduced import times by setting logger names, #1981 <https://github.com/qutip/qutip/pull/1981>)
- Pieter Eendebak (Allow scipy 1.12 to be used with qutip, #2354 <https://github.com/qutip/qutip/pull/2354>)
- Xavier Sproken (included C header files in the source distribution, #1971 <https://github.com/qutip/qutip/pull/1971>)
- Christian Staufenbiel (added support for multiple collapse operators to the Floquet solver, #1962 <https://github.com/qutip/qutip/pull/1962>)
- Christian Staufenbiel (fixed the basis used in the Floquet Master Equation solver, #1952 <https://github.com/qutip/qutip/pull/1952>)
- Christian Staufenbiel (allowed the `bloch_redfield_tensor` function to accept strings and callables for `a_ops`, #1951 <https://github.com/qutip/qutip/pull/1951>)
- Christian Staufenbiel (Add a guide on Superoperators, Pauli Basis and Channel Contraction, #1984 <https://github.com/qutip/qutip/pull/1984>)
- Henrique Silvéro (allowed `qutip_qip` to be imported as `qutip.qip`, #1920 <https://github.com/qutip/qutip/pull/1920>)
- Florian Hopfmueller (added a vastly improved implementations of `process_fidelity` and `average_gate_fidelity`, #1712 <https://github.com/qutip/qutip/pull/1712>, #1748 <https://github.com/qutip/qutip/pull/1748>, #1788 <https://github.com/qutip/qutip/pull/1788>)
- Felipe Bivort Haiek (fixed inaccuracy in docstring of the dense implementation of negation, #1608 <https://github.com/qutip/qutip/pull/1608/>)
- Rajath Shetty (added support for specifying colors for individual points, vectors and states display by `qutip.Bloch`, #1335 <https://github.com/qutip/qutip/pull/1335>)
- Rochisha Agarwal (Add dtype to printed output of `qobj`, #2352 <https://github.com/qutip/qutip/pull/2352>)
- Kosuke Mizuno (Add arguments of `plot_wigner()` and `plot_wigner_fock_distribution()` to specify parameters for `wigner()`, #2057 <https://github.com/qutip/qutip/pull/2057>)
- Matt Ord (Only pre-compute density matrices if `keep_runs_results` is False, #2303 <https://github.com/qutip/qutip/pull/2303>)

- Daniel Moreno Galán (Add the possibility to customize point colors as in V4 and fix point plot behavior for 'l' style, #2303 <<https://github.com/qutip/qutip/pull/2303>>)
- Sola85 (Fixed simdiag not returning orthonormal eigenvectors, #2269 <<https://github.com/qutip/qutip/pull/2269>>)
- Edward Thomas (Fix LaTeX display of Qobj state in Jupyter cell outputs, #2272 <<https://github.com/qutip/qutip/pull/2272>>)
- Bogdan Reznichenko (Rework kraus\_to\_choi making it faster, #2284 <<https://github.com/qutip/qutip/pull/2284>>)
- gabbence95 (Fix typos in expect documentation, #2331 <<https://github.com/qutip/qutip/pull/2331>>)
- lklivingstone (Added \_\_repr\_\_ to QobjEvo, #2111 <<https://github.com/qutip/qutip/pull/2111>>)
- Yuji Tamakoshi (Improve print(qutip.settings) by make it shorter, #2113 <<https://github.com/qutip/qutip/pull/2113>>)
- khnikhil (Added fermionic annihilation and creation operators, #2166 <<https://github.com/qutip/qutip/pull/2166>>)
- Daniel Weiss (Improved sampling algorithm for mcsolve, #2218 <<https://github.com/qutip/qutip/pull/2218>>)
- SJUW (Increase missing colorbar padding for matrix\_histogram\_complex() from 0 to 0.05, #2181 <<https://github.com/qutip/qutip/pull/2181>>)
- Valan Baptist Mathuranayagam (Changed qutip-notebooks to qutip-tutorials and fixed the typo in the link redirecting to the changelog section in the PR template, #2107 <<https://github.com/qutip/qutip/pull/2107>>)
- Gerardo Jose Suarez (Added information on sec\_cutoff to the documentation, #2136 <<https://github.com/qutip/qutip/pull/2136>>)
- Cristian Emiliano Godinez Ramirez (Added inherited members to API doc of MESolver, SMESolver, SSE-Solver, NonMarkovianMCSolver, #2167 <<https://github.com/qutip/qutip/pull/2167>>)
- Andrey Rakhubovsky (Corrected grammar in Bloch-Redfield master equation documentation, #2174 <<https://github.com/qutip/qutip/pull/2174>>)
- Rushiraj Gadhvi (qutip.ipynbtools.version\_table() can now be called without Cython installed, #2110 <<https://github.com/qutip/qutip/pull/2110>>)
- Harsh Khilawala (Moved HTMLProgressBar from qutip/ipynbtools.py to qutip/ui/progressbar.py, #2112 <<https://github.com/qutip/qutip/pull/2112>>)
- Avatar Srinidhi P V (Added new argument bc\_type to take boundary conditions when creating QobjEvo, #2114 <<https://github.com/qutip/qutip/pull/2114>>)
- Andrey Rakhubovsky (Fix types in docstring of projection(), #2363 <<https://github.com/qutip/qutip/pull/2363>>)

## 6.1.2 Qobj changes

Previously Qobj data was stored in a SciPy-like sparse matrix. Now the representation is flexible. Implementations for dense and sparse formats are included in QuTiP and custom implementations are possible. QuTiP's performance on dense states and operators is significantly improved as a result.

Some highlights:

- The data is still accessible via the `.data` attribute, but is now an instance of the underlying data type instead of a SciPy-like sparse matrix. The operations available in `qutip.core.data` may be used on `.data`, regardless of the data type.
- Qobj with different data types may be mixed in arithmetic and other operations. A sensible output type will be automatically determined.
- The new `.to(...)` method may be used to convert a Qobj from one data type to another. E.g. `.to("dense")` will convert to the dense representation and `.to("csr")` will convert to the sparse type.

- Many `Qobj` methods and methods that create `Qobj` now accepted a `dtype` parameter that allows the data type of the returned `Qobj` to be specified.
- The new `&` operator may be used to obtain the tensor product.
- The new `@` operator may be used to obtain the matrix / operator product. `bar @ ket` returns a scalar.
- The new `.contract()` method will collapse 1D subspaces of the dimensions of the `Qobj`.
- The new `.logm()` method returns the matrix logarithm of an operator.
- The methods `.set_data`, `.get_data`, `.extract_state`, `.eliminate_states`, `.evaluate` and `.check_isunitary` have been removed.
- The property `dtype` returns the representation of the data used.
- The new `data_as` allows to obtain the data as a common python format: numpy array, scipy sparse matrix, JAX Array, etc.

### 6.1.3 QobjEvo changes

The `QobjEvo` type for storing time-dependent quantum objects has been significantly expanded, standardized and extended. The time-dependent coefficients are now represented using a new `Coefficient` type that may be independently created and manipulated if required.

Some highlights:

- The `.compile()` method has been removed. Coefficients specified as strings are automatically compiled if possible and the compilation is cached across different Python runs and instances.
- Mixing coefficient types within a single `Qobj` is now supported.
- Many new attributes were added to `QobjEvo` for convenience. Examples include `.dims`, `.shape`, `.superrep` and `.isconstant`.
- Many old attributes such as `.cte`, `.use_cython`, `.type`, `.const`, and `.coeff_file` were removed.
- A new `Spline` coefficient supports spline interpolations of different orders. The old `Cubic_Spline` coefficient has been removed.
- The new `.arguments(...)` method allows additional arguments to the underlying coefficient functions to be updated.
- The `_step_func_coeff` argument has been replaced by the `order` parameter. `_step_func_coeff=False` is equivalent to `order=3`. `_step_func_coeff=True` is equivalent to `order=0`. Higher values of `order` give spline interpolations of higher orders.
- The spline type can take `bc_type` to control the boundary conditions.
- `QobjEvo` can be created from the multiplication of a `Qobj` with a coefficient: `oper * qutip.coefficient(f, args=args)` is equivalent to `qutip.QobjEvo([[oper, f]], args=args)`.
- Coefficient function can be defined in a pythonic manner: `def f(t, A, w)`. The dictionary `args` second argument is no longer needed. Function using the exact `f(t, args)` signature will use the old method for backward compatibility.



### 6.1.4 Solver changes

The solvers in QuTiP have been heavily reworked and standardized. Under the hood solvers now make use of swappable ODE Integrators. Many Integrators are included (see the list below) and custom implementations are possible. Solvers now consistently accept a QobjEvo instance at the Hamiltonian or Liouvillian, or any object which can be passed to the QobjEvo constructor.

A breakdown of highlights follows.

All solvers:

- Solver options are now supplied in an ordinary Python dict. `qutip.Options` is deprecated and returns a dict for backwards compatibility.
- A specific ODE integrator may be selected by supplying a `method` option.
- Each solver provides a class interface. Creating an instance of the class allows a solver to be run multiple times for the same system without having to repeatedly reconstruct the right-hand side of the ODE to be integrated.
- A QobjEvo instance is accepted for most operators, e.g., `H`, `c_ops`, `e_ops`, `a_ops`.
- The progress bar is now selected using the `progress_bar` option. A new progress bar using the `tqdm` Python library is provided.
- Dynamic arguments, where the value of an operator depends on the current state of the evolution interface reworked. Now a property of the solver is to be used as an arguments: `args={"state": MESolver.StateFeedback(default=rho0)}`

Integrators:

- The SciPy `zode` integrator is available with the BDF and Adams methods as `bdf` and `adams`.
- The SciPy `dop853` integrator (an eighth order Runge-Kutta method by Dormand & Prince) is available as `dop853`.
- The SciPy `lsoda` integrator is available as `lsoda`.
- QuTiP's own implementation of Verner's "most efficient" Runge-Kutta methods of order 7 and 9 are available as `vern7` and `vern9`. See <http://people.math.sfu.ca/~jverner/> for a description of the methods.
- QuTiP's own implementation of a solver that directly diagonalizes the the system to be integrated is available as `diag`. It only works on time-independent systems and is slow to setup, but once the diagonalization is complete, it generates solutions very quickly.
- QuTiP's own implementation of an approximate Krylov subspace integrator is available as `krylov`. This integrator is only usable with `sesolve`.

Result class:

- A new `.e_data` attribute provides expectation values as a dictionary. Unlike `.expect`, the values are provided in a Python list rather than a numpy array, which better supports non-numeric types.
- The contents of the `.stats` attribute changed significantly and is now more consistent across solvers.

Monte-Carlo Solver (`mcsolve`):

- The system, `H`, may now be a super-operator.
- The `seed` parameter now supports supplying numpy `SeedSequence` or `Generator` types.
- The new `timeout` and `target_tol` parameters allow the solver to exit early if a timeout or target tolerance is reached.
- The `ntraj` option no longer supports a list of numbers of trajectories. Instead, just run the solver multiple times and use the class `MCSolver` if setting up the solver uses a significant amount of time.
- The `map_func` parameter has been replaced by the `map` option.
- A `loky` based parallel map as been added.

- A mpi based parallel map as been added.
- The result returned by `mcsolve` now supports calculating photocurrents and calculating the steady state over `N` trajectories.
- The old `parfor` parallel execution function has been removed from `qutip.parallel`. Use `parallel_map`, `loky_map` or `mpi_pmap` instead.
- Added improved sampling options which converge much faster when the probability of collapse is small.

Non Markovian Monte-Carlo Solver (`nm_mcsolve`):

- New Monte-Carlo Solver supporting negative decay rates.
- Based on the influence martingale approach, Donvil et al., Nat Commun 13, 4140 (2022).
- Most of the improvements made to the regular Monte-Carlo solver are also available here.
- The value of the influence martingale is available through the `.trace` attribute of the result.

Stochastic Equation Solvers (`ssesolve`, `smesolve`)

- Function call greatly changed: many keyword arguments are now options.
- `m_ops` and `dW_factors` are now changed from the default from the new class interface only.
- Use the same parallel maps as `mcsolve`: support for `loky` and `mpi` map added.
- End conditions `timeout` and `target_tol` added.
- The `seed` parameter now supports supplying numpy `SeedSequence`.
- Wiener function is now available as a feedback.

Bloch-Redfield Master Equation Solver (`brmesolve`):

- The `a_ops` and `spectra` support implementations been heavily reworked to reuse the techniques from the new `Coefficient` and `QobjEvo` classes.
- The `use_secular` parameter has been removed. Use `sec_cutoff=-1` instead.
- The required tolerance is now read from `qutip.settings`.

Krylov Subspace Solver (`krylovsolve`):

- The Krylov solver is now implemented using `SESolver` and the `krylov` ODE integrator. The function `krylovsolve` is maintained for convenience and now supports many more options.
- The `sparse` parameter has been removed. Supply a sparse `Qobj` for the Hamiltonian instead.

Floquet Solver (`fsesolve` and `fmmsolve`):

- The Floquet solver has been rewritten to use a new `FloquetBasis` class which manages the transformations from lab to Floquet basis and back.
- Many of the internal methods used by the old Floquet solvers have been removed. The Floquet tensor may still be retrieved using the function `floquet_tensor`.
- The Floquet Markov Master Equation solver has had many changes and new options added. The environment temperature may be specified using `w_th`, and the result states are stored in the lab basis and optionally in the Floquet basis using `store_floquet_state`.
- The spectra functions supplied to `fmmsolve` must now be vectorized (i.e. accept and return numpy arrays for frequencies and densities) and must accept negative frequency (i.e. usually include a `w > 0` factor so that the returned densities are zero for negative frequencies).
- The number of sidebands to keep, `kmax` may only be supplied when using the `FMESolver`
- The `Tsteps` parameter has been removed from both `fsesolve` and `fmmsolve`. The `precompute` option to `FloquetBasis` may be used instead.

Evolution of State Solver (`essolve`):

- The function `essolve` has been removed. Use the `diag` integration method with `sesolve` or `mesolve` instead.

Steady-state solvers (steadystate module):

- The `method` parameter and `solver` parameters have been separated. Previously they were mixed together in the `method` parameter.
- The previous options are now passed as parameters to the steady state solver and mostly passed through to the underlying SciPy functions.
- The logging and statistics have been removed.

Correlation functions (correlation module):

- A new `correlation_3op` function has been added. It supports `MESolver` or `BRMESolver`.
- The `correlation`, `correlation_4op`, and `correlation_ss` functions have been removed.
- Support for calculating correlation with `mcsolve` has been removed.

Propagators (propagator module):

- A class interface, `qutip.Propagator`, has been added for propagators.
- Propagation of time-dependent systems is now supported using `QobjEvo`.
- The `unitary_mode` and `parallel` options have been removed.

Correlation spectra (spectrum module):

- The functions `spectrum_ss` and `spectrum_pi` have been removed and are now internal functions.
- The `use_pinv` parameter for `spectrum` has been removed and the functionality merged into the `solver` parameter. Use `solver="pi"` instead.

Hierarchical Equation of Motion Solver (HEOM)

- Updated the solver to use the new QuTiP integrators and data layer.
- Updated all the HEOM tutorials to QuTiP 5.
- Added support for combining bosonic and fermionic baths.
- Sped up the construction of the RHS of the HEOM solver by a factor of 4x.
- As in QuTiP 4, the HEOM supports arbitrary spectral densities, bosonic and fermionic baths, Páde and Matsubara expansions of the correlation functions, calculating the Matsubara terminator and inspection of the ADOs (auxiliary density operators).

### 6.1.5 QuTiP core

There have been numerous other small changes to core QuTiP features:

- `qft(...)` the function that returns the quantum Fourier transform operator was moved from `qutip.qip.algorithm` into `qutip`.
- The Bloch-Redfield solver tensor, `brtensor`, has been moved into `qutip.core`. See the section above on the Bloch-Redfield solver for details.
- The functions `mat2vec` and `vec2mat` for transforming states to and from super-operator states have been renamed to `stack_columns` and `unstack_columns`.
- The function `liouvillian_ref` has been removed. Used `liouvillian` instead.
- The superoperator transforms `super_to_choi`, `choi_to_super`, `choi_to_kraus`, `choi_to_chi` and `chi_to_choi` have been removed. Used `to_choi`, `to_super`, `to_kraus` and `to_chi` instead.
- All of the random object creation functions now accepted a numpy `Generator` as a seed.

- The `dims` parameter of all random object creation functions has been removed. Supply the dimensions as the first parameter if explicit dimensions are required.
- The function `rand_unitary_haar` has been removed. Use `rand_unitary(distribution="haar")` instead.
- The functions `rand_dm_hs` and `rand_dm_ginibre` have been removed. Use `rand_dm(distribution="hs")` and `rand_dm(distribution="ginibre")` instead.
- The function `rand_ket_haar` has been removed. Use `rand_ket(distribution="haar")` instead.
- The measurement functions have had the `target` parameter for expanding the measurement operator removed. Used `expand_operator` to expand the operator instead.
- `qutip.Bloch` now supports applying colours per-point, state or vector in `add_point`, `add_states`, and `add_vectors`.
- Dimensions use a class instead of layered lists.
- Allow measurement functions to support degenerate operators.
- Add `qeye_like` and `qzero_like`.
- Added fermionic annihilation and creation operators.

### 6.1.6 QuTiP settings

Previously `qutip.settings` was an ordinary module. Now `qutip.settings` is an instance of a settings class. All the runtime modifiable settings for core operations are in `qutip.settings.core`. The other settings are not modifiable at runtime.

- Removed `load`, `reset` and `save` functions.
- Removed `.debug`, `.fortran`, `.openmp_thresh`.
- New `.compile` stores the compilation options for compiled coefficients.
- New `.core["rtol"]` core option gives the default relative tolerance used by QuTiP.
- The absolute tolerance setting `.atol` has been moved to `.core["atol"]`.

### 6.1.7 Visualization

- Added arguments to `plot_wigner` and `plot_wigner_fock_distribution` to specify parameters for wigner.
- Removed `Bloch3D`. The same functionality is provided by `Bloch`.
- Added `fig`, `ax` and `cmap` keyword arguments to all visualization functions.
- Most visualization functions now respect the `colorblind_safe` setting.
- Added new functions to create animations from a list of `Qobj` or directly from solver results with saved states.

### 6.1.8 Package reorganization

- `qutip.qip` has been moved into its own package, `qutip-qip`. Once installed, `qutip-qip` is available as either `qutip.qip` or `qutip_qip`. Some widely useful gates have been retained in `qutip.gates`.
- `qutip.control` has been moved to `qutip-qtrl` and once installed `qutip-qtrl` is available as either `qutip.control` or `qutip_qtrl`. Note that `qutip_qtrl` is provided primarily for backwards compatibility. Improvements to optimal control will take place in the new `qutip_qoc` package.
- `qutip.lattice` has been moved into its own package, `qutip-lattice`. It is available from <https://github.com/qutip/qutip-lattice>.
- `qutip.sparse` has been removed. It contained the old sparse matrix representation and is replaced by the new implementation in `qutip.data`.
- `qutip.piqs` functions are no longer available from the `qutip` namespace. They are accessible from `qutip.piqs` instead.

### 6.1.9 Miscellaneous

- Support has been added for 64-bit integer sparse matrix indices, allowing sparse matrices with up to  $2^{63}$  rows and columns. This support needs to be enabled at compilation time by calling `setup.py` and passing `--with-idxint-64`.

### 6.1.10 Feature removals

- Support for OpenMP has been removed. If there is enough demand and a good plan for how to organize it, OpenMP support may return in a future QuTiP release.
- The `qutip.parfor` function has been removed. Use `qutip.parallel_map` instead.
- `qutip.graph` has been removed and replaced by SciPy's graph functions.
- `qutip.topology` has been removed. It contained only one function `berry_curvature`.
- The `~/.qutip/qutiprc` config file is no longer supported. It contained settings for the OpenMP support.
- Deprecate `three_level_atom`
- Deprecate `orbital`

### 6.1.11 Changes from QuTiP 5.0.0b1:

### 6.1.12 Features

- Add dtype to printed output of `qobj` (#2352 by Rochisha Agarwal)

### 6.1.13 Miscellaneous

- Allow `scipy 1.12` to be used with `qutip`. (#2354 by Pieter Eendebak)

## 6.2 QuTiP 5.0.0b1 (2024-03-04)

### 6.2.1 Features

- Create a Dimension class (#1996)
- Add arguments of `plot_wigner()` and `plot_wigner_fock_distribution()` to specify parameters for `wigner()`. (#2057, by Kosuke Mizuno)
- Restore feedback to solvers (#2210)
- Added `mpi_pmap`, which uses the `mpi4py` module to run computations in parallel through the MPI interface. (#2296, by Paul)
- Only pre-compute density matrices if `keep_runs_results` is `False` (#2303, by Matt Ord)

### 6.2.2 Bug Fixes

- Add the possibility to customize point colors as in V4 and fix point plot behavior for 'l' style (#1974, by Daniel Moreno Galán)
- Disabled broken “improved sampling” for `nm_mcsolve`. (#2234, by Paul)
- Fixed result objects storing a reference to the solver through `options._feedback`. (#2262, by Paul)
- Fixed `simdiag` not returning orthonormal eigenvectors. (#2269, by Sola85)
- Fix LaTeX display of `Qobj` state in Jupyter cell outputs (#2272, by Edward Thomas)
- Improved behavior of `parallel_map` and `loky_pmap` in the case of timeouts, errors or keyboard interrupts (#2280, by Paul)
- Ignore deprecation warnings from cython 0.29.X in tests. (#2288)
- Fixed two problems with the `steady_state()` solver in the HEOM method. (#2333)

### 6.2.3 Miscellaneous

- Improve fidelity doc-string (#2257)
- Improve documentation in `guide/dynamics` (#2271)
- Improve states and operator parameters documentation. (#2289)
- Rework `kraus_to_choi` making it faster (#2284, by Bogdan Reznichenko)
- Remove Bloch3D: redundant to Bloch (#2306)
- Allow tests to run without matplotlib and ipython. (#2311)
- Add too small step warnings in fixed dt SODE solver (#2313)
- Add `dtype` to `Qobj` and `QobjEvo` (#2325)
- Fix typos in `expect` documentation (#2331, by gabbence95)
- Allow measurement functions to support degenerate operators. (#2342)

## 6.3 QuTiP 5.0.0a2 (2023-09-06)

### 6.3.1 Features

- Add support for different spectra types for `bloch_redfield_tensor` (#1951)
- Improve qutip import times by setting logger names explicitly. (#1981, by Pieter Eendebak)
- Change the order of parameters in `expand_operator` (#1991)
- Add `svn` and `solve` to dispatched (#2002)
- Added `nm_mcsolve` to provide support for Monte-Carlo simulations of master equations with possibly negative rates. The method implemented here is described in arXiv:2209.08958 [quant-ph]. (#2070 by pmenczel)
- Add support for combining bosonic and fermionic HEOM baths (#2089)
- Added `__repr__` to `QobjEvo` (#2111 by lklivingstone)
- Improve `print(qutip.settings)` by make it shorter (#2113 by tamakoshi2001)
- Create the `trace_oper_ket` operation (#2126)
- Speed up the construction of the RHS of the HEOM solver by a factor of 4x by converting the final step to Cython. (#2128)
- Rewrite the stochastic solver to use the v5 solver interface. (#2131)
- Add `Qobj.get` to extract underlying data in original format. (#2141)
- Add `qeye_like` and `qzero_like` (#2153)
- Add capacity to dispatch on `Data` (#2157)
- Added fermionic annihilation and creation operators. (#2166 by khnikhil)
- Changed arguments and applied `colorblind_safe` to functions in `visualization.py` (#2170 by Yuji Tamakoshi)
- Changed arguments and applied `colorblind_safe` to `plot_wigner_sphere` and `matrix_histogram` in `visualization.py` (#2193 by Yuji Tamakoshi)
- Added Dia data layer which represents operators as multi-diagonal matrices. (#2196)
- Added support for animated plots. (#2203 by Yuji Tamakoshi)
- Improved sampling algorithm for `mcsolve` (#2218 by Daniel Weiss)
- Added support for early termination of map functions. (#2222)

### 6.3.2 Bug Fixes

- Add missing state transformation to `floquet_markov_mesolve` (#1952 by christian512)
- Added default `_isherm` value (True) for momentum and position operators. (#2032 by Asier Galicia)
- Changed qutip-notebooks to qutip-tutorials and fixed the typo in the link redirecting to the changelog section in the PR template. (#2107 by Valan Baptist Mathuranayagam)
- Increase missing colorbar padding for `matrix_histogram_complex()` from 0 to 0.05. (#2181 by SJUW)
- Raise error on insufficient memory. (#2224)
- Fixed fallback to `fsolve` call in `fmmsolve` (#2225)

### 6.3.3 Removals

- Remove `qutip.control` and replace with `qutip_qtrl`. (#2116)
- Deleted `_solve` in `countstat.py` and used `_data.solve`. (#2120 by Yuji Tamakoshi)
- Deprecate `three_level_atom` (#2221)
- Deprecate `orbital` (#2223)

### 6.3.4 Documentation

- Add a guide on Superoperators, Pauli Basis and Channel Contraction. (#1984 by christian512)
- Added information on `sec_cutoff` to the documentation (#2136 by Gerardo Jose Suarez)
- Added inherited members to API doc of `MESolver`, `SMESolver`, `SSESolver`, `NonMarkovianMCSolver` (#2167 by Cristian Emiliano Godinez Ramirez)
- Corrected grammar in Bloch-Redfield master equation documentation (#2174 by Andrey Rakhubovsky)

### 6.3.5 Miscellaneous

- Update `scipy` version requirement to 1.5+ (#1982 by Pieter Eendebak)
- Added `__all__` to `qutip/measurements.py` and `qutip/core/semidefinite.py` (#2103 by Rushiraj Gadhvi)
- Restore `towncrier` check (#2105)
- `qutip.ipynbtools.version_table()` can now be called without Cython installed (#2110 by Rushiraj Gadhvi)
- Moved `HTMLProgressBar` from `qutip/ipynbtools.py` to `qutip/ui/progressbar.py` (#2112 by Harsh Khilawala)
- Added new argument `bc_type` to take boundary conditions when creating `QobjEvo` (#2114 by Avatar Srinidhi P V)
- Remove Windows build warning suppression. (#2119)
- Optimize dispatcher by dispatching on positional only args. (#2135)
- Clean `semidefinite` (#2138)
- Migrate `transfertensor.py` to `solver` (#2142)
- Add a test for `progress_bar` (#2150)
- Enable cython 3 (#2151)
- Added tests for `visualization.py` (#2192 by Yuji Tamakoshi)
- Sorted arguments of `sphereplot` so that the order is similar to those of `plot_spin_distribution` (#2219 by Yuji Tamakoshi)

### Version 5.0.0a1 (February 7, 2023)

QuTiP 5 is a redesign of many of the core components of QuTiP (`Qobj`, `QobjEvo`, solvers) to make them more consistent and more flexible.

`Qobj` may now be stored in either sparse or dense representations, and the two may be mixed sensibly as needed. `QobjEvo` is now used consistently throughout QuTiP, and the implementation has been substantially cleaned up. A new `Coefficient` class is used to represent the time-dependent factors inside `QobjEvo`.

The solvers have been rewritten to work well with the new data layer and the concept of `Integrators` which solve ODEs has been introduced. In future, new data layers may provide their own `Integrators` specialized to their representation of the underlying data.



Much of the user-facing API of QuTiP remains familiar, but there have had to be many small breaking changes. If we can make changes to easy migrating code from QuTiP 4 to QuTiP 5, please let us know.

Any extensive list of changes follows.

### 6.3.6 Contributors

QuTiP 5 has been a large effort by many people over the last three years.

In particular:

- Jake Lishman led the implementation of the new data layer and coefficients.
- Eric Giguère led the implementation of the new QobjEvo interface and solvers.
- Boxi Li led the updating of QuTiP's QIP support and the creation of `qutip_qip`.

Other members of the QuTiP Admin team have been heavily involved in reviewing, testing and designing QuTiP 5:

- Alexander Pitchford
- Asier Galicia
- Nathan Shammah
- Shahnawaz Ahmed
- Neill Lambert
- Simon Cross

Two Google Summer of Code contributors updated the tutorials and benchmarks to QuTiP 5:

- Christian Staufienbiel updated many of the tutorials (<https://github.com/qutip/qutip-tutorials/>).
- Xavier Sproken update the benchmarks (<https://github.com/qutip/qutip-benchmark/>).

Four experimental data layers backends were written either as part of Google Summer of Code or as separate projects. While these are still alpha quality, they helped significantly to test the data layer API:

- `qutip-tensorflow`: a TensorFlow backend by Asier Galicia (<https://github.com/qutip/qutip-tensorflow>)
- `qutip-cupy`: a CuPy GPU backend by Felipe Bivort Haiek (<https://github.com/qutip/qutip-cupy/>)
- `qutip-tensornetwork`: a TensorNetwork backend by Asier Galicia (<https://github.com/qutip/qutip-tensornetwork>)
- `qutip-jax`: a JAX backend by Eric Giguère (<https://github.com/qutip/qutip-jax/>)

We have also had many other contributors, whose specific contributions are detailed below:

- Pieter Eendebak (updated the required SciPy to 1.4+, #1982 <https://github.com/qutip/qutip/pull/1982>).
- Pieter Eendebak (reduced import times by setting logger names, #1981 <https://github.com/qutip/qutip/pull/1981>)
- Xavier Sproken (included C header files in the source distribution, #1971 <https://github.com/qutip/qutip/pull/1971>)
- Christian Staufienbiel (added support for multiple collapse operators to the Floquet solver, #1962 <https://github.com/qutip/qutip/pull/1962>)
- Christian Staufienbiel (fixed the basis used in the Floquet Master Equation solver, #1952 <https://github.com/qutip/qutip/pull/1952>)
- Christian Staufienbiel (allowed the `bloch_redfield_tensor` function to accept strings and callables for `a_ops`, #1951 <https://github.com/qutip/qutip/pull/1951>)

- Henrique Silvéro (allowed `qutip_qip` to be imported as `qutip.qip`, #1920 <<https://github.com/qutip/qutip/pull/1920>>)
- Florian Hopfmueller (added a vastly improved implementations of `process_fidelity` and `average_gate_fidelity`, #1712 <<https://github.com/qutip/qutip/pull/1712>>, #1748 <<https://github.com/qutip/qutip/pull/1748>>, #1788 <<https://github.com/qutip/qutip/pull/1788>>)
- Felipe Bivort Haiek (fixed inaccuracy in docstring of the dense implementation of negation, #1608 <<https://github.com/qutip/qutip/pull/1608>>)
- Rajath Shetty (added support for specifying colors for individual points, vectors and states display by `qutip.Bloch`, #1335 <<https://github.com/qutip/qutip/pull/1335>>)

### 6.3.7 Qobj changes

Previously Qobj data was stored in a SciPy-like sparse matrix. Now the representation is flexible. Implementations for dense and sparse formats are included in QuTiP and custom implementations are possible. QuTiP's performance on dense states and operators is significantly improved as a result.

Some highlights:

- The data is still accessible via the `.data` attribute, but is now an instance of the underlying data type instead of a SciPy-like sparse matrix. The operations available in `qutip.core.data` may be used on `.data`, regardless of the data type.
- Qobj with different data types may be mixed in arithmetic and other operations. A sensible output type will be automatically determined.
- The new `.to(...)` method may be used to convert a Qobj from one data type to another. E.g. `.to("dense")` will convert to the dense representation and `.to("csr")` will convert to the sparse type.
- Many Qobj methods and methods that create Qobj now accepted a `dtype` parameter that allows the data type of the returned Qobj to be specified.
- The new `&` operator may be used to obtain the tensor product.
- The new `@` operator may be used to obtain the matrix / operator product. `bar @ ket` returns a scalar.
- The new `.contract()` method will collapse 1D subspaces of the dimensions of the Qobj.
- The new `.logm()` method returns the matrix logarithm of an operator.
- The methods `.set_data`, `.get_data`, `.extract_state`, `.eliminate_states`, `.evaluate` and `.check_isunitary` have been removed.

### 6.3.8 QobjEvo changes

The QobjEvo type for storing time-dependent quantum objects has been significantly expanded, standardized and extended. The time-dependent coefficients are now represented using a new `Coefficient` type that may be independently created and manipulated if required.

Some highlights:

- The `.compile()` method has been removed. Coefficients specified as strings are automatically compiled if possible and the compilation is cached across different Python runs and instances.
- Mixing coefficient types within a single Qobj is now supported.
- Many new attributes were added to QobjEvo for convenience. Examples include `.dims`, `.shape`, `.superrep` and `.isconstant`.
- Many old attributes such as `.cte`, `.use_cython`, `.type`, `.const`, and `.coeff_file` were removed.
- A new `Spline` coefficient supports spline interpolations of different orders. The old `Cubic_Spline` coefficient has been removed.

- The new `.arguments(...)` method allows additional arguments to the underlying coefficient functions to be updated.
- The `_step_func_coeff` argument has been replaced by the `order` parameter. `_step_func_coeff=False` is equivalent to `order=3`. `_step_func_coeff=True` is equivalent to `order=0`. Higher values of `order` gives spline interpolations of higher orders.

### 6.3.9 Solver changes

The solvers in QuTiP have been heavily reworked and standardized. Under the hood solvers now make use of swappable ODE Integrators. Many Integrators are included (see the list below) and custom implementations are possible. Solvers now consistently accept a `QobjEvo` instance at the Hamiltonian or Liouvillian, or any object which can be passed to the `QobjEvo` constructor.

A breakdown of highlights follows.

All solvers:

- Solver options are now supplied in an ordinary Python dict. `qutip.Options` is deprecated and returns a dict for backwards compatibility.
- A specific ODE integrator may be selected by supplying a `method` option.
- Each solver provides a class interface. Creating an instance of the class allows a solver to be run multiple times for the same system without having to repeatedly reconstruct the right-hand side of the ODE to be integrated.
- A `QobjEvo` instance is accepted for most operators, e.g., `H`, `c_ops`, `e_ops`, `a_ops`.
- The progress bar is now selected using the `progress_bar` option. A new progress bar using the `tqdm` Python library is provided.
- Dynamic arguments, where the value of an operator depends on the current state of the evolution, have been removed. They may be re-implemented later if there is demand for them.

Integrators:

- The SciPy `zode` integrator is available with the BDF and Adams methods as `bdf` and `adams`.
- The SciPy `dop853` integrator (an eighth order Runge-Kutta method by Dormand & Prince) is available as `dop853`.
- The SciPy `lsoda` integrator is available as `lsoda`.
- QuTiP's own implementation of Verner's "most efficient" Runge-Kutta methods of order 7 and 9 are available as `vern7` and `vern9`. See <http://people.math.sfu.ca/~jverner/> for a description of the methods.
- QuTiP's own implementation of a solver that directly diagonalizes the the system to be integrated is available as `diag`. It only works on time-independent systems and is slow to setup, but once the diagonalization is complete, it generates solutions very quickly.
- QuTiP's own implementation of an approximate Krylov subspace integrator is available as `krylov`. This integrator is only usable with `sesolve`.

Result class:

- A new `.e_data` attribute provides expectation values as a dictionary. Unlike `.expect`, the values are provided in a Python list rather than a numpy array, which better supports non-numeric types.
- The contents of the `.stats` attribute changed significantly and is now more consistent across solvers.

Monte-Carlo Solver (`mcsolve`):

- The system, `H`, may now be a super-operator.
- The `seed` parameter now supports supplying numpy `SeedSequence` or `Generator` types.
- The new `timeout` and `target_tol` parameters allow the solver to exit early if a timeout or target tolerance is reached.

- The `ntraj` option no longer supports a list of numbers of trajectories. Instead, just run the solver multiple times and use the class `MCSolver` if setting up the solver uses a significant amount of time.
- The `map_func` parameter has been replaced by the `map` option. In addition to the existing `serial` and `parallel` values, the value `loky` may be supplied to use the `loky` package to parallelize trajectories.
- The result returned by `mcsolve` now supports calculating photocurrents and calculating the steady state over `N` trajectories.
- The old `parfor` parallel execution function has been removed from `qutip.parallel`. Use `parallel_map` or `loky_map` instead.

Bloch-Redfield Master Equation Solver (`brmesolve`):

- The `a_ops` and `spectra` support implementations have been heavily reworked to reuse the techniques from the new `Coefficient` and `QobjEvo` classes.
- The `use_secular` parameter has been removed. Use `sec_cutoff=-1` instead.
- The required tolerance is now read from `qutip.settings`.

Krylov Subspace Solver (`krylovsolve`):

- The Krylov solver is now implemented using `SESolver` and the `krylov` ODE integrator. The function `krylovsolve` is maintained for convenience and now supports many more options.
- The `sparse` parameter has been removed. Supply a sparse `Qobj` for the Hamiltonian instead.

Floquet Solver (`fsesolve` and `fmmsolve`):

- The Floquet solver has been rewritten to use a new `FloquetBasis` class which manages the transformations from lab to Floquet basis and back.
- Many of the internal methods used by the old Floquet solvers have been removed. The Floquet tensor may still be retrieved using the function `floquet_tensor`.
- The Floquet Markov Master Equation solver has had many changes and new options added. The environment temperature may be specified using `w_th`, and the result states are stored in the lab basis and optionally in the Floquet basis using `store_floquet_state`.
- The spectra functions supplied to `fmmsolve` must now be vectorized (i.e. accept and return numpy arrays for frequencies and densities) and must accept negative frequency (i.e. usually include a  $\omega > 0$  factor so that the returned densities are zero for negative frequencies).
- The number of sidebands to keep, `kmax` may only be supplied when using the `FMESolver`.
- The `Tsteps` parameter has been removed from both `fsesolve` and `fmmsolve`. The `precompute` option to `FloquetBasis` may be used instead.

Evolution of State Solver (`essolve`):

- The function `essolve` has been removed. Use the `diag` integration method with `sesolve` or `mesolve` instead.

Steady-state solvers (`steadystate` module):

- The `method` parameter and `solver` parameters have been separated. Previously they were mixed together in the `method` parameter.
- The previous options are now passed as parameters to the steady state solver and mostly passed through to the underlying SciPy functions.
- The logging and statistics have been removed.

Correlation functions (`correlation` module):

- A new `correlation_3op` function has been added. It supports `MESolver` or `BRMESolver`.
- The `correlation`, `correlation_4op`, and `correlation_ss` functions have been removed.
- Support for calculating correlation with `mcsolve` has been removed.

Propagators (propagator module):

- A class interface, `qutip.Propagator`, has been added for propagators.
- Propagation of time-dependent systems is now supported using `QobjEvo`.
- The `unitary_mode` and `parallel` options have been removed.

Correlation spectra (spectrum module):

- The functions `spectrum_ss` and `spectrum_pi` have been removed and are now internal functions.
- The `use_pinv` parameter for `spectrum` has been removed and the functionality merged into the `solver` parameter. Use `solver="pi"` instead.

### 6.3.10 QuTiP core

There have been numerous other small changes to core QuTiP features:

- `qft(...)` the function that returns the quantum Fourier transform operator was moved from `qutip.qip.algorithm` into `qutip`.
- The Bloch-Redfield solver tensor, `brtensor`, has been moved into `qutip.core`. See the section above on the Bloch-Redfield solver for details.
- The functions `mat2vec` and `vec2mat` for transforming states to and from super-operator states have been renamed to `stack_columns` and `unstack_columns`.
- The function `liouvillian_ref` has been removed. Used `liouvillian` instead.
- The superoperator transforms `super_to_choi`, `choi_to_super`, `choi_to_kraus`, `choi_to_chi` and `chi_to_choi` have been removed. Used `to_choi`, `to_super`, `to_kraus` and `to_chi` instead.
- All of the random object creation functions now accepted a numpy Generator as a seed.
- The `dims` parameter of all random object creation functions has been removed. Supply the dimensions as the first parameter if explicit dimensions are required.
- The function `rand_unitary_haar` has been removed. Use `rand_unitary(distribution="haar")` instead.
- The functions `rand_dm_hs` and `rand_dm_ginibre` have been removed. Use `rand_dm(distribution="hs")` and `rand_dm(distribution="ginibre")` instead.
- The function `rand_ket_haar` has been removed. Use `rand_ket(distribution="haar")` instead.
- The measurement functions have had the `target` parameter for expanding the measurement operator removed. Used `expand_operator` to expand the operator instead.
- `qutip.Bloch` now supports applying colours per-point, state or vector in `add_point`, `add_states`, and `add_vectors`.

### 6.3.11 QuTiP settings

Previously `qutip.settings` was an ordinary module. Now `qutip.settings` is an instance of a settings class. All the runtime modifiable settings for core operations are in `qutip.settings.core`. The other settings are not modifiable at runtime.

- Removed `load`, `reset` and `save` functions.
- Removed `.debug`, `.fortran`, `.openmp_thresh`.
- New `.compile` stores the compilation options for compiled coefficients.
- New `.core["rtol"]` core option gives the default relative tolerance used by QuTiP.
- The absolute tolerance setting `.atol` has been moved to `.core["atol"]`.

### 6.3.12 Package reorganization

- `qutip.qip` has been moved into its own package, `qutip-qip`. Once installed, `qutip-qip` is available as either `qutip.qip` or `qutip_qip`. Some widely useful gates have been retained in `qutip.gates`.
- `qutip.lattice` has been moved into its own package, `qutip-lattice`. It is available from [<https://github.com/qutip/qutip-lattice>](https://github.com/qutip/qutip-lattice).
- `qutip.sparse` has been removed. It contained the old sparse matrix representation and is replaced by the new implementation in `qutip.data`.
- `qutip.piqs` functions are no longer available from the `qutip` namespace. They are accessible from `qutip.piqs` instead.

### 6.3.13 Miscellaneous

- Support has been added for 64-bit integer sparse matrix indices, allowing sparse matrices with up to  $2^{63}$  rows and columns. This support needs to be enabled at compilation time by calling `setup.py` and passing `--with-idxint-64`.

### 6.3.14 Feature removals

- Support for OpenMP has been removed. If there is enough demand and a good plan for how to organize it, OpenMP support may return in a future QuTiP release.
- The `qutip.parfor` function has been removed. Use `qutip.parallel_map` instead.
- `qutip.graph` has been removed and replaced by SciPy's graph functions.
- `qutip.topology` has been removed. It contained only one function `berry_curvature`.
- The `~/.qutip/qutiprc` config file is no longer supported. It contained settings for the OpenMP support.

## 6.4 QuTiP 4.7.5 (2024-01-29)

Patch release for QuTiP 4.7. It adds support for SciPy 1.12.

### 6.4.1 Bug Fixes

- Remove use of `scipy.<numpy-func>` in `parallel.py`, incompatible with `scipy==1.12` (#2305 by Evan McKinney)

## 6.5 QuTiP 4.7.4 (2024-01-15)

### 6.5.1 Bug Fixes

- Adapt to deprecation from matplotlib 3.8 (#2243, reported by Bogdan Reznichenko)
- Fix name of temp files for removal after use. (#2251, reported by Qile Su)
- Avoid integer overflow in `Qobj` creation. (#2252, reported by KianHwee-Lim)
- Ignore `DeprecationWarning` from `pyximport` (#2287)
- Add partial support and tests for python 3.12. (#2294)

### 6.5.2 Miscellaneous

- Rework *choi\_to\_kraus*, making it rely on an eigenstates solver that can choose *eigh* if the Choi matrix is Hermitian, as it is more numerically stable. (#2276, by Bogdan Reznichenko)
- Rework *kraus\_to\_choi*, making it faster (#2283, by Bogdan Reznichenko and Rafael Haenel)

## 6.6 QuTiP 4.7.3 (2023-08-22)

### 6.6.1 Bug Fixes

- Non-oper qobj + scalar raise an error. (#2208 reported by vikramkashyap)
- Fixed issue where *extract\_states* did not preserve hermiticity. Fixed issue where *rand\_herm* did not set the private attribute *\_isherm* to True. (#2214 by AGaliciaMartinez)
- ssesolve average states to density matrices (#2216 reported by BenjaminDAnjou)

### 6.6.2 Miscellaneous

- Exclude cython 3.0.0 from requirement (#2204)
- Run in no cython mode with cython >=3.0.0 (#2207)

## 6.7 QuTiP 4.7.2 (2023-06-28)

This is a bugfix release for QuTiP 4.7.X. It adds support for numpy 1.25 and scipy 1.11.

### 6.7.1 Bug Fixes

- Fix setting of *sso.m\_ops* in heterodyne smesolver and passing through of *sc\_ops* to photocurrent solver. (#2081 by Bogdan Reznichenko and Simon Cross)
- Update calls to SciPy *eigvalsh* and *eigsh* to pass the range of eigenvalues to return using *subset\_by\_index=*. (#2081 by Simon Cross)
- Fixed bug where some matrices were wrongly found to be hermitian. (#2082 by AGaliciaMartinez)

### 6.7.2 Miscellaneous

- Fixed typo in *stochastic.py* (#2049, by eltociear)
- *ptrace* always return density matrix (#2185, issue by udevd)
- *mesolve* can support mixed callable and Qobj for *e\_ops* (#2184 issue by balopat)

### Version 4.7.1 (December 11, 2022)

This is a bugfix release for QuTiP 4.7.X. In addition to the minor fixes listed below, the release adds builds for Python 3.11 and support for packaging 22.0.

## 6.7.3 Features

- Improve qutip import times by setting logger names explicitly. (#1980)

## 6.7.4 Bug Fixes

- Change `floquet_master_equation_rates(...)` to use an adaptive number of time steps scaled by the number of sidebands, `kmax`. (#1961)
- Change `fidelity(A, B)` to use the reduced fidelity formula for pure states which is more numerically efficient and accurate. (#1964)
- Change `brmesolve` to raise an exception when ode integration is not successful. (#1965)
- Backport fix for IPython helper `Bloch._repr_svg_` from dev.major. Previously the `print_figure` function returned bytes, but since `ipython/ipython#5452` (in 2014) it returns a Unicode string. This fix updates QuTiP's helper to match. (#1970)
- Fix correlation for case where only the collapse operators are time dependent. (#1979)
- Fix the hinton visualization method to plot the matrix instead of its transpose. (#2011)
- Fix the hinton visualization method to take into account all the matrix coefficients to set the squares scale, instead of only the diagonal coefficients. (#2012)
- Fix parsing of package versions in `setup.py` to support packaging 22.0. (#2037)
- Add back `.qu` suffix to objects saved with `qsave` and loaded with `qload`. The suffix was accidentally removed in QuTiP 4.7.0. (#2038)
- Add a default `max_step` to processors. (#2040)

## 6.7.5 Documentation

- Add towncrier for managing the changelog. (#1927)
- Update the version of numpy used to build documentation to 1.22.0. (#1940)
- Clarify returned objects from `bloch_redfield_tensor()`. (#1950)
- Update Floquet Markov solver docs. (#1958)
- Update the roadmap and ideas to show completed work as of August 2022. (#1967)

## 6.7.6 Miscellaneous

- Return `TypeError` instead of `Exception` for type error in `sesolve` argument. (#1924)
- Add towncrier draft build of changelog to CI tests. (#1946)
- Add Python 3.11 to builds. (#2041)
- Simplify version parsing by using `packaging.version.Version`. (#2043)
- Update builds to use `cibuildwheel 2.11`, and to build with `manylinux2014` on Python 3.8 and 3.9, since `numpy` and `SciPy` no longer support `manylinux2010` on those versions of Python. (#2047)



## Version 4.7.0 (April 13, 2022)

This release sees the addition of two new solvers – `qutip.krylovsolve` based on the Krylov subspace approximation and `qutip.nonmarkov.heom` that reimplements the BoFiN HEOM solver.

Bloch sphere rendering gained support for drawing arcs and lines on the sphere, and for setting the transparency of rendered points and vectors, Hinton plots gained support for specifying a coloring style, and matrix histograms gained better default colors and more flexible styling options.

Other significant improvements include better scaling of the Floquet solver, support for passing `Path` objects when saving and loading files, support for passing callable functions as `e_ops` to `mesolve` and `sesolve`, and faster state number enumeration and Husimi  $Q$  functions.

Import bugfixes include some bugs affecting plotting with matplotlib 3.5 and fixing support for qutrits (and other non-qubit) quantum circuits.

The many other small improvements, bug fixes, documentation enhancements, and behind the scenes development changes are included in the list below.

QuTiP 4.7.X will be the last series of releases for QuTiP 4. Patch releases will continue for the 4.7.X series but the main development effort will move to QuTiP 5.

The many, many contributors who filed issues, submitted or reviewed pull requests, and improved the documentation for this release are listed next to their contributions below. Thank you to all of you.

## 6.7.7 Improvements

- **MAJOR** Added `krylovsolve` as a new solver based on krylov subspace approximation. (#1739 by Emiliano Fortes)
- **MAJOR** Imported BoFiN HEOM (<https://github.com/tehruhn/bofin/>) into QuTiP and replaced the HEOM solver with a compatibility wrapper around BoFiN bosonic solver. (#1601, #1726, and #1724 by Simon Cross, Tarun Raheja and Neill Lambert)
- **MAJOR** Added support for plotting lines and arcs on the Bloch sphere. (#1690 by Gaurav Saxena, Asier Galicia and Simon Cross)
- Added transparency parameter to the `add_point`, `add_vector` and `add_states` methods in the `Bloch` and `Bloch3d` classes. (#1837 by Xavier Spronken)
- Support `Path` objects in `qutip.fileio`. (#1813 by Adrià Labay)
- Improved the weighting in steadystate solver, so that the default weight matches the documented behaviour and the dense solver applies the weights in the same manner as the sparse solver. (#1275 and #1802 by NS2 Group at LPS and Simon Cross)
- Added a `color_style` option to the `hinton` plotting function. (#1595 by Cassandra Granade)
- Improved the scaling of `floquet_master_equation_rates` and `floquet_master_equation_tensor` and fixed transposition and basis change errors in `floquet_master_equation_tensor` and `floquet_markov_mesolve`. (#1248 by Camille Le Calonnec, Jake Lishman and Eric Giguère)
- Removed `linspace_with` and `view_methods` from `qutip.utilities`. For the former it is far better to use `numpy.linspace` and for the later Python’s in-built `help` function or other tools. (#1680 by Eric Giguère)
- Added support for passing callable functions as `e_ops` to `mesolve` and `sesolve`. (#1655 by Marek Narożniak)
- Added the function `steadystate_floquet`, which returns the “effective” steadystate of a periodic driven system. (#1660 by Alberto Mercurio)
- Improved `mcsolve` memory efficiency by not storing final states when they are not needed. (#1669 by Eric Giguère)

- Improved the default colors and styling of `matrix_histogram` and provided additional styling options. (#1573 and #1628 by Mahdi Aslani)
- Sped up `state_number_enumerate`, `state_number_index`, `state_index_number`, and added some error checking. `enr_state_dictionaries` now returns a list for `idx2state`. (#1604 by Johannes Feist)
- Added new Husimi Q algorithms, improving the speed for density matrices, and giving a near order-of-magnitude improvement when calculating the Q function for many different states, using the new `qutip.QFunc` class, instead of the `qutip.qfunc` function. (#934 and #1583 by Daniel Weigand and Jake Lishman)
- Updated licence holders with regards to new governance model, and remove extraneous licensing information from source files. (#1579 by Jake Lishman)
- Removed the vendored copy of LaTeX's `qcircuit` package which is GPL licensed. We now rely on the package being installed by user. It is installed by default with `TeXLive`. (#1580 by Jake Lishman)
- The signatures of `rand_ket` and `rand_ket_haar` were changed to allow `N` (the size of the random ket) to be determined automatically when `dims` are specified. (#1509 by Purva Thakre)

### 6.7.8 Bug Fixes

- Fix circuit index used when plotting circuits with non-reversed states. (#1847 by Christian Staufenbiel)
- Changed implementation of `qutip.orbital` to use `scipy.special.spy_harm` to remove bugs in angle interpretation. (#1844 by Christian Staufenbiel)
- Fixed `QobjEvo.tidyup` to use `settings.auto_tidyup_atol` when removing small elements in sparse matrices. (#1832 by Eric Giguère)
- Ensured that `tidyup`'s default tolerance is read from settings at each call. (#1830 by Eric Giguère)
- Fixed `scipy.sparse` deprecation warnings raised by `qutip.fast_csr_matrix`. (#1827 by Simon Cross)
- Fixed rendering of vectors on the Bloch sphere when using `matplotlib` 3.5 and above. (#1818 by Simon Cross)
- Fixed the displaying of `Lattice1d` instances and their unit cells. Previously calling them raised exceptions in simple cases. (#1819, #1697 and #1702 by Simon Cross and Saumya Biswas)
- Fixed the displaying of the title for `hinton` and `matrix_histogram` plots when a title is given. Previously the supplied title was not displayed. (#1707 by Vladimir Vargas-Calderón)
- Removed an incorrect check on the initial state dimensions in the `QubitCircuit` constructor. This allows, for example, the construction of `qutrit` circuits. (#1807 by Boxi Li)
- Fixed the checking of `method` and `offset` parameters in `coherent` and `coherent_dm`. (#1469 and #1741 by Joseph Fox-Rabinovitz and Simon Cross)
- Removed the Hamiltonian saved in the `sesolve` solver results. (#1689 by Eric Giguère)
- Fixed a bug in `rand_herm` with `pos_def=True` and `density>0.5` where the diagonal was incorrectly filled. (#1562 by Eric Giguère)

### 6.7.9 Documentation Improvements

- Added contributors image to the documentation. (#1828 by Leonard Assis)
- Fixed the Theory of Quantum Information bibliography link. (#1840 by Anto Luketina)
- Fixed minor grammar errors in the dynamics guide. (#1822 by Victor Omole)
- Fixed many small documentation typos. (#1569 by Ashish Panigrahi)
- Added `Pulser` to the list of libraries that use QuTiP. (#1570 by Ashish Panigrahi)
- Corrected typo in the states and operators guide. (#1567 by Laurent Ajdnik)

- Converted http links to https. (#1555 by Jake Lishamn)

### 6.7.10 Developer Changes

- Add GitHub actions test run on windows-latest. (#1853 and #1855 by Simon Cross)
- Bumped the version of pillow used to build documentation from 9.0.0 to 9.0.1. (#1835 by dependabot)
- Migrated the `qutip.superop_reps` tests to pytest. (#1825 by Felipe Bivort Haiek)
- Migrated the `qutip.steadystates` tests to pytest. (#1679 by Eric Giguère)
- Changed the README.md CI badge to the GitHub Actions badge. (#1581 by Jake Lishman)
- Updated CodeClimate configuration to treat our Python source files as Python 3. (#1577 by Jake Lishman)
- Reduced cyclomatic complexity in `qutip._mkl`. (#1576 by Jake Lishman)
- Fixed PEP8 warnings in `qutip.control`, `qutip.mcsolve`, `qutip.random_objects`, and `qutip.stochastic`. (#1575 by Jake Lishman)
- Bumped the version of urllib3 used to build documentation from 1.26.4 to 1.26.5. (#1563 by dependabot)
- Moved tests to GitHub Actions. (#1551 by Jake Lishman)
- The GitHub contributing guidelines were re-added and updated to point to the more complete guidelines in the documentation. (#1549 by Jake Lishman)
- The release documentation was reworked after the initial 4.6.1 to match the actual release process. (#1544 by Jake Lishman)

### Version 4.6.3 (February 9, 2022)

This minor release adds support for numpy 1.22 and Python 3.10 and removes some blockers for running QuTiP on the Apple M1.

The performance of the `enr_destroy`, `state_number_enumerate` and `hadamard_transform` functions was drastically improved (up to 70x or 200x faster in some common cases), and support for the drift Hamiltonian was added to the `qutip.qip.Processor`.

The `qutip.hardware_info` module was removed as part of adding support for the Apple M1. We hope the removal of this little-used module does not adversely affect many users – it was largely unrelated to QuTiP’s core functionality and its presence was a continual source of blockers to importing `qutip` on new or changed platforms.

A new check on the dimensions of `Qobj`’s were added to prevent segmentation faults when invalid shape and dimension combinations were passed to Cython code.

In addition, there were many small bugfixes, documentation improvements, and improvements to our building and testing processes.

### 6.7.11 Improvements

- The `enr_destroy` function was made ~200x faster in many simple cases. (#1593 by Johannes Feist)
- The `state_number_enumerate` function was made significantly faster. (#1594 by Johannes Feist)
- Added the missing drift Hamiltonian to the method `run_analytically` of `Processor`. (#1603 Boxi Li)
- The `hadamard_transform` was made much faster, e.g., ~70x faster for  $N=10$ . (#1688 by Asier Galicia)
- Added support for computing the power of a scalar-like `Qobj`. (#1692 by Asier Galicia)
- Removed the `hardware_info` module. This module wasn’t used inside QuTiP and regularly broke when new operating systems were released, and in particular prevented importing QuTiP on the Apple M1. (#1754, #1758 by Eric Giguère)

## 6.7.12 Bug Fixes

- Fixed support for calculating the propagator of a density matrix with collapse operators. QuTiP 4.6.2 introduced extra sanity checks on the dimensions of inputs to `mesolve` (Fix `mesolve` segfault with bad initial state [#1459](#)), but the propagator function's calls to `mesolve` violated these checks by supplying initial states with the dimensions incorrectly set. `propagator` now calls `mesolve` with the correct dimensions set on the initial state. ([#1588](#) by Simon Cross)
- Fixed support for calculating the propagator for a superoperator without collapse operators. This functionality was not tested by the test suite and appears to have broken sometime during 2019. Tests have now been added and the code breakages fixed. ([#1588](#) by Simon Cross)
- Fixed the ignoring of the random number seed passed to `rand_dm` in the case where `pure` was set to true. ([#1600](#) Pontus Wikstahl)
- Fixed `qutip.control.optimize_pulse` support for sparse eigenvector decomposition with the `Qobj` `oper_dtype` (the `Qobj` `oper_dtype` is the default for large systems). ([#1621](#) by Simon Cross)
- Removed `qutip.control.optimize_pulse` support for `scipy.sparse.csr_matrix` and generic ndarray-like matrices. Support for these was non-functional. ([#1621](#) by Simon Cross)
- Fixed errors in the calculation of the Husimi `spin_q_function` and `spin_wigner` functions and added tests for them. ([#1632](#) by Mark Johnson)
- Fixed setting of OpenMP compilation flag on Linux. Previously when compiling the OpenMP functions were compiled without parallelization. ([#1693](#) by Eric Giguère)
- Fixed tracking the state of the Bloch sphere figure and axes to prevent exceptions during rendering. ([#1619](#) by Simon Cross)
- Fixed compatibility with numpy configuration in numpy's 1.22.0 release. ([#1752](#) by Matthew Treinish)
- Added `dims` checks for `e_ops` passed to solvers to prevent hanging the calling process when `e_ops` of the wrong dimensions were passed. ([#1778](#) by Eric Giguère)
- Added a check in `Qobj` constructor that the respective members of `data.shape` cannot be larger than what the corresponding `dims` could contain to prevent a segmentation fault caused by inconsistencies between `dims` and `shapes`. ([#1783](#), [#1785](#), [#1784](#) by Lajos Palanki & Eric Giguère)

## 6.7.13 Documentation Improvements

- Added docs for the `num_cbits` parameter of the `QubitCircuit` class. ([#1652](#) by Jon Crall)
- Fixed the parameters in the call to `fsesolve` in the Floquet guide. ([#1675](#) by Simon Cross)
- Fixed the description of random number usage in the Monte Carlo solver guide. ([#1677](#) by Ian Thorvaldson)
- Fixed the rendering of equation numbers in the documentation (they now appear on the right as expected, not above the equation). ([#1678](#) by Simon Cross)
- Updated the installation requirements in the documentation to match what is specified in `setup.py`. ([#1715](#) by Asier Galicia)
- Fixed a typo in the `chi_to_choi` documentation. Previously the documentation mixed up `chi` and `choi`. ([#1731](#) by Pontus Wikstahl)
- Improved the documentation for the stochastic equation solvers. Added links to notebooks with examples, API documentation and external references. ([#1743](#) by Leonardo Assis)
- Fixed a typo in `qutip.settings` in the settings guide. ([#1786](#) by Mahdi Aslani)
- Made numerous small improvements to the text of the QuTiP basics guide. ([#1768](#) by Anna Naden)
- Made a small phrasing improvement to the README. ([#1790](#) by Rita Abani)

## 6.7.14 Developer Changes

- Improved test coverage of states and operators functions. ([#1578](#) by Eric Giguère)
- Fixed test\_interpolate mcsolve use ([#1645](#) by Eric Giguère)
- Ensured figure plots are explicitly closed during tests so that the test suite passes when run headless under Xvfb. ([#1648](#) by Simon Cross)
- Bumped the version of pillow used to build documentation from 8.2.0 to 9.0.0. ([#1654](#), [#1760](#) by dependabot)
- Bumped the version of babel used to build documentation from 2.9.0 to 2.9.1. ([#1695](#) by dependabot)
- Bumped the version of numpy used to build documentation from 1.19.5 to 1.21.0. ([#1767](#) by dependabot)
- Bumped the version of ipython used to build documentation from 7.22.0 to 7.31.1. ([#1780](#) by dependabot)
- Rename qutip.bib to CITATION.bib to enable GitHub’s citation support. ([#1662](#) by Ashish Panigrahi)
- Added tests for simdiags. ([#1681](#) by Eric Giguère)
- Added support for specifying the numpy version in the CI test matrix. ([#1696](#) by Simon Cross)
- Fixed the skipping of the dnorm metric tests if cvxpy is not installed. Previously all metrics tests were skipped by accident. ([#1704](#) by Florian Hopfmueller)
- Added bug report, feature request and other options to the GitHub issue reporting template. ([#1728](#) by Aryaman Kolhe)
- Updated the build process to support building on Python 3.10 by removing the build requirement for numpy < 1.20 and replacing it with a requirement on oldest-supported-numpy. ([#1747](#) by Simon Cross)
- Updated the version of cibuildwheel used to build wheels to 2.3.0. ([#1747](#), [#1751](#) by Simon Cross)
- Added project urls to linking to the source repository, issue tracker and documentation to setup.cfg. ([#1779](#) by Simon Cross)
- Added a numpy 1.22 and Python 3.10 build to the CI test matrix. ([#1777](#) by Simon Cross)
- Ignore deprecation warnings from SciPy 1.8.0 scipy.sparse.X imports in CI tests. ([#1797](#) by Simon Cross)
- Add building of wheels for Python 3.10 to the cibuildwheel job. ([#1796](#) by Simon Cross)

### Version 4.6.2 (June 2, 2021)

This minor release adds a function to calculate the quantum relative entropy, fixes a corner case in handling time-dependent Hamiltonians in `mesolve` and adds back support for a wider range of matplotlib versions when plotting or animating Bloch spheres.

It also adds a section in the README listing the papers which should be referenced while citing QuTiP.

## 6.7.15 Improvements

- Added a “Citing QuTiP” section to the README, containing a link to the QuTiP papers. ([#1554](#))
- Added `entropy_relative` which returns the quantum relative entropy between two density matrices. ([#1553](#))

### 6.7.16 Bug Fixes

- Fixed Bloch sphere distortion when using Matplotlib  $\geq 3.3.0$ . (#1496)
- Removed use of integer-like floats in `math.factorial` since it is deprecated as of Python 3.9. (#1550)
- Simplified call to `ffmpeg` used in the the Bloch sphere animation tutorial to work with recent versions of `ffmpeg`. (#1557)
- Removed blitting in Bloch sphere `FuncAnimation` example. (#1558)
- Added a version checking condition to handle specific functionalities depending on the matplotlib version. (#1556)
- Fixed `mesolve` handling of time-dependent Hamiltonian with a custom `tlist` and `c_ops`. (#1561)

### 6.7.17 Developer Changes

- Read documentation version and release from the `VERSION` file.

#### Version 4.6.1 (May 4, 2021)

This minor release fixes bugs in QIP gate definitions, fixes building from the source tarball when `git` is not installed and works around an MKL bug in versions of SciPy  $\leq 1.4$ .

It also adds the `[full]` pip install target so that `pip install qutip[full]` installs qutip and all of its optional and developer dependencies.

### 6.7.18 Improvements

- Add the `[full]` pip install target (by **Jake Lishman**)

### 6.7.19 Bug Fixes

- Work around pointer MKL eigh bug in SciPy  $\leq 1.4$  (by **Felipe Bivort Haiek**)
- Fix `berkeley`, `swapalpha` and `cz` gate operations (by **Boxi Li**)
- Expose the CPHASE control gate (by **Boxi Li**)
- Fix building from the `sdist` when `git` is not installed (by **Jake Lishman**)

### 6.7.20 Developer Changes

- Move the `qutip-doc` documentation into the qutip repository (by **Jake Lishman**)
- Fix warnings in documentation build (by **Jake Lishman**)
- Fix warnings in pytest runs and make pytest treat warnings as errors (by **Jake Lishman**)
- Add Simon Cross as author (by **Simon Cross**)

## Version 4.6.0 (April 11, 2021)

This release brings improvements for qubit circuits, including a pulse scheduler, measurement statistics, reading/writing OpenQASM and optimisations in the circuit simulations.

This is the first release to have full binary wheel releases on pip; you can now do `pip install qutip` on almost any machine to get a correct version of the package without needing any compilers set up. The support for Numpy 1.20 that was first added in QuTiP 4.5.3 is present in this version as well, and the same build considerations mentioned there apply here too. If building using the now-supported PEP 517 mechanisms (e.g. `python -mbuild /path/to/qutip`), all build dependencies will be correctly satisfied.

### 6.7.21 Improvements

- **MAJOR** Add saving, loading and resetting functionality to `qutip.settings` for easy re-configuration. (by **Eric Giguère**)
- **MAJOR** Add a quantum gate scheduler in `qutip.qip.scheduler`, to help parallelise the operations of quantum gates. This supports two scheduling modes: as late as possible, and as soon as possible. (by **Boxi Li**)
- **MAJOR** Improved qubit circuit simulators, including OpenQASM support and performance optimisations. (by **Sidhant Saraogi**)
- **MAJOR** Add tools for quantum measurements and their statistics. (by **Simon Cross** and **Sidhant Saraogi**)
- Add support for Numpy 1.20. QuTiP should be compiled against a version of Numpy  $\geq 1.16.6$  and  $< 1.20$  (note: does `_not_` include 1.20 itself), but such an installation is compatible with any modern version of Numpy. Source installations from pip understand this constraint.
- Improve the error message when circuit plotting fails. (by **Boxi Li**)
- Add support for parsing M1 Mac hardware information. (by **Xiaoliang Wu**)
- Add more single-qubit gates and controlled gates. (by **Mateo Laguna** and **Martín Sande Costa**)
- Support decomposition of X, Y and Z gates in circuits. (by **Boxi Li**)
- Refactor `QubitCircuit.resolve_gate()` (by **Martín Sande Costa**)

### 6.7.22 Bug Fixes

- Fix dims in the returns from `Qobj.eigenstates` on superoperators. (by **Jake Lishman**)
- Calling Numpy ufuncs on `Qobj` will now correctly raise a `TypeError` rather than returning a nonsense ndarray. (by **Jake Lishman**)
- Convert segfault into Python exception when creating too-large tensor products. (by **Jake Lishman**)
- Correctly set `num_collapse` in the output of `mesolve`. (by **Jake Lishman**)
- Fix `ptrace` when all subspaces are being kept, or the subspaces are passed in order. (by **Jake Lishman**)
- Fix sorting bug in `Bloch3d.add_points()`. (by **pschindler**)
- Fix invalid string literals in docstrings and some unclosed files. (by **Élie Gouzien**)
- Fix Hermiticity tests for matrices with values that are within the tolerance of 0. (by **Jake Lishman**)
- Fix the trace norm being incorrectly reported as 0 for small matrices. (by **Jake Lishman**)
- Fix issues with `dnorm` when using CVXPY 1.1 with sparse matrices. (by **Felipe Bivort Haiek**)
- Fix segfaults in `mesolve` when passed a bad initial `Qobj` as the state. (by **Jake Lishman**)
- Fix sparse matrix construction in PIQS when using Scipy 1.6.1. (by **Drew Parsons**)
- Fix `zspmv_openmp.cpp` missing from the pip sdist. (by **Christoph Gohlke**)



- Fix correlation functions throwing away imaginary components. (by **Asier Galicia Martinez**)
- Fix `QubitCircuit.add_circuit()` for SWAP gate. (by **Canoming**)
- Fix the broken LaTeX image conversion. (by **Jake Lishman**)
- Fix gate resolution of the FREDKIN gate. (by **Bo Yang**)
- Fix broken formatting in docstrings. (by **Jake Lishman**)

### 6.7.23 Deprecations

- `eseries`, `essolve` and `ode2es` are all deprecated, pending removal in QuTiP 5.0. These are legacy functions and classes that have been left unmaintained for a long time, and their functionality is now better achieved with `QobjEvo` or `mesolve`.

### 6.7.24 Developer Changes

- **MAJOR** Overhaul of setup and packaging code to make it satisfy PEP 517, and move the build to a matrix on GitHub Actions in order to release binary wheels on pip for all major platforms and supported Python versions. (by **Jake Lishman**)
- Default arguments in `Qobj` are now `None` rather than mutable types. (by **Jake Lishman**)
- Fixed consumable iterators being used to parametrise some tests, preventing the testing suite from being re-run within the same session. (by **Jake Lishman**)
- Remove unused imports, simplify some floats and remove unnecessary list conversions. (by **jakobjakobson13**)
- Improve Travis jobs matrix for specifying the testing containers. (by **Jake Lishman**)
- Fix coverage reporting on Travis. (by **Jake Lishman**)
- Added a `pyproject.toml` file. (by **Simon Humpohl** and **Eric Giguère**)
- Add doctests to documentation. (by **Sidhant Saraogi**)
- Fix all warnings in the documentation build. (by **Jake Lishman**)

### Version 4.5.3 (February 19, 2021)

This patch release adds support for Numpy 1.20, made necessary by changes to how array-like objects are handled. There are no other changes relative to version 4.5.2.

Users building from source should ensure that they build against Numpy versions  $\geq 1.16.6$  and  $< 1.20$  (not including 1.20 itself), but after that or for those installing from conda, an installation will support any current Numpy version  $\geq 1.16.6$ .

### 6.7.25 Improvements

- Add support for Numpy 1.20. QuTiP should be compiled against a version of Numpy  $\geq 1.16.6$  and  $< 1.20$  (note: does `_not_` include 1.20 itself), but such an installation is compatible with any modern version of Numpy. Source installations from pip understand this constraint.



### Version 4.5.2 (July 14, 2020)

This is predominantly a hot-fix release to add support for Scipy 1.5, due to changes in private sparse matrix functions that QuTiP also used.

#### 6.7.26 Improvements

- Add support for Scipy 1.5. (by **Jake Lishman**)
- Improved speed of `zcsr_inner`, which affects `Qobj.overlap`. (by **Jake Lishman**)
- Better error messages when installation requirements are not satisfied. (by **Eric Giguère**)

#### 6.7.27 Bug Fixes

- Fix `zcsr_proj` acting on matrices with unsorted indices. (by **Jake Lishman**)
- Fix errors in Milstein's heterodyne. (by **Eric Giguère**)
- Fix datatype bug in `qutip.lattice` module. (by **Boxi Li**)
- Fix issues with `eigh` on Mac when using OpenBLAS. (by **Eric Giguère**)

#### 6.7.28 Developer Changes

- Converted more of the codebase to PEP 8.
- Fix several instances of unsafe mutable default values and unsafe `is` comparisons.

### Version 4.5.1 (May 15, 2020)

#### 6.7.29 Improvements

- `husimi` and `wigner` now accept half-integer spin (by **maij**)
- Better error messages for failed string coefficient compilation. (issue raised by **nohchangsubk**)

#### 6.7.30 Bug Fixes

- Safer naming for temporary files. (by **Eric Giguère**)
- Fix `clebsch` function for half-integer (by **Thomas Walker**)
- Fix `randint`'s dtype to `uint32` for compatibility with Windows. (issue raised by **Boxi Li**)
- Corrected stochastic's heterodyne's `m_ops` (by **eliegeois**)
- Mac pool use spawn. (issue raised by **goerz**)
- Fix typos in `QobjEvo._shift`. (by **Eric Giguère**)
- Fix warning on Travis CI. (by **Ivan Carvalho**)

### 6.7.31 Deprecations

- `qutip.graph` functions will be deprecated in QuTiP 5.0 in favour of `scipy.sparse.csgraph`.

### 6.7.32 Developer Changes

- Add Boxi Li to authors. (by **Alex Pitchford**)
- Skip some tests that cause segfaults on Mac. (by **Nathan Shammah** and **Eric Giguère**)
- Use Python 3.8 for testing on Mac and Linux. (by **Simon Cross** and **Eric Giguère**)

### Version 4.5.0 (January 31, 2020)

### 6.7.33 Improvements

- **MAJOR FEATURE:** Added *qip.noise*, a module with pulse level description of quantum circuits allowing to model various types of noise and devices (by **Boxi Li**).
- **MAJOR FEATURE:** Added *qip.lattice*, a module for the study of lattice dynamics in 1D (by **Saumya Biswas**).
- Migrated testing from Nose to PyTest (by **Tarun Raheja**).
- Optimized testing for PyTest and removed duplicated test runners (by **Jake Lishman**).
- Deprecated importing *qip* functions to the `qutip` namespace (by **Boxi Li**).
- Added the possibility to define non-square superoperators relevant for quantum circuits (by **Arne Grimsmo** and **Josh Combes**).
- Implicit tensor product for *qeye*, *qzero* and *basis* (by **Jake Lishman**).
- *QObjEvo* no longer requires Cython for string coefficient (by **Eric Giguère**).
- Added marked tests for faster tests in *testing.run()* and made faster OpenMP benchmarking in CI (by **Eric Giguère**).
- Added entropy and purity for Dicke density matrices, refactored into more general *dicke\_trace* (by **Nathan Shammah**).
- Added option for specifying resolution in *Bloch.save* function (by **Tarun Raheja**).
- Added information related to the value of  $\hbar$  in *wigner* and *continuous\_variables* (by **Nicolas Quesada**).
- Updated requirements for *scipy 1.4* (by **Eric Giguère**).
- Added previous lead developers to the `qutip.about()` message (by **Nathan Shammah**).
- Added improvements to *Qobj* introducing the *inv* method and making the partial trace, *ptrace*, faster, keeping both sparse and dense methods (by **Eric Giguère**).
- Allowed general callable objects to define a time-dependent Hamiltonian (by **Eric Giguère**).
- Added feature so that *QobjEvo* no longer requires Cython for string coefficients (by **Eric Giguère**).
- Updated authors list on Github and added *my binder* link (by **Nathan Shammah**).

### 6.7.34 Bug Fixes

- Fixed *PolyDataMapper* construction for *Bloch3d* (by **Sam Griffiths**).
- Fixed error checking for null matrix in *essolve* (by **Nathan Shammah**).
- Fixed name collision for parallel propagator (by **Nathan Shammah**).
- Fixed dimensional incongruence in *propagator* (by **Nathan Shammah**).
- Fixed bug by rewriting *clebsch* function based on long integer fraction (by **Eric Giguère**).
- Fixed bugs in *QobjEvo*'s args depending on state and added solver tests using them (by **Eric Giguère**).
- Fixed bug in *sesolve* calculation of average states when summing the timeslot states (by **Alex Pitchford**).
- Fixed bug in *steadystate* solver by removing separate arguments for MKL and Scipy (by **Tarun Raheja**).
- Fixed *Bloch.add\_ponts* by setting *edgecolor* = *None* in *plot\_points* (by **Nathan Shammah**).
- Fixed error checking for null matrix in *essolve* solver affecting also *ode2es* (by **Peter Kirton**).
- Removed unnecessary shebangs in .pyx and .pxd files (by **Samesh Lakhotia**).
- Fixed *sesolve* and import of *os* in *codegen* (by **Alex Pitchford**).
- Updated *plot\_fock\_distribution* by removing the offset value 0.4 in the plot (by **Rajiv-B**).

#### Version 4.4.1 (August 29, 2019)

### 6.7.35 Improvements

- *QobjEvo* do not need to start from 0 anymore (by **Eric Giguère**).
- Add a quantum object purity function (by **Nathan Shammah** and **Shahnawaz Ahmed**).
- Add step function interpolation for array time-coefficient (by **Boxi Li**).
- Generalize *expand\_oper* for arbitrary dimensions, and new method for cyclic permutations of given target cubits (by **Boxi Li**).

### 6.7.36 Bug Fixes

- Fixed the pickling but that made solver unable to run in parallel on Windows (Thank **lrunze** for reporting).
- Removed warning when *mesolve* fall back on *sesolve* (by **Michael Goerz**).
- Fixed dimension check and confusing documentation in *random ket* (by **Yariv Yanay**).
- Fixed *Qobj* *isherm* not working after using *Qobj.permute* (Thank **llorz1207** for reporting).
- Correlation functions call now properly handle multiple time dependant functions (Thank **taw181** for reporting).
- Removed mutable default values in *mesolve*/*sesolve* (by **Michael Goerz**).
- Fixed *simdiag* bug (Thank **Croydon-Brixton** for reporting).
- Better support of constant *QobjEvo* (by **Boxi Li**).
- Fixed potential cyclic import in the control module (by **Alexander Pitchford**).

## Version 4.4.0 (July 03, 2019)

### 6.7.37 Improvements

- **MAJOR FEATURE:** Added methods and techniques to the stochastic solvers (by **Eric Giguère**) which allows to use a much broader set of solvers and much more efficiently.
- **MAJOR FEATURE:** Optimization of the montecarlo solver (by **Eric Giguère**). Computation are faster in many cases. Collapse information available to time dependant information.
- Added the QObjEvo class and methods (by **Eric Giguère**), which is used behind the scenes by the dynamical solvers, making the code more efficient and tidier. More built-in function available to string coefficients.
- The coefficients can be made from interpolated array with variable timesteps and can obtain state information more easily. Time-dependant collapse operator can have multiple terms.
- New wigner\_transform and plot\_wigner\_sphere function. (by **Nithin Ramu**).
- ptrace is faster and work on bigger systems, from 15 Qbits to 30 Qbits.
- QIP module: added the possibility for user-defined gates, added the possibility to remove or add gates in any point of an already built circuit, added the molmer\_sorensen gate, and fixed some bugs (by **Boxi Li**).
- Added the quantum Hellinger distance to qutip.metrics (by **Wojciech Rzadkowski**).
- Implemented possibility of choosing a random seed (by **Marek Marekyygdrasil**).
- Added a code of conduct to Github.

### 6.7.38 Bug Fixes

- Fixed bug that made QuTiP incompatible with SciPy 1.3.

## Version 4.3.0 (July 14, 2018)

### 6.7.39 Improvements

- **MAJOR FEATURE:** Added the Permutational Invariant Quantum Solver (PIQS) module (by **Nathan Shammah** and **Shahnawaz Ahmed**) which allows the simulation of large TLSs ensembles including collective and local Lindblad dissipation. Applications range from superradiance to spin squeezing.
- **MAJOR FEATURE:** Added a photon scattering module (by **Ben Bartlett**) which can be used to study scattering in arbitrary driven systems coupled to some configuration of output waveguides.
- Cubic\_Spline functions as time-dependent arguments for the collapse operators in mesolve are now allowed.
- Added a faster version of bloch\_redfield\_tensor, using components from the time-dependent version. About 3x+ faster for secular tensors, and 10x+ faster for non-secular tensors.
- Computing Q.overlap() [inner product] is now ~30x faster.
- Added projector method to Qobj class.
- Added fast projector method, Q.proj().
- Computing matrix elements, Q.matrix\_element is now ~10x faster.
- Computing expectation values for ket vectors using expect is now ~10x faster.
- Q.tr() is now faster for small Hilbert space dimensions.
- Unitary operator evolution added to sesolve
- Use OPENMP for tidyup if installed.

### 6.7.40 Bug Fixes

- Fixed bug that stopped simdiag working for python 3.
- Fixed semidefinite cvxpy Variable and Parameter.
- Fixed iterative lu solve atol keyword issue.
- Fixed unitary op evolution rhs matrix in ssesolve.
- Fixed interpolating function to return zero outside range.
- Fixed dnorm complex casting bug.
- Fixed control.io path checking issue.
- Fixed ENR fock dimension.
- Fixed hard coded options in propagator 'batch' mode
- Fixed bug in trace-norm for non-Hermitian operators.
- Fixed bug related to args not being passed to coherence\_function\_g2
- Fixed MKL error checking dict key error

### Version 4.2.0 (July 28, 2017)

### 6.7.41 Improvements

- **MAJOR FEATURE:** Initial implementation of time-dependent Bloch-Redfield Solver.
- Qobj tidyup is now an order of magnitude faster.
- Time-dependent codegen now generates output NumPy arrays faster.
- Improved calculation for analytic coefficients in coherent states (Sebastian Kramer).
- Input array to correlation FFT method now checked for validity.
- Function-based time-dependent mesolve and sesolve routines now faster.
- Codegen now makes sure that division is done in C, as opposed to Python.
- Can now set different controls for a each timeslot in quantum optimization. This allows time-varying controls to be used in pulse optimisation.

### 6.7.42 Bug Fixes

- rcsolve importing old Odeoptions Class rather than Options.
- Non-int issue in spin Q and Wigner functions.
- Qobj's should tidyup before determining isherm.
- Fixed time-dependent RHS function loading on Win.
- Fixed several issues with compiling with Cython 0.26.
- Liouvillian superoperators were hard setting isherm=True by default.
- Fixed an issue with the solver safety checks when inputting a list with Python functions as time-dependence.
- Fixed non-int issue in Wigner\_cmap.
- MKL solver error handling not working properly.

#### Version 4.1.0 (March 10, 2017)

### 6.7.43 Improvements

#### *Core libraries*

- **MAJOR FEATURE:** QuTiP now works for Python 3.5+ on Windows using Visual Studio 2015.
- **MAJOR FEATURE:** Cython and other low level code switched to C++ for MS Windows compatibility.
- **MAJOR FEATURE:** Can now use interpolating cubic splines as time-dependent coefficients.
- **MAJOR FEATURE:** Sparse matrix - vector multiplication now parallel using OPENMP.
- Automatic tuning of OPENMP threading threshold.
- Partial trace function is now up to 100x+ faster.
- Hermitian verification now up to 100x+ faster.
- Internal Qobj objects now created up to 60x faster.
- Inplace conversion from COO -> CSR sparse formats (e.g. Memory efficiency improvement.)
- Faster reverse Cuthill-Mckee and sparse one and inf norms.

### 6.7.44 Bug Fixes

- Cleanup of temp. Cython files now more robust and working under Windows.

#### Version 4.0.2 (January 5, 2017)

### 6.7.45 Bug Fixes

- td files no longer left behind by correlation tests
- Various fast sparse fixes

#### Version 4.0.0 (December 22, 2016)

### 6.7.46 Improvements

#### *Core libraries*

- **MAJOR FEATURE:** Fast sparse: New subclass of `csr_matrix` added that overrides commonly used methods to avoid certain checks that incur execution cost. All `Qobj.data` now `fast_csr_matrix`
- HEOM performance enhancements
- `spmv` now faster
- `mcsolve` codegen further optimised

#### *Control modules*

- Time dependent drift (through list of pwc dynamics generators)
- memory optimisation options provided for `control.dynamics`

### 6.7.47 Bug Fixes

- recompilation of pyx files on first import removed
- tau array in control.pulseoptim funcs now works

### Version 3.2.0 (Never officially released)

### 6.7.48 New Features

#### Core libraries

- **MAJOR FEATURE:** Non-Markovian solvers: Hierarchy (**Added by Neill Lambert**), Memory-Cascade, and Transfer-Tensor methods.
- **MAJOR FEATURE:** Default steady state solver now up to 100x faster using the Intel Pardiso library under the Anaconda and Intel Python distributions.
- The default Wigner function now uses a Clenshaw summation algorithm to evaluate a polynomial series that is applicable for any number of excitations (previous limitation was ~50 quanta), and is ~3x faster than before. (**Added by Denis Vasilyev**)
- Can now define a given eigen spectrum for random Hermitian and density operators.
- The Qobj `expm` method now uses the equivalent SciPy routine, and performs a much faster `exp` operation if the matrix is diagonal.
- One can now build zero operators using the `qzero` function.

#### Control modules

- **MAJOR FEATURE:** CRAB algorithm added This is an alternative to the GRAPE algorithm, which allows for analytical control functions, which means that experimental constraints can more easily be added into optimisation. See tutorial notebook for full information.

### 6.7.49 Improvements

#### Core libraries

- Two-time correlation functions can now be calculated for fully time-dependent Hamiltonians and collapse operators. (**Added by Kevin Fischer**)
- The code for the inverse-power method for the steady state solver has been simplified.
- Bloch-Redfield tensor creation is now up to an order of magnitude faster. (**Added by Johannes Feist**)
- Q.transform now works properly for arrays directly from `sp_eigs` (or `eig`).
- Q.groundstate now checks for degeneracy.
- Added `sinm` and `cosm` methods to the Qobj class.
- Added `charge` and `tunneling` operators.
- Time-dependent Cython code is now easier to read and debug.

#### Control modules

- The internal state / quantum operator data type can now be either Qobj or ndarray Previous only ndarray was possible. This now opens up possibility of using Qobj methods in fidelity calculations The attributes and functions that return these operators are now preceded by an underscore, to indicate that the data type could change depending on the configuration options. In most cases these functions were for internal processing only anyway, and should have been 'private'. Accessors to the properties that could be useful outside of the library have been added. These always return Qobj. If the internal operator data type is not Qobj, then there could be significant overhead in the conversion, and so this should be avoided during pulse optimisation. If custom sub-classes are developed that use Qobj properties and methods (e.g. partial trace), then it is very likely

that it will be more efficient to set the internal data type to Qobj. The internal operator data will be chosen automatically based on the size and sparsity of the dynamics generator. It can be forced by setting `dynamics.oper_dtype = <type>` Note this can be done by passing `dyn_params={'oper_dtype':<type>}` in any of the pulseoptim functions.

Some other properties and methods were renamed at the same time. A full list is given here.

- All modules - function: `set_log_level` -> property: `log_level`
- dynamics functions
  - \* `_init_lists` now `_init_evo`
  - \* `get_num_ctrls` now property: `num_ctrls`
  - \* `get_owd_evo_target` now property: `onto_evo_target`
  - \* `combine_dyn_gen` now `_combine_dyn_gen` (no longer returns a value)
  - \* `get_dyn_gen` now `_get_phased_dyn_gen`
  - \* `get_ctrl_den_gen` now `_get_phased_ctrl_dyn_gen`
  - \* `ensure_decomp_curr` now `_ensure_decomp_curr`
  - \* `spectral_decomp` now `_spectral_decomp`
- dynamics properties
  - \* `evo_init2t` now `_fwd_evo` (`fwd_evo` as Qobj)
  - \* `evo_t2end` now `_onwd_evo` (`onwd_evo` as Qobj)
  - \* `evo_t2targ` now `_onto_evo` (`onto_evo` as Qobj)
- fidcomp properties
  - \* `uses_evo_t2end` now `uses_onwd_evo`
  - \* `uses_evo_t2targ` now `uses_onto_evo`
  - \* `set_phase_option` function now property `phase_option`
- propcomp properties
  - \* `grad_exact` (now read only)
- propcomp functions
  - \* `compute_propagator` now `_compute_propagator`
  - \* `compute_diff_prop` now `_compute_diff_prop`
  - \* `compute_prop_grad` now `_compute_prop_grad`
- tslocomp functions
  - \* `get_timeslot_for_fidelity_calc` now `_get_timeslot_for_fidelity_calc`

#### *Miscellaneous*

- QuTiP Travis CI tests now use the Anaconda distribution.
- The about box and `ipynb_version_table` now display additional system information.
- Updated Cython cleanup to remove deprecation warning in `sysconfig`.
- Updated `ipynb_parallel` to look for `ipyparallel` module in V4 of the notebooks.



### 6.7.50 Bug Fixes

- Fixes for countstat and psuedo-inverse functions
- Fixed Qobj division tests on 32-bit systems.
- Removed extra call to Python in time-dependent Cython code.
- Fixed issue with repeated Bloch sphere saving.
- Fixed T\_0 triplet state not normalized properly. **(Fixed by Eric Hontz)**
- Simplified compiler flags (support for ARM systems).
- Fixed a decoding error in qload.
- Fixed issue using complex.h math and np.kind\_t variables.
- Corrected output states mismatch for ntraj=1 in the mcf90 solver.
- Qobj data is now copied by default to avoid a bug in multiplication. **(Fixed by Richard Brierley)**
- Fixed bug overwriting hardware\_info in \_\_init\_\_. **(Fixed by Johannes Feist)**
- Restored ability to explicitly set Q.isherm, Q.type, and Q.superrep.
- Fixed integer depreciation warnings from NumPy.
- Qobj \* (dense vec) would result in a recursive loop.
- Fixed args=None -> args={} in correlation functions to be compatible with mesolve.
- Fixed depreciation warnings in mcsolve.
- Fixed neagative only real parts in rand\_ket.
- Fixed a complicated list-cast-map-list antipattern in super operator reps. **(Fixed by Stefan Krastanov)**
- Fixed incorrect isherm for sigmam spin operator.
- Fixed the dims when using final\_state\_output in mesolve and sesolve.

### Version 3.1.0 (January 1, 2015)

#### 6.7.51 New Features

- **MAJOR FEATURE:** New module for quantum control (qutip.control).
- **NAMESPACE CHANGE:** QuTiP no longer exports symbols from NumPy and matplotlib, so those modules must now be explicitly imported when required.
- New module for counting statistics.
- Stochastic solvers now run trajectories in parallel.
- New superoperator and tensor manipulation functions (super\_tensor, composite, tensor\_contract).
- New logging module for debugging (qutip.logging).
- New user-available API for parallelization (parallel\_map).
- New enhanced (optional) text-based progressbar (qutip.ui.EnhancedTextProgressBar)
- Faster Python based monte carlo solver (mcsolve).
- Support for progress bars in propagator function.
- Time-dependent Cython code now calls complex cmath functions.
- Random numbers seeds can now be reused for successive calls to mcsolve.
- The Bloch-Redfield master equation solver now supports optional Lindblad type collapse operators.

- Improved handling of ODE integration errors in `mesolve`.
- Improved correlation function module (for example, improved support for time-dependent problems).
- Improved parallelization of `mc_solve` (can now be interrupted easily, support for `IPython.parallel`, etc.)
- Many performance improvements, and much internal code restructuring.

### 6.7.52 Bug Fixes

- Cython build files for time-dependent string format now removed automatically.
- Fixed incorrect solution time from inverse-power method steady state solver.
- `mc_solve` now supports `Options(store_states=True)`
- Fixed bug in `hadamard` gate function.
- Fixed compatibility issues with NumPy 1.9.0.
- Progressbar in `mc_solve` can now be suppressed.
- Fixed bug in `gate_expand_3toN`.
- Fixed bug for time-dependent problem (list string format) with multiple terms in coefficient to an operator.

### Version 3.0.1 (Aug 5, 2014)

### 6.7.53 Bug Fixes

- Fix bug in `create()`, which returned a `Qobj` with CSC data instead of CSR.
- Fix several bugs in `mc_solve`: Incorrect storing of collapse times and collapse operator records. Incorrect averaging of expectation values for different trajectories when using only 1 CPU.
- Fix bug in parsing of time-dependent Hamiltonian/collapse operator arguments that occurred when the `args` argument is not a dictionary.
- Fix bug in internal `_version2int` function that cause a failure when parsing the version number of the Cython package.
- 

### Version 3.0.0 (July 17, 2014)

### 6.7.54 New Features

- New module `qutip.stochastic` with stochastic master equation and stochastic Schrödinger equation solvers.
- Expanded steady state solvers. The function `steady` has been deprecated in favor of `steadystate`. The `steadystate` solver no longer use `umfpack` by default. New pre-processing methods for reordering and balancing the linear equation system used in direct solution of the steady state.
- New module `qutip.qip` with utilities for quantum information processing, including pre-defined quantum gates along with functions for expanding arbitrary 1, 2, and 3 qubit gates to N qubit registers, circuit representations, library of quantum algorithms, and basic physical models for some common QIP architectures.
- New module `qutip.distributions` with unified API for working with distribution functions.
- New format for defining time-dependent Hamiltonians and collapse operators, using a pre-calculated numpy array that specifies the values of the `Qobj`-coefficients for each time step.
- New functions for working with different superoperator representations, including Kraus and Chi representation.

- New functions for visualizing quantum states using Qubism and Schimdt plots: `plot_qubism` and `plot_schmidt`.
- Dynamics solver now support taking argument `e_ops` (expectation value operators) in dictionary form.
- Public plotting functions from the `qutip.visualization` module are now prefixed with `plot_` (e.g., `plot_fock_distribution`). The `plot_wigner` and `plot_wigner_fock_distribution` now supports 3D views in addition to contour views.
- New API and new functions for working with spin operators and states, including for example `spin_Jx`, `spin_Jy`, `spin_Jz` and `spin_state`, `spin_coherent`.
- The `expect` function now supports a list of operators, in addition to the previously supported list of states.
- Simplified creation of qubit states using `ket` function.
- The module `qutip.cyQ` has been renamed to `qutip.cy` and the sparse matrix-vector functions `spmv` and `spmv1d` has been combined into one function `spmv`. New functions for operating directly on the underlying sparse CSR data have been added (e.g., `spmv_csr`). Performance improvements. New and improved Cython functions for calculating expectation values for state vectors, density matrices in matrix and vector form.
- The `concurrence` function now supports both pure and mixed states. Added function for calculating the entangling power of a two-qubit gate.
- Added function for generating (generalized) Lindblad dissipator superoperators.
- New functions for generating Bell states, and singlet and triplet states.
- QuTiP no longer contains the demos GUI. The examples are now available on the QuTiP web site. The `qutip.gui` module has been renamed to `qutip.ui` and does no longer contain graphical UI elements. New text-based and HTML-based progressbar classes.
- Support for harmonic oscillator operators/states in a Fock state basis that does not start from zero (e.g., in the range  $[M, N+1]$ ). Support for eliminating and extracting states from `Qobj` instances (e.g., removing one state from a two-qubit system to obtain a three-level system).
- Support for time-dependent Hamiltonian and Liouvillian callback functions that depend on the instantaneous state, which for example can be used for solving master equations with mean field terms.

### 6.7.55 Improvements

- Restructured and optimized implementation of `Qobj`, which now has significantly lower memory footprint due to avoiding excessive copying of internal matrix data.
- The classes `OdeData`, `Odeoptions`, `Odeconfig` are now called `Result`, `Options`, and `Config`, respectively, and are available in the module `qutip.solver`.
- The `squeez` function has been renamed to `squeeze`.
- Better support for sparse matrices when calculating propagators using the `propagator` function.
- Improved Bloch sphere.
- Restructured and improved the module `qutip.sparse`, which now only operates directly on sparse matrices (not on `Qobj` instances).
- Improved and simplified implement of the `tensor` function.
- Improved performance, major code cleanup (including namespace changes), and numerous bug fixes.
- Benchmark scripts improved and restructured.
- QuTiP is now using continuous integration tests (TravisCI).

## Version 2.2.0 (March 01, 2013)

### 6.7.56 New Features

- **Added Support for Windows**
- New Bloch3d class for plotting 3D Bloch spheres using Mayavi.
- Bloch sphere vectors now look like arrows.
- Partial transpose function.
- Continuous variable functions for calculating correlation and covariance matrices, the Wigner covariance matrix and the logarithmic negativity for multimode fields in Fock basis.
- The master-equation solver (mesolve) now accepts pre-constructed Liouvillian terms, which makes it possible to solve master equations that are not on the standard Lindblad form.
- Optional Fortran Monte Carlo solver (mcsolve\_f90) by Arne Grimsmo.
- A module of tools for using QuTiP in IPython notebooks.
- Increased performance of the steady state solver.
- New Wigner colormap for highlighting negative values.
- More graph styles to the visualization module.

### 6.7.57 Bug Fixes

- Function based time-dependent Hamiltonians now keep the correct phase.
- mcsolve no longer prints to the command line if ntraj=1.

## Version 2.1.0 (October 05, 2012)

### 6.7.58 New Features

- New method for generating Wigner functions based on Laguerre polynomials.
- coherent(), coherent\_dm(), and thermal\_dm() can now be expressed using analytic values.
- Unittests now use nose and can be run after installation.
- Added iswap and sqrt-iswap gates.
- Functions for quantum process tomography.
- Window icons are now set for Ubuntu application launcher.
- The propagator function can now take a list of times as argument, and returns a list of corresponding propagators.

### 6.7.59 Bug Fixes

- mesolver now correctly uses the user defined rhs\_filename in Odeoptions().
- rhs\_generate() now handles user defined filenames properly.
- Density matrix returned by propagator\_steadystate is now Hermitian.
- eseries\_value returns real list if all imag parts are zero.
- mcsolver now gives correct results for strong damping rates.
- Odeoptions now prints mc\_avg correctly.

- Do not check for PyObj in mcsolve when gui=False.
- Eseries now correctly handles purely complex rates.
- thermal\_dm() function now uses truncated operator method.
- Cython based time-dependence now Python 3 compatible.
- Removed call to NSAutoPool on mac systems.
- Progress bar now displays the correct number of CPU's used.
- Qobj.diag() returns reals if operator is Hermitian.
- Text for progress bar on Linux systems is no longer cutoff.

### Version 2.0.0 (June 01, 2012)

The second version of QuTiP has seen many improvements in the performance of the original code base, as well as the addition of several new routines supporting a wide range of functionality. Some of the highlights of this release include:

#### 6.7.60 New Features

- QuTiP now includes solvers for both Floquet and Bloch-Redfield master equations.
- The Lindblad master equation and Monte Carlo solvers allow for time-dependent collapse operators.
- It is possible to automatically compile time-dependent problems into c-code using Cython (if installed).
- Python functions can be used to create arbitrary time-dependent Hamiltonians and collapse operators.
- Solvers now return Odedata objects containing all simulation results and parameters, simplifying the saving of simulation results.

---

**Important:** This breaks compatibility with QuTiP version 1.x.

---

- mesolve and mcsolve can reuse Hamiltonian data when only the initial state, or time-dependent arguments, need to be changed.
- QuTiP includes functions for creating random quantum states and operators.
- The generation and manipulation of quantum objects is now more efficient.
- Quantum objects have basis transformation and matrix element calculations as built-in methods.
- The quantum object eigensolver can use sparse solvers.
- The partial-trace (ptrace) function is up to 20x faster.
- The Bloch sphere can now be used with the Matplotlib animation function, and embedded as a subplot in a figure.
- QuTiP has built-in functions for saving quantum objects and data arrays.
- The steady-state solver has been further optimized for sparse matrices, and can handle much larger system Hamiltonians.
- The steady-state solver can use the iterative bi-conjugate gradient method instead of a direct solver.
- There are three new entropy functions for concurrence, mutual information, and conditional entropy.
- Correlation functions have been combined under a single function.
- The operator norm can now be set to trace, Frobius, one, or max norm.
- Global QuTiP settings can now be modified.

- QuTiP includes a collection of unit tests for verifying the installation.
- Demos window now lets you copy and paste code from each example.

#### **Version 1.1.4 (May 28, 2012)**

##### **6.7.61 Bug Fixes**

- Fixed bug pointed out by Brendan Abolins.
- `Qobj.tr()` returns zero-dim ndarray instead of float or complex.
- Updated factorial import for scipy version 0.10+

#### **Version 1.1.3 (November 21, 2011)**

##### **6.7.62 New Functions**

- Allow custom naming of Bloch sphere.

##### **6.7.63 Bug Fixes**

- Fixed text alignment issues in AboutBox.
- Added fix for SciPy V>0.10 where factorial was moved to `scipy.misc` module.
- Added `tidyup` function to tensor function output.
- Removed `openmp` flags from `setup.py` as new Mac Xcode compiler does not recognize them.
- `Qobj.diag` method now returns real array if all imaginary parts are zero.
- Examples GUI now links to new documentation.
- Fixed zero-dimensional array output from metrics module.

#### **Version 1.1.2 (October 27, 2011)**

##### **6.7.64 Bug Fixes**

- Fixed issue where Monte Carlo states were not output properly.

#### **Version 1.1.1 (October 25, 2011)**

**THIS POINT-RELEASE INCLUDES VASTLY IMPROVED TIME-INDEPENDENT MCSOLVE AND ODESOLVE PERFORMANCE**

##### **6.7.65 New Functions**

- Added linear entropy function.
- Number of CPU's can now be changed.

### 6.7.66 Bug Fixes

- Metrics no longer use dense matrices.
- Fixed Bloch sphere grid issue with matplotlib 1.1.
- Qobj trace operation uses only sparse matrices.
- Fixed issue where GUI windows do not raise to front.

### Version 1.1.0 (October 04, 2011)

**THIS RELEASE NOW REQUIRES THE GCC COMPILER TO BE INSTALLED**

### 6.7.67 New Functions

- tidyup function to remove small elements from a Qobj.
- Added concurrence function.
- Added simdiag for simultaneous diagonalization of operators.
- Added eigenstates method returning eigenstates and eigenvalues to Qobj class.
- Added fileio for saving and loading data sets and/or Qobj's.
- Added hinton function for visualizing density matrices.

### 6.7.68 Bug Fixes

- Switched Examples to new Signals method used in PySide 1.0.6+.
- Switched ProgressBar to new Signals method.
- Fixed memory issue in expm functions.
- Fixed memory bug in isherm.
- Made all Qobj data complex by default.
- Reduced ODE tolerance levels in Odeoptions.
- Fixed bug in ptrace where dense matrix was used instead of sparse.
- Fixed issue where PyQt4 version would not be displayed in about box.
- Fixed issue in Wigner where xvec was used twice (in place of yvec).

### Version 1.0.0 (July 29, 2011)

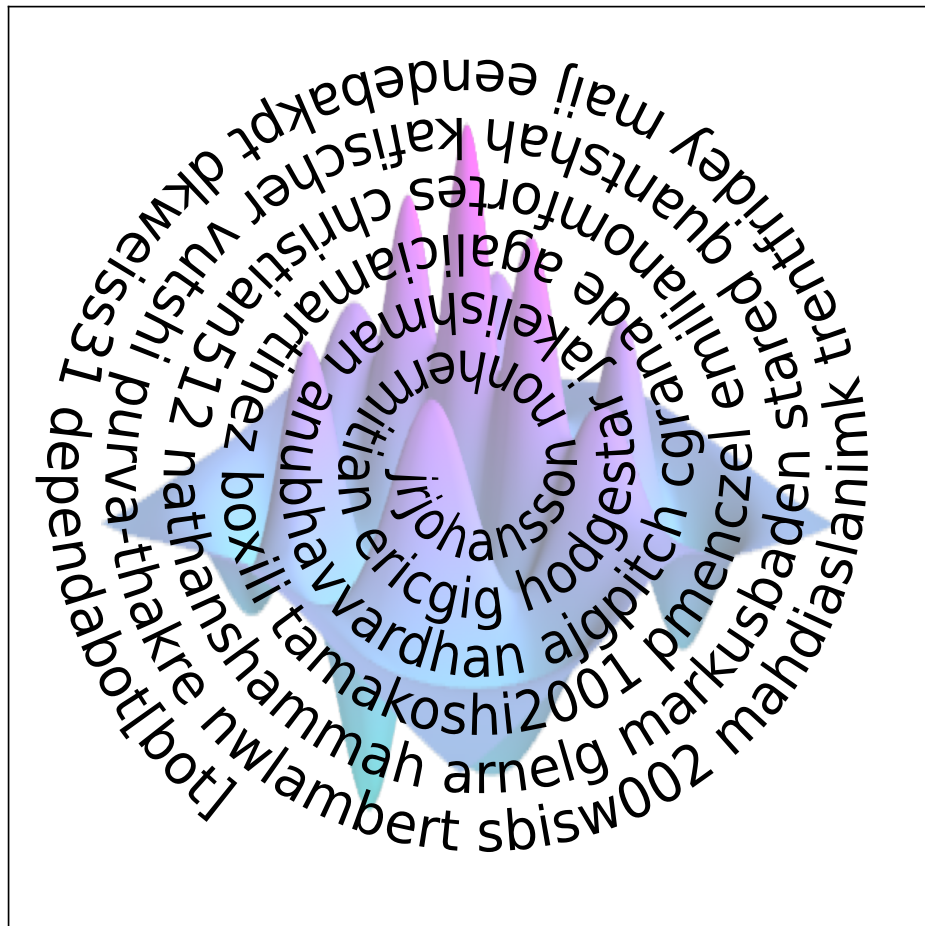
- **Initial release.**





## Chapter 7

# Developers



## 7.1 Lead Developers

- Alex Pitchford
- Nathan Shammah
- Shahnawaz Ahmed
- Neill Lambert
- Eric Giguère
- Boxi Li
- Simon Cross
- Asier Galicia

## 7.2 Past Lead Developers

- Robert Johansson (RIKEN)
- Paul Nation (Korea University)
- Chris Granade
- Arne Grimsmo
- Jake Lishman

## 7.3 Contributors

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**Note:** Anyone is welcome to contribute to QuTiP. If you are interested in helping, please let us know!

---

- Abhisek Upadhyaya
- Adriaan
- Alexander Pitchford
- Alexios-xi
- Amit
- Anubhav Vardhan
- Arie van Deursen
- Arne Grimsmo
- Arne Hamann
- Asier Galicia Martinez
- Ben Bartlett
- Ben Criger
- Ben Jones
- Bo Yang
- Boxi Li
- Canoming

- Christoph Gohlke
- Christopher Granade
- Craig Gidney
- Denis Vasilyev
- Dominic Meiser
- Drew Parsons
- Eric Giguère
- Eric Hontz
- Felipe Bivort Haiek
- Florestan Ziem
- Gilbert Shih
- Harry Adams
- Ivan Carvalho
- Jake Lishman
- Jevon Longdell
- Johannes Feist
- Jonas Hoersch
- Jonas Neergaard-Nielsen
- Jonathan A. Gross
- Julian Iacoponi
- Kevin Fischer
- Laurence Stant
- Louis Tessler
- Lucas Verney
- Marco David
- Marek Narozniak
- Markus Baden
- Martín Sande
- Mateo Laguna
- Matthew O'Brien
- Michael Goerz
- Michael V. DePalatis
- Moritz Oberhauser
- Nathan Shammah
- Neill Lambert
- Nicolas Quesada
- Nikolas Tezak
- Nithin Ramu
- Paul Nation

- Peter Kirton
- Philipp Schindler
- Piotr Migdal
- Rajiv-B
- Ray Ganardi
- Reinier Heeres
- Richard Brierley
- Robert Johansson
- Sam Griffiths
- Samesh Lakhotia
- Sebastian Krämer
- Shahnawaz Ahmed
- Sidhant Saraogi
- Simon Cross
- Simon Humpohl
- Simon Whalen
- Stefan Krastanov
- Tarun Raheja
- Thomas Walker
- Viacheslav Ostroukh
- Vlad Negnevitsky
- Wojciech Rzadkowski
- Xiaodong Qi
- Xiaoliang Wu
- Yariv Yanay
- YouWei Zhao
- alex
- eliegenois
- essence-of-waqf
- fhenneke
- gecrooks
- jakobjakobson13
- maij
- sbisw002
- [yuri@FreeBSD](#)
- Élie Gouzien

## Chapter 8

# Development Documentation

This chapter covers the development of QuTiP and its subpackages, including a roadmap for upcoming releases and ideas for future improvements.

## 8.1 Contributing to QuTiP Development

### 8.1.1 Quick Start

QuTiP is developed through wide collaboration using the `git` version-control system, with the main repositories hosted in the [qutip organisation on GitHub](#). You will need to be familiar with `git` as a tool, and the [GitHub Flow](#) workflow for branching and making pull requests. The exact details of environment set-up, build process and testing vary by repository and are discussed below, however in overview, the steps to contribute are:

1. Consider creating an issue on the GitHub page of the relevant repository, describing the change you think should be made and why, so we can discuss details with you and make sure it is appropriate.
2. (If this is your first contribution.) Make a fork of the relevant repository on GitHub and clone it to your local computer. Also add our copy as a remote (`git remote add qutip https://github.com/qutip/<repo>`)
3. Begin on the `master` branch (`git checkout master`), and pull in changes from the main QuTiP repository to make sure you have an up-to-date copy (`git pull qutip master`).
4. Switch to a new `git` branch (`git checkout -b <branch-name>`).
5. Make the changes you want to make, then create some commits with short, descriptive names (`git add <files>` then `git commit`).
6. Follow the build process for this repository to build the final result so you can check your changes work sensibly.
7. Run the tests for the repository (if it has them).
8. Push the changes to your fork (`git push -u origin <branch-name>`). You won't be able to push to the main QuTiP repositories directly.
9. Go to the GitHub website for the repository you are contributing to, click on the "Pull Requests" tab, click the "New Pull Request" button, and follow the instructions there.

Once the pull request is created, some members of the QuTiP admin team will review the code to make sure it is suitable for inclusion in the library, to check the programming, and to ensure everything meets our standards. For some repositories, several automated tests will run whenever you create or modify a pull request; in general these will be the same tests you can run locally, and all tests are required to pass online before your changes are merged. There may be some feedback and possibly some requested changes. You can add more commits to address these, and push them to the relevant branch of your fork to update the pull request.

The rest of this document covers programming standards, and particular considerations for some of the more complicated repositories.

### 8.1.2 Core Library: `qutip/qutip`

The core library is in the [qutip/qutip repository on GitHub](#).

#### Building

Building the core library from source is typically a bit more difficult than simply installing the package for regular use. You will most likely want to do this in a clean Python environment so that you do not compromise a working installation of a release version, for example by starting from

```
conda create -n qutip-dev python
```

*Complete instructions for the build* are elsewhere in this guide, however beware that you will need to follow the *installation from source using setuptools section*, not the general installation. You will need all the *build* and *tests* “optional” requirements for the package. The build requirements can be found in the `pyproject.toml` file, and the testing requirements are in the `tests` key of the `options.extras_require` section of `setup.cfg`. You will also need the requirements for any optional features you want to test as well.

Refer to the main instructions for the most up-to-date version, however as of version 4.6 the requirements can be installed into a conda environment with

```
conda install setuptools wheel numpy scipy cython packaging pytest pytest-  
↳rerunfailures
```

Note that `qutip` should *not* be installed with `conda install`.

---

**Note:** If you prefer, you can also use `pip` to install all the dependencies. We typically recommend `conda` when doing main-library development because it is easier to switch low-level packages around like BLAS implementations, but if this doesn’t mean anything to you, feel free to use `pip`.

---

You will need to make sure you have a functioning C++ compiler to build QuTiP. If you are on Linux or Mac, this is likely already done for you, however if you are on Windows, refer to the [Windows installation](#) section of the installation guide.

The command to build QuTiP in editable mode is

```
python setup.py develop
```

from the repository directory. If you now load up a Python interpreter, you should be able to `import qutip` from anywhere as long as the correct Python environment is active. Any changes you make to the Python files in the git repository should be immediately present if you restart your Python interpreter and re-import `qutip`.

On the first run, the `setup` command will compile many C++ extension modules built from Cython sources (files ending `.pxd` and `.pyx`). Generally the low-level linear algebra routines that QuTiP uses are written in these files, not in pure Python. Unlike Python files, changes you make to Cython files will not appear until you run `python setup.py develop` again; you will only need to re-run this if you are changing Cython files. Cython will detect and compile only the files that have been changed, so this command will be faster on subsequent runs.

---

**Note:** When undertaking Cython development, the reason we use `python setup.py develop` instead of `pip install -e .` is because Cython’s changed-file detection does not reliably work in the latter. `pip` tends to build in temporary virtual environments, which often makes Cython think its core library files have been updated, triggering a complete, slow rebuild of everything.

---

---

**Note:** QuTiP follows [NEP29](#) when selecting the supported version of its dependencies. To see which versions are planned to be supported in the next release, please refer to the [QuTiP major release roadmap](#). These coincide with the versions employed for testing in continuous integration.

In the event of a feature requiring a version upgrade of python or a dependency, it will be considered appropriately in the pull request. In any case, python and dependency upgrades will only happen in mayor or minor versions of QuTiP, not in a patch.

---

## Code Style

The biggest concern you should always have is to make it easy for your code to be read and understood by the person who comes next.

All new contributions must follow [PEP 8 style](#); all pull requests will be passed through a linter that will complain if you violate it. You should use the `pycodestyle` package locally (available on `pip`) to test you satisfy the requirements before you push your commits, since this is rather faster than pushing 10 different commits trying to fix minor niggles. Keep in mind that there is quite a lot of freedom in this style, especially when it comes to line breaks. If a line is too long, consider the *best* way to split it up with the aim of making the code readable, not just the first thing that doesn't generate a warning.

Try to stay consistent with the style of the surrounding code. This includes using the same variable names, especially if they are function arguments, even if these “break” PEP 8 guidelines. *Do not* change existing parameter, attribute or method names to “match” PEP 8; these are breaking user-facing changes, and cannot be made except in a new major release of QuTiP.

Other than this, general “good-practice” Python standards apply: try not to duplicate code; try to keep functions short, descriptively-named and side-effect free; provide a docstring for every new function; and so on.

## Documenting

When you make changes in the core library, you should update the relevant documentation if needed. If you are making a bug fix, or other relatively minor changes, you will probably only need to make sure that the docstrings of the modified functions and classes are up-to-date; changes here will propagate through to the documentation the next time it is built. Be sure to follow the [Numpy documentation standards \(numpydoc\)](#) when writing docstrings. All docstrings will be parsed as `reStructuredText`, and will form the API documentation section of the documentation.

## Testing

We use `pytest` as our test runner. The base way to run every test is

```
pytest /path/to/repo/qutip/tests
```

This will take around 10 to 30 minutes, depending on your computer and how many of the optional requirements you have installed. It is normal for some tests to be marked as “skip” or “xfail” in yellow; these are not problems. True failures will appear in red and be called “fail” or “error”.

While prototyping and making changes, you might want to use some of the filtering features of `pytest`. Instead of passing the whole `tests` directory to the `pytest` command, you can also pass a list of files. You can also use the `-k` selector to only run tests whose names include a particular pattern, for example

```
pytest qutip/tests/test_qobj.py -k "expm"
```

to run the tests of `Qobj.expm`.

## Changelog Generation

We use `towncrier` for tracking changes and generating a changelog. When making a pull request, we require that you add a `towncrier` entry along with the code changes. You should create a file named `<PR number>.<change type>` in the `doc/changes` directory, where the PR number should be substituted for `<PR number>`, and `<change type>` is either `feature`, `bugfix`, `doc`, `removal`, `misc`, or `deprecation`, depending on the type of change included in the PR.

You can also create this file by installing `towncrier` and running

```
towncrier create <PR number>.<change type>
```

Running this will create a file in the `doc/changes` directory with a filename corresponding to the argument you passed to `towncrier create`. In this file, you should add a short description of the changes that the PR introduces.

## 8.1.3 Documentation: qutip/qutip (doc directory)

The core library is in the [qutip/qutip repository on GitHub](#), inside the `doc` directory.

### Building

The documentation is built using `sphinx`, `matplotlib` and `numpydoc`, with several additional extensions including `sphinx-gallery` and `sphinx-rtd-theme`. The most up-to-date instructions and dependencies will be in the `README.md` file of the documentation directory. You can see the rendered version of this file simply by going to the [documentation GitHub page](#) and scrolling down.

Building the documentation can be a little finnick on occasion. You likely will want to keep a separate Python environment to build the documentation in, because some of the dependencies can have tight requirements that may conflict with your favourite tools for Python development. We recommend creating an empty `conda` environment containing only Python with

```
conda create -n qutip-doc python=3.8
```

and install all further dependencies with `pip`. There is a `requirements.txt` file in the repository root that fixes all package versions exactly into a known-good configuration for a completely empty environment, using

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

This known-good configuration was intended for Python 3.8, though in principle it is possible that other Python versions will work.

---

**Note:** We recommend you use `pip` to install dependencies for the documentation rather than `conda` because several necessary packages can be slower to update their `conda` recipes, so suitable versions may not be available.

---

The documentation build includes running many components of the main QuTiP library to generate figures and to test the output, and to generate all the API documentation. You therefore need to have a version of QuTiP available in the same Python environment. If you are only interested in updating the users' guide, you can use a release version of QuTiP, for example by running `pip install qutip`. If you are also modifying the main library, you need to make your development version accessible in this environment. See the [above section on building QuTiP](#) for more details, though the `requirements.txt` file will have already installed all the build requirements, so you should be able to simply run

```
python setup.py develop
```

in the main library repository.

The documentation is built by running the `make` command. There are several targets to build, but the most useful will be `html` to build the webpage documentation, `latexpdf` to build the PDF documentation (you will also need



a full `pdflatex` installation), and `clean` to remove all built files. The most important command you will want to run is

```
make html
```

You should re-run this any time you make changes, and it should only update files that have been changed.

---

**Important:** The documentation build includes running almost all the optional features of QuTiP. If you get failure messages in red, make sure you have installed all of the optional dependencies for the main library.

---

The HTML files will be placed in the `_build/html` directory. You can open the file `_build/html/index.html` in your web browser to check the output.

## Code Style

All user guide pages and docstrings are parsed by Sphinx using reStructuredText. There is a general [Sphinx usage guide](#), which has a lot of information that can sometimes be a little tricky to follow. It may be easier just to look at other `.rst` files already in the documentation to copy the different styles.

---

**Note:** reStructuredText is a very different language to the Markdown that you might be familiar with. It's always worth checking your work in a web browser to make sure it's appeared the way you intended.

---

## Testing

There are unfortunately no automated tests for the documentation. You should ensure that no errors appeared in red when you ran `make html`. Try not to introduce any new warnings during the build process. The main test is to open the HTML pages you have built (open `_build/html/index.html` in your web browser), and click through to the relevant pages to make sure everything has rendered the way you expected it to.

# 8.2 QuTiP Development Roadmap

## 8.2.1 Preamble

This document outlines plan and ideas for the current and future development of QuTiP. The document is maintained by the QuTiP Admin team. Contributions from the QuTiP Community are very welcome.

In particular this document outlines plans for the next major release of qutip, which will be version 5. And also plans and dreams beyond the next major version.

There is lots of development going on in QuTiP that is not recorded in here. This is just an attempt at coordinated strategy and ideas for the future.

## What is QuTiP?

The name QuTiP refers to a few things. Most famously, qutip is a Python library for simulating quantum dynamics. To support this, the library also contains various software tools (functions and classes) that have more generic applications, such as linear algebra components and visualisation utilities, and also tools that are specifically quantum related, but have applications beyond just solving dynamics (for instance partial trace computation).

QuTiP is also an organisation, in the Github sense, and in the sense of a group of people working collaboratively towards common objectives, and also a web presence [qutip.org](http://qutip.org). The QuTiP Community includes all the people who have supported the project since in conception in 2010, including manager, funders, developers, maintainers and users.

These related, and overlapping, uses of the QuTiP name are of little consequence until one starts to consider how to organise all the software packages that are somehow related to QuTiP, and specifically those that are maintained by the QuTiP Admin Team. Herein QuTiP will refer to the project / organisation and qutip to the library for simulating quantum dynamics.

Should we be starting again from scratch, then we would probably choose another name for the main qutip library, such as qutip-quantdyn. However, qutip is famous, and the name will stay.

## 8.2.2 Library package structure

With a name as general as Quantum Toolkit in Python, the scope for new code modules to be added to qutip is very wide. The library was becoming increasingly difficult to maintain, and in c. 2020 the QuTiP Admin Team decided to limit the scope of the ‘main’ (for want of a better name) qutip package. This scope is restricted to components for the simulation (solving) of the dynamics of quantum systems. The scope includes utilities to support this, including analysis and visualisation of output.

At the same time, again with the intention of easing maintenance, a decision to limit dependences was agreed upon. Main qutip runtime code components should depend only upon Numpy and Scipy. Installation (from source) requires Cython, and some optional components also require Cython at runtime. Unit testing requires Pytest. Visualisation (optional) components require Matplotlib.

Due to the all encompassing nature of the plan to abstract the linear algebra data layer, this enhancement (developed as part of a GSOC project) was allowed the freedom (potential for non-backward compatibility) of requiring a major release. The timing of such allows for a restructuring of the qutip components, such that some that could be deemed out of scope could be packaged in a different way – that is, not installed as part of the main qutip package. Hence the proposal for different types of package described next. With reference to the [discussion above](#) on the name QuTiP/qutip, the planned restructuring suffers from confusing naming, which seems unavoidable without remaining either the organisation or the main package (neither of which are desirable).

### QuTiP family packages

The main qutip package already has sub-packages, which are maintained in the main qutip repo. Any packages maintained by the QuTiP organisation will be called QuTiP ‘family’ packages. Sub-packages within qutip main will be called ‘integrated’ sub-packages. Some packages will be maintained in their own repos and installed separately within the main qutip folder structure to provide backwards compatibility, these are (will be) called qutip optional sub-packages. Others will be installed in their own folders, but (most likely) have qutip as a dependency – these will just be called ‘family’ packages.

### QuTiP affiliated packages

Other packages have been developed by others outside of the QuTiP organisation that work with, and are complementary to, qutip. The plan is to give some recognition to those that we deem worthy of such [this needs clarification]. These packages will not be maintained by the QuTiP Team.

## Family packages

### qutip main

- **current package status:** family package *qutip*
- **planned package status:** family package *qutip*

The in-scope components of the main qutip package all currently reside in the base folder. The plan is to move some components into integrated subpackages as follows:

- *core* quantum objects and operations
- *solver* quantum dynamics solvers

What will remain in the base folder will be miscellaneous modules. There may be some opportunity for grouping some into a *visualisation* subpackage. There is also some potential for renaming, as some module names have underscores, which is unconventional.

## Qtrl

- **current package status:** integrated sub-package *qutip.control*
- **planned package status:** family package *qtrl*

There are many OSS Python packages for quantum control optimisation. There are also many different algorithms. The current *control* integrated subpackage provides the GRAPE and CRAB algorithms. It is too ambitious for QuTiP to attempt (or want) to provide for all options. Control optimisation has been deemed out of scope and hence these components will be separated out into a family package called Qtrl.

Potentially Qtrl may be replaced by separate packages for GRAPE and CRAB, based on the QuTiP Control Framework.

## QIP

- **current package status:** integrated sub-package *qutip.qip*
- **planned package status:** family package *qutip-qip*

The QIP subpackage has been deemed out of scope (feature-wise). It also depends on *qutip.control* and hence would be out of scope for dependency reasons. A separate repository has already been made for *qutip-qip*.

## qutip-symbolic

- **current package status:** independent package *sympsi*
- **planned package status:** family package *qutip-symbolic*

Long ago Robert Johansson and Eunjong Kim developed Sympsi. It is a fairly complete library for quantum computer algebra (symbolic computation). It is primarily a quantum wrapper for *Sympy*.

It has fallen into unmaintained status. The latest version on the [sympsi repo](#) does not work with recent versions of Sympy. Alex Pitchford has a [fork](#) that does ‘work’ with recent Sympy versions – unit tests pass, and most examples work. However, some (important) examples fail, due to lack of respect for non-commuting operators in Sympy simplification functions (note this was true as of Nov 2019, may be fixed now).

There is a [not discussed with RJ & EK] plan to move this into the QuTiP family to allow the Admin Team to maintain, develop and promote it. The ‘Sympsi’ name is cute, but a little abstract, and *qutip-symbolic* is proposed as an alternative, as it is plainer and more distinct from Sympy.

## Affiliated packages

### qucontrol-krotov

- **code repository:** <https://github.com/qucontrol/krotov>

A package for quantum control optimisation using Krotov, developed mainly by Michael Goerz.

Generally accepted by the Admin Team as well developed and maintained. A solid candidate for affiliation.

## 8.2.3 Development Projects

### Solver data layer integration

**tag**  
solve-dl

**status**  
development ongoing

**admin lead**  
Eric

**main dev**  
Eric

The new data layer gives opportunity for significantly improving performance of the qutip solvers. Eric has been revamping the solvers by deploying *QobjEvo* (the time-dependent quantum object) that he developed. *QobjEvo* will exploit the data layer, and the solvers in turn exploit *QobjEvo*.

### Qtrl migration

**tag**  
qtrl-mig

**status**  
conceptualised

**admin lead**  
Alex

**main dev**  
TBA

The components currently packaged as an integrated subpackage of qutip main will be moved to separate package called Qtrl. This is the original codename of the package before it was integrated into qutip. Also changes to exploit the new data layer will be implemented.

### QuTiP control framework

**tag**  
ctrl-fw

**status**  
conceptualised

**admin lead**  
Alex

**main dev**  
TBA

Create new package qutip-ctrlfw “QuTiP Control Framework”. The aim is provide a common framework that can be adopted by control optimisation packages, such that different packages (algorithms) can be applied to the same problem.

Classes for defining a controlled system:

- named control parameters. Scalar and n-dim. Continuous and discrete variables
- mapping of control parameters to dynamics generator args
- masking for control parameters to be optimised

Classes for time-dependent variable parameterisation

- piecewise constant
- piecewise linear
- Fourier basis
- more

Classes for defining an optimisation problem:

- single and multiple objectives

## QuTiP optimisation

**tag**  
qutip-optim

**status**  
conceptualised

**admin lead**  
Alex

**main dev**  
TBA

A wrapper for multi-variable optimisation functions. For instance those in *scipy.optimize* (Nelder-Mead, BFGS), but also others, such as Bayesian optimisation and other machine learning based approaches. Initially just providing a common interface for quantum control optimisation, but applicable more generally.

## Sympsi migration

**tag**  
sympsi-mig

**status**  
conceptualised

**admin lead**  
Alex

**main dev**  
TBA

Create a new family package qutip-symbolic from ajgpitch fork of Sympy. Must gain permission from Robert Johansson and Eunjong Kim. Extended Sympy simplify to respect non-commuting operators. Produce user documentation.

## Status messaging and recording

**tag**  
status-msg

**status**  
conceptualised

**admin lead**  
Alex

**main dev**  
TBA

QuTiP has various ways of recording and reporting status and progress.

- *ProgressBar* used by some solvers

- Python logging used in `qutip.control`
- *Dump* used in `qutip.control`
- heom records *solver.Stats*

Some consolidation of these would be good.

Some processes (some solvers, correlation, control optimisation) have many stages and many layers. *Dump* was initially developed to help with debugging, but it is also useful for recording data for analysis. `qutip.logging_utils` has been criticised for the way it uses Python logging. The output goes to `stderr` and hence the output looks like errors in Jupyter notebooks.

Clearly, storing process stage data is costly in terms of memory and cpu time, so any implementation must be able to be optionally switched on/off, and avoided completely in low-level processes (cythonized components).

Required features:

- optional recording (storing) of process stage data (states, operators etc)
- optionally write subsets to `stdout`
- maybe other graphical representations
- option to save subsets to file
- should ideally replace use of *ProgressBar*, Python logging, *control.Dump*, *solver.Stats*

### qutip Interactive

**status**

conceptualised

**tag**

qutip-gui

**admin lead**

Alex

**main dev**

TBA

QuTiP is pretty simple to use at an entry level for anyone with basic Python skills. However, *some* Python skills are necessary. A graphical user interface (GUI) for some parts of qutip could help make qutip more accessible. This could be particularly helpful in education, for teachers and learners.

This would make an good GSoC project. It is independent and the scope is flexible.

The scope for this is broad and flexible. Ideas including, but not limited to:

### Interactive Bloch sphere

Matplotlib has some interactive features (sliders, radio buttons, cmd buttons) that can be used to control parameters. They are a bit clunky to use, but they are there. Could maybe avoid these and develop our own GUI. An interactive Bloch sphere could have sliders for qubit state angles. Buttons to add states, toggle state evolution path.

## Interactive solvers

Options to configure dynamics generators (Lindbladian / Hamiltonian args etc) and expectation operators. Then run solver and view state evolution.

## Animated circuits

QIP circuits could be animated. Status lights showing evolution of states during the processing. Animated Bloch spheres for qubits.

## 8.2.4 Completed Development Projects

### data layer abstraction

```

tag
  dl-abs

status
  completed

admin lead
  Eric

main dev
  Jake Lishman

```

Development completed as a GSoC project. Fully implemented in the dev.major branch. Currently being used by some research groups.

Abstraction of the linear algebra data from code qutip components, allowing for alternatives, such as sparse, dense etc. Difficult to summarize. Almost every file in qutip affected in some way. A major milestone for qutip. Significant performance improvements throughout qutip.

Some developments tasks remain, including providing full control over how the data-layer dispatchers choose the most appropriate output type.

### qutip main reorganization

```

tag
  qmain-reorg

status
  completed

admin lead
  Eric

main dev
  Jake Lishman

```

Reorganise qutip main components to the structure *described above*.

### qutip user docs migration

**tag**  
qmain-docs

**status**  
completed

**admin lead**  
Jake Lishman

**main dev**  
Jake Lishman

The qutip user documentation build files are to be moved to the qutip/qutip repo. This is more typical for an OSS package.

As part of the move, the plan is to reconstruct the Sphinx structure from scratch. Historically, there have been many issues with building the docs. Sphinx has come a long way since qutip docs first developed. The main source (rst) files will remain [pretty much] as they are, although there is a lot of scope to improve them.

The qutip-doc repo will afterwards just be used for documents, such as this one, pertaining to the QuTiP project.

### QIP migration

**tag**  
qip-mig

**status**  
completed

**admin lead**  
Boxi

**main dev**  
Sidhant Saraogi

A separate package for qutip-qip was created during Sidhant's GSoC project. There is some fine tuning required, especially after qutip.control is migrated.

### HEOM revamp

**tag**  
heom-revamp

**status**  
completed

**admin lead**  
Neill

**main dev**  
Simon Cross, Tarun Raheja

An overhaul of the HEOM solver, to incorporate the improvements pioneered in BoFiN.



## 8.2.5 QuTiP major release roadmap

### QuTiP v.5

These Projects need to be completed for the qutip v.5 release.

- *data layer abstraction* (completed)
- *qutip main reorganization* (completed)
- *qutip user docs migration* (completed)
- *Solver data layer integration* (in-progress)
- *QIP migration* (completed)
- *Qtrl migration*
- *HEOM revamp* (completed)

The planned timeline for the release is:

- **alpha version, December 2022.** Core features packaged and available for experienced users to test.
- **beta version, January 2023.** All required features and documentation complete, packaged and ready for community testing.
- **full release, April 2023.** Full tested version released.

Planned supported environment:

- python 3.8 .. 3.11
- numpy 1.20 .. 1.23
- scipy 1.5 .. 1.8

## 8.3 Ideas for future QuTiP development

Ideas for significant new features are listed here. For the general roadmap, see [QuTiP Development Roadmap](#).

### 8.3.1 QuTiP Interactive

#### Contents

- *Interactive Bloch sphere*
- *Interactive solvers*
- *Animated circuits*
  - *Expected outcomes*
  - *Skills*
  - *Difficulty*
  - *Mentors*

QuTiP is pretty simple to use at an entry level for anyone with basic Python skills. However, *some* Python skills are necessary. A graphical user interface (GUI) for some parts of qutip could help make qutip more accessible. This could be particularly helpful in education, for teachers and learners.

Ideally, interactive components could be embedded in web pages. Including, but not limited to, Jupyter notebooks.

The scope for this is broad and flexible. Ideas including, but not limited to:

### Interactive Bloch sphere

QuTiP has a Bloch sphere virtualisation for qubit states. This could be made interactive through sliders, radio buttons, cmd buttons etc. An interactive Bloch sphere could have sliders for qubit state angles. Buttons to add states, toggle state evolution path. Potential for recording animations. Matplotlib has some interactive features (sliders, radio buttons, cmd buttons) that can be used to control parameters. that could potentially be used.

### Interactive solvers

Options to configure dynamics generators (Lindbladian / Hamiltonian args etc) and expectation operators. Then run solver and view state evolution.

### Animated circuits

QIP circuits could be animated. Status lights showing evolution of states during the processing. Animated Bloch spheres for qubits.

### Expected outcomes

- Interactive graphical components for demonstrating quantum dynamics
- Web pages for [qutip.org](http://qutip.org) or Jupyter notebooks introducing quantum dynamics using the new components

### Skills

- Git, Python and familiarity with the Python scientific computing stack
- elementary understanding of quantum dynamics

### Difficulty

- Variable

### Mentors

- Nathan Shammah ([nathan.shammah@gmail.com](mailto:nathan.shammah@gmail.com))
- Alex Pitchford ([alex.pitchford@gmail.com](mailto:alex.pitchford@gmail.com))
- Simon Cross ([hodgestar@gmail.com](mailto:hodgestar@gmail.com))
- Boxi Li ([etamin1201@gmail.com](mailto:etamin1201@gmail.com)) [QuTiP GSoC 2019 graduate]

## 8.3.2 Pulse level description of quantum circuits

### Contents

- *Expected outcomes*
- *Skills*
- *Difficulty*
- *Mentors*

## • References

The aim of this proposal is to enhance QuTiP quantum-circuit compilation features with regard to quantum information processing. While QuTiP core modules deal with dynamics simulation, there is also a module for quantum circuits simulation. The two subsequent Google Summer of Code projects, in 2019 and 2020, enhanced them in capabilities and features, allowing the simulation both at the level of gates and at the level of time evolution. To connect them, a compiler is implemented to compile quantum gates into the Hamiltonian model. We would like to further enhance this feature in QuTiP and the connection with other libraries.

## Expected outcomes

- APIs to import and export pulses to other libraries. Quantum compiler is a current research topic in quantum engineering. Although QuTiP has a simple compiler, many may want to try their own compiler which is more compatible with their quantum device. Allowing importation and exportation of control pulses will make this much easier. This will include a study of existing libraries, such as *qiskit.pulse* and *OpenPulse*<sup>1</sup>, comparing them with *qutip.qip.pulse* module and building a more general and comprehensive description of the pulse.
- More examples of quantum system in the *qutip.qip.device* module. The circuit simulation and compilation depend strongly on the physical system. At the moment, we have two models: spin chain and cavity QED. We would like to include some other commonly used platform such as Superconducting system<sup>2</sup>, Ion trap system<sup>3</sup> or silicon system. Each model will need a new set of control Hamiltonian and a compiler that finds the control pulse of a quantum gate. More involved noise models can also be added based on the physical system. This part is going to involve some physics and study of commonly used hardware platforms. The related code can be found in *qutip.qip.device* and *qutip.qip.compiler*.

## Skills

- Git, Python and familiarity with the Python scientific computing stack
- quantum information processing and quantum computing (quantum circuit formalism)

## Difficulty

- Medium

## Mentors

- Boxi Li ([etamin1201@gmail.com](mailto:etamin1201@gmail.com)) [QuTiP GSoC 2019 graduate]
- Nathan Shammah ([nathan.shammah@gmail.com](mailto:nathan.shammah@gmail.com))
- Alex Pitchford ([alex.pitchford@gmail.com](mailto:alex.pitchford@gmail.com))

<sup>1</sup> McKay D C, Alexander T, Bello L, et al. Qiskit backend specifications for openqasm and openpulse experiments[J]. arXiv preprint arXiv:1809.03452, 2018.

<sup>2</sup> Häffner H, Roos C F, Blatt R, **Quantum computing with trapped ions**, Physics reports, 2008, 469(4): 155-203.

<sup>3</sup> Krantz P, Kjaergaard M, Yan F, et al. **A quantum engineer's guide to superconducting qubits**, Applied Physics Reviews, 2019, 6(2): 021318.

## References

### 8.3.3 Quantum Error Mitigation

#### Contents

- *Expected outcomes*
- *Skills*
- *Difficulty*
- *Mentors*
- *References*

From the QuTiP 4.5 release, the `qutip.qip` module now contains the noisy quantum circuit simulator (which was a GSoC project) providing enhanced features for a pulse-level description of quantum circuits and noise models. A new class *Processor* and several subclasses are added to represent different platforms for quantum computing. They can transfer a quantum circuit into the corresponding control sequence and simulate the dynamics with QuTiP solvers. Different noise models can be added to *qutip.qip.noise* to simulate noise in a quantum device.

This module is still young and many features can be improved, including new device models, new noise models and integration with the existing general framework for quantum circuits (*qutip.qip.circuit*). There are also possible applications such as error mitigation techniques (<sup>1,2,3</sup>).

The tutorial notebooks can be found in the Quantum information processing section of <https://qutip.org/qutip-tutorials/index-v5.html>. A recent presentation on the FOSDEM conference may help you get an overview ([https://fosdem.org/2020/schedule/event/quantum\\_qutip/](https://fosdem.org/2020/schedule/event/quantum_qutip/)). See also the Github Project page for a collection of related issues and ongoing Pull Requests.

#### Expected outcomes

- Make an overview of existing libraries and features in error mitigation, similarly to a literature survey for a research article, but for a code project (starting from Refs.<sup>4,5</sup>). This is done in order to best integrate the features in QuTiP with existing libraries and avoid reinventing the wheel.
- Features to perform error mitigation techniques in QuTiP, such as zero-noise extrapolation by pulse stretching.
- Tutorials implementing basic quantum error mitigation protocols
- Possible integration with Mitiq<sup>6</sup>

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<sup>1</sup> Kristan Temme, Sergey Bravyi, Jay M. Gambetta, **Error mitigation for short-depth quantum circuits**, Phys. Rev. Lett. 119, 180509 (2017)

<sup>2</sup> Abhinav Kandala, Kristan Temme, Antonio D. Corcoles, Antonio Mezzacapo, Jerry M. Chow, Jay M. Gambetta, **Extending the computational reach of a noisy superconducting quantum processor**, Nature 567, 491 (2019)

<sup>3</sup>

S. Endo, S.C. Benjamin, Y. Li, **Practical quantum error mitigation for near-future applications**, Physical Review X 8, 031027 (2018)

<sup>4</sup> Boxi Li's blog on the GSoC 2019 project on pulse-level control, <https://gsoc2019-boxili.blogspot.com/>

<sup>5</sup> Video of a recent talk on the GSoC 2019 project, [https://fosdem.org/2020/schedule/event/quantum\\_qutip/](https://fosdem.org/2020/schedule/event/quantum_qutip/)

<sup>6</sup> Mitiq

## Skills

- Background in quantum physics and quantum circuits.
- Git, python and familiarity with the Python scientific computing stack

## Difficulty

- Medium

## Mentors

- Nathan Shammah ([nathan.shammah@gmail.com](mailto:nathan.shammah@gmail.com))
- Alex Pitchford ([alex.pitchford@gmail.com](mailto:alex.pitchford@gmail.com))
- Eric Giguère ([eric.giguere@usherbrooke.ca](mailto:eric.giguere@usherbrooke.ca))
- Neill Lambert ([nwlambert@gmail.com](mailto:nwlambert@gmail.com))
- Boxi Li ([etamin1201@gmail.com](mailto:etamin1201@gmail.com)) [QuTiP GSoC 2019 graduate]

## References

### 8.3.4 GPU implementation of the Hierarchical Equations of Motion

#### Contents

- *Expected outcomes*
- *Skills*
- *Difficulty*
- *Mentors*
- *References*

The Hierarchical Equations of Motion (HEOM) method is a non-perturbative approach to simulate the evolution of the density matrix of dissipative quantum systems. The underlying equations are a system of coupled ODEs which can be run on a GPU. This will allow the study of larger systems as discussed in<sup>1</sup>. The goal of this project would be to extend QuTiP's HEOM method<sup>2</sup> and implement it on a GPU.

Since the method is related to simulating large, coupled ODEs, it can also be quite general and extended to other solvers.

<sup>1</sup> <https://pubs.acs.org/doi/abs/10.1021/ct200126d?src=recsys&journalCode=jctcce>

<sup>2</sup> <https://arxiv.org/abs/2010.10806>

### Expected outcomes

- A version of HEOM which runs on a GPU.
- Performance comparison with the CPU version.
- Implement dynamic scaling.

### Skills

- Git, python and familiarity with the Python scientific computing stack
- CUDA and OpenCL knowledge

### Difficulty

- Hard

### Mentors

- Neill Lambert ([nwlambert@gmail.com](mailto:nwlambert@gmail.com))
- Alex Pitchford ([alex.pitchford@gmail.com](mailto:alex.pitchford@gmail.com))
- Shahnawaz Ahmed ([shahnawaz.ahmed95@gmail.com](mailto:shahnawaz.ahmed95@gmail.com))
- Simon Cross ([hodgestar@gmail.com](mailto:hodgestar@gmail.com))

### References

## 8.3.5 Google Summer of Code

Many possible extensions and improvements to QuTiP have been documented as part of [Google Summer of Code](#):

- [GSoC 2021](#)
- [GSoC 2022](#)

## 8.3.6 Completed Projects

These projects have been completed:

### TensorFlow Data Backend

#### Contents

- *Why a TensorFlow backend?*
- *Challenges*
  - *Expected outcomes*
  - *Skills*
  - *Difficulty*
  - *Mentors*
  - *References*

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**Note:** This project was completed as part of GSoC 2021<sup>3</sup>.

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QuTiP's data layer provides the mathematical operations needed to work with quantum states and operators, i.e. `Qobj`, inside QuTiP. As part of Google Summer of Code 2020, the data layer was rewritten to allow new backends to be added more easily and for different backends to interoperate with each other. Backends using in-memory spares and dense matrices already exist, and we would like to add a backend that implements the necessary operations using TensorFlow<sup>1</sup>.

### Why a TensorFlow backend?

TensorFlow supports distributing matrix operations across multiple GPUs and multiple machines, and abstracts away some of the complexities of doing so efficiently. We hope that by using TensorFlow we might enable QuTiP to scale to bigger quantum systems (e.g. more qubits) and decrease the time taken to simulate them.

There is particular interest in trying the new backend with the BoFiN HEOM (Hierarchical Equations of Motion) solver<sup>2</sup>.

### Challenges

TensorFlow is a very different kind of computational framework to the existing dense and sparse matrix backends. It uses flow graphs to describe operations, and to work efficiently. Ideally large graphs of operations need to be executed together in order to efficiently compute results.

The QuTiP data layer might need to be adjusted to accommodate these differences, and it is possible that this will prove challenging or even that we will not find a reasonable way to achieve the desired performance.

### Expected outcomes

- Add a `qutip.core.data.tensorflow` data type.
- Implement specialisations for some important operations (e.g. `add`, `mul`, `matmul`, `eigen`, etc).
- Write a small benchmark to show how `Qobj` operations scale on the new backend in comparison to the existing backends. Run the benchmark both with and without using a GPU.
- Implement enough for a solver to run on top of the new TensorFlow data backend and benchmark that (stretch goal).

### Skills

- Git, Python and familiarity with the Python scientific computing stack
- Familiarity with TensorFlow (beneficial, but not required)
- Familiarity with Cython (beneficial, but not required)

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<sup>3</sup> <https://github.com/qutip/qutip-tensorflow/>

<sup>1</sup> <https://www.tensorflow.org/>

<sup>2</sup> <https://github.com/tehrunn/bofin>

## Difficulty

- Medium

## Mentors

- Simon Cross ([hodgestar@gmail.com](mailto:hodgestar@gmail.com))
- Jake Lishman ([jake@binhbar.com](mailto:jake@binhbar.com))
- Alex Pitchford ([alex.pitchford@gmail.com](mailto:alex.pitchford@gmail.com))

## References

## 8.4 Working with the QuTiP Documentation

The user guide provides an overview of QuTiP’s functionality. The guide is composed of individual reStructured-Text (`.rst`) files which each get rendered as a webpage. Each page typically tackles one area of functionality. To learn more about how to write `.rst` files, it is useful to follow the [sphinx guide](#).

The documentation build also utilizes a number of [Sphinx Extensions](#) including but not limited to [doctest](#), [autodoc](#), [sphinx gallery](#) and [plot](#). Additional extensions can be configured in the `conf.py` file.

### 8.4.1 Directives

There are two Sphinx directives that can be used to write code examples in the user guide:

- [Doctest](#)
- [Plot](#)

For a more comprehensive account of the usage of each directive, please refer to their individual pages. Here we outline some general guidelines on how to these directives while making a user guide.

#### Doctest

The doctest directive enables tests on interactive code examples. The simplest way to do this is by specifying a prompt along with its respective output:

```
.. doctest::

    >>> a = 2
    >>> a
    2
```

This is rendered in the documentation as follows:

```
>>> a = 2
>>> a
2
```

While specifying code examples under the `.. doctest::` directive, either all statements must be specified by the `>>>` prompt or without it. For every prompt, any potential corresponding output must be specified immediately after it. This directive is ideally used when there are a number of examples that need to be checked in quick succession.

A different way to specify code examples (and test them) is using the associated `.. testcode::` directive which is effectively a code block:



```
.. testcode::

    a = 2
    print(a)
```

followed by its results. The result can be specified with the `.. testoutput::` block:

```
.. testoutput::

    2
```

The advantage of the `testcode` directive is that it is a lot simpler to specify and amenable to copying the code to clipboard. Usually, tests are more easily specified with this directive as the input and output are specified in different blocks. The rendering is neater too.

---

**Note:** The `doctest` and `testcode` directives should not be assumed to have the same namespace.

---

### Output:

```
a = 2
print(a)
```

```
2
```

A few notes on using the `doctest` extension:

- By default, each `testcode` and `doctest` block is run in a fresh namespace. To share a common namespace, we can specify a common group across the blocks (within a single `.rst` file). For example,

```
.. doctest:: [group_name]

>>> a = 2
```

can be followed by some explanation followed by another code block sharing the same namespace

```
.. doctest:: [group_name]

>>> print(a)
2
```

- To only print the code blocks (or the output), use the option `+SKIP` to specify the block without the code being tested when running `make doctest`.
- To check the result of a Qobj output, it is useful to make sure that spacing irregularities between the expected and actual output are ignored. For that, we can use the option `+NORMALIZE_WHITESPACE`.

### Plot

Since the `doctest` directive cannot render matplotlib figures, we use Matplotlib's `Plot` directive when rendering to LaTeX or HTML.

The plot directive can also be used in the `doctest` format. In this case, when running doctests (which is enabled by specifying all statements with the `>>>` prompts), tests also include those specified under the plot directive.

### Example:

First we specify some data:

```
.. plot::

>>> import numpy as np
>>> x = np.linspace(0, 2 * np.pi, 1000)
>>> x[:10] # doctest: +NORMALIZE_WHITESPACE
array([ 0.          ,  0.00628947,  0.01257895,  0.01886842,  0.0251579 ,
        0.03144737,  0.03773685,  0.04402632,  0.0503158 ,  0.05660527])

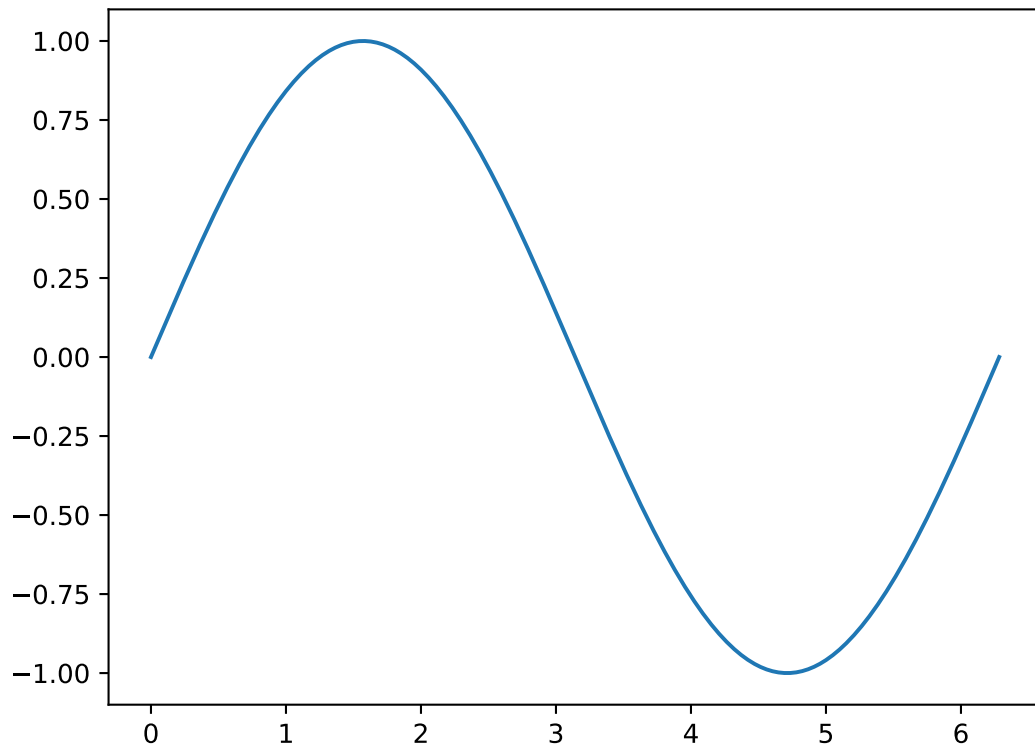
.. plot::
:context:

>>> import matplotlib.pyplot as plt
>>> plt.plot(x, np.sin(x))
[...]
```

Note the use of the `NORMALIZE_WHITESPACE` option to ensure that the multiline output matches.

**Render:**

```
>>> import numpy as np
>>> x = np.linspace(0, 2 * np.pi, 1000)
>>> x[:10]
array([ 0.          ,  0.00628947,  0.01257895,  0.01886842,  0.0251579 ,
        0.03144737,  0.03773685,  0.04402632,  0.0503158 ,  0.05660527])
>>> import matplotlib.pyplot as plt
>>> plt.plot(x, np.sin(x))
[...]
```



A few notes on using the plot directive:

- A useful argument to specify in plot blocks is that of `context` which ensures that the code is being run in the namespace of the previous plot block within the same file.
- By default, each rendered figure in one plot block (when using `:context:`) is carried over to the next block.
- When the `context` argument is specified with the `reset` option as `:context: reset`, the namespace is reset to a new one and all figures are erased.
- When the `context` argument is specified with the `close-figs` option as `:context: reset`, the namespace is reset to a new one and all figures are erased.

The Plot directive cannot be used in conjunction with Doctest because they do not share the same namespace when used in the same file. Since Plot can also be used in doctest mode, in the case where code examples require both testing and rendering figures, it is easier to use the Plot directive. To learn more about each directive, it is useful to refer to their individual pages.

## 8.5 Release and Distribution

### 8.5.1 Preamble

This document covers the process for managing updates to the current minor release and making new releases. Within this document, the git remote `upstream` refers to the main QuTiP organisation repository, and `origin` refers to your personal fork.

In short, the steps you need to take are:

1. Prepare the release branch (see [git](#)).

2. Run the “Build wheels, optionally deploy to PyPI” GitHub action to build binary and source packages and upload them to PyPI (see [deploy](#)).
3. Retrieve the built documentation from GitHub (see [docbuild](#)).
4. Create a GitHub release and uploaded the built files to it (see [github](#)).
5. Update [qutip.org](#) with the new links and documentation ([web](#)).
6. Update the conda feedstock, deploying the package to conda ([cforge](#)).

## 8.5.2 Setting Up The Release Branch

In this step you will prepare a git branch on the main QuTiP repository that has the state of the code that is going to be released. This procedure is quite different if you are releasing a new minor or major version compared to if you are making a bugfix patch release. For a new minor or major version, do [update-changelog](#) and then jump to [release](#). For a bug fix to an existing release, do [update-changelog](#) and then jump to [bugfix](#).

Changes that are not backwards-compatible may only be made in a major release. New features that do not affect backwards-compatibility can be made in a minor release. Bug fix releases should be small, only fix bugs, and not introduce any new features.

There are a few steps that *should* have been kept up-to-date during day-to-day development, but might not be quite accurate. For every change that is going to be part of your release, make sure that:

- The user guide in the documentation is updated with any new features, or changes to existing features.
- Any new API classes or functions have entries in a suitable RST file in `doc/apidoc`.
- Any new or changed docstrings are up-to-date and render correctly in the API documentation.

Please make a normal PR to `master` correcting anything missing from these points and have it merged before you begin the release, if necessary.

### Updating the Requirements

Ensure that QuTiP’s tests pass on the oldest version supported in the requirements. On major and minor version, requirements can be adjusted upwards, but patch release must not change minimum requirements. We follow [NEP29](#) for minimum supported versions

- All minor versions of Python released 42 months prior to the project, and at minimum the two latest minor versions.
  - All minor versions of numpy and scipy released in the 24 months prior to the project, and at minimum the last three minor versions.

If dependency versions need to be updated, update them in the master branch. The following files may need to be updated: `.github/workflows/tests.yml`, `setup.cfg` and `roadmap.rst`. Finally, ensure that PyPI wheels and conda builds cover at least these versions.

### Updating the Changelog

This needs to be done no matter what type of release is being made.

1. Create a new branch to use to make a pull request.
2. Update the changelog using `towncrier`:  
`towncrier build --version=<version-number>`

Where `<version-number>` is the expected version number of the release

1. Make a pull request on the main `qutip/qutip` repository with this changelog, and get other members of the admin team to approve it.

2. Merge this into master.

Now jump to [release](#) if you are making a major or minor release, or [bugfix](#) if you are only fixing bugs in a previous release.

## Create a New Minor or Major Release

This involves making a new branch to hold the release and adding some commits to set the code into “release” mode. This release should be done by branching directly off the master branch at its current head.

1. On your machine, make sure your copy of master is up-to-date (`git checkout master; git pull upstream master`). This should at least involve fetching the changelog PR that you just made. Now create a new branch off a commit in master that has the state of the code you want to release. The command is `git checkout -b qutip-<major>.<minor>.X`, for example `qutip-4.7.X`. This branch name will be public, and must follow this format.
2. Push the new branch (with no commits in it relative to master) to the main qutip/qutip repository (`git push upstream qutip-4.7.X`). Creating a branch is one of the only situations in which it is ok to push to qutip/qutip without making a pull request.
3. Create a second new branch, which will be pushed to your fork and used to make a pull request against the `qutip-<major>.<minor>.X` branch on qutip/qutip you just created. You can call this branch whatever you like because it is not going to the main repository, for example `git checkout -b prepare-qutip-4.7.0`.
4.
  - Change the VERSION file to contain the new version number exactly, removing the .dev suffix. For example, if you are releasing the first release of the minor 4.7 track, set VERSION to contain the string 4.7.0. (*Special circumstances:* if you are making an alpha, beta or release candidate release, append a .a<n>, .b<n> or .rc<n> to the version string, where <n> is an integer starting from 0 that counts how many of that pre-release track there have been.)
  - Edit setup.cfg by changing the “Development Status” line in the classifiers section to

```
Development Status :: 5 - Production/Stable
```

Commit both changes (`git add VERSION setup.cfg; git commit -m "Set release mode for 4.7.0"`), and then push them to your fork (`git push -u origin prepare-qutip-4.7.0`)

5. Using GitHub, make a pull request to the release branch (e.g. `qutip-4.7.X`) using this branch that you just created. You will need to change the “base branch” in the pull request, because GitHub will always try to make the PR against master at first. When the tests have passed, merge this in.
6. Finally, back on master, make a new pull request that changes the VERSION file to be <next-expected-version>.dev, for example 4.8.0.dev. The “Development Status” in setup.cfg on master should not have changed, and should be

```
Development Status :: 2 - Pre-Alpha
```

because master is never directly released.

You should now have a branch that you can see on the GitHub website that is called `qutip-4.7.X` (or whatever minor version), and the state of the code in it should be exactly what you want to release as the new minor release. If you notice you have made a mistake, you can make additional pull requests to the release branch to fix it. master should look pretty similar, except the VERSION will be higher and have a .dev suffix, and the “Development Status” in setup.cfg will be different.

You are now ready to actually perform the release. Go to [deploy](#).

## Create a Bug Fix Release

In this you will modify an already-released branch by “cherry-picking” one or more pull requests that have been merged to `master` (including your new changelog), and bump the “patch” part of the version number.

1. On your machine, make sure your copy of `master` is up-to-date (`git checkout master; git pull upstream master`). In particular, make sure the changelog you wrote in the first step is visible.
2. Find the branch of the release that you will be modifying. This should already exist on the `qutip/qutip` repository, and be called `qutip-<major>.<minor>.X` (e.g. `qutip-4.6.X`). If you cannot see it, run `git fetch upstream` to update all the branch references from the main repository. Checkout a new private branch, starting from the head of the release branch (`git checkout -b prepare-qutip-4.6.1 upstream/qutip-4.6.X`). You can call this branch whatever you like (in the example it is `prepare-qutip-4.6.1`), because it will only be used to make a pull request.
3. Cherry-pick all the commits that will be added to this release in order, including your PR that wrote the new changelog entries (this will be the last one you cherry-pick). You will want to use `git log` to find the relevant commits, going from **oldest to newest** (their “age” is when they were merged into `master`, not when the PR was first opened). The command is slightly different depending on which merge strategy was used for a particular PR:
  - “merge”: you only need to find one commit though the log will have included several; there will be an entry in `git log` with a title such as “Merge pull request #1000 from <...>”. Note the first 7 characters of its hash. Cherry-pick this by `git cherry-pick --mainline 1 <hash>`.
  - “squash and merge”: there will only be a single commit for the entire PR. Its name will be “<Name of the pull request> (#1000)”. Note the first 7 characters of its hash. Cherry-pick this by `git cherry-pick <hash>`.
  - “rebase and merge”: this is the most difficult, because there will be many commits that you will have to find manually, and cherry-pick all of them. Go to the GitHub page for this PR, and go to the “Commits” tab. Using your local `git log` (you may find `git log --oneline` useful), find the hash for every single commit that is listed on the GitHub page, in order from **oldest to newest** (top-to-bottom in the GitHub view, which is bottom-to-top in `git log`). You will need to use the commit message to do this; the hashes that GitHub reports will probably not be the same as how they appear locally. Find the first 7 characters of each of the hashes. Cherry-pick these all in one go by `git cherry-pick <hash1> <hash2> ... <hash10>`, where `<hash1>` is the oldest.

If any of the cherry-picks have merge conflicts, first verify that you are cherry-picking in order from oldest to newest. If you still have merge conflicts, you will either need to manually fix them (if it is a *very* simple fix), or else you will need to find which additional PR this patch depends on, and restart the bug fix process including this additional patch. This generally should not happen if you are sticking to very small bug fixes; if the fixes had far-reaching changes, a new minor release may be more appropriate.

4. Change the `VERSION` file by bumping the last number up by one (double-digit numbers are fine, so `4.6.10` comes after `4.6.9`), and commit the change.
5. Push this branch to your fork, and make a pull request against the release branch. On GitHub in the PR screen, you will need to change the “Base” branch to `qutip-4.6.X` (or whatever version), because GitHub will default to making it against `master`. It should be quite clear if you have forgotten to do this, because there will probably be many merge conflicts. Once the tests have passed and you have another admin’s approval, merge the PR.

You should now see that the `qutip-4.6.X` (or whatever) branch on GitHub has been updated, and now includes all the changes you have just made. If you have made a mistake, feel free to make additional PRs to rectify the situation.

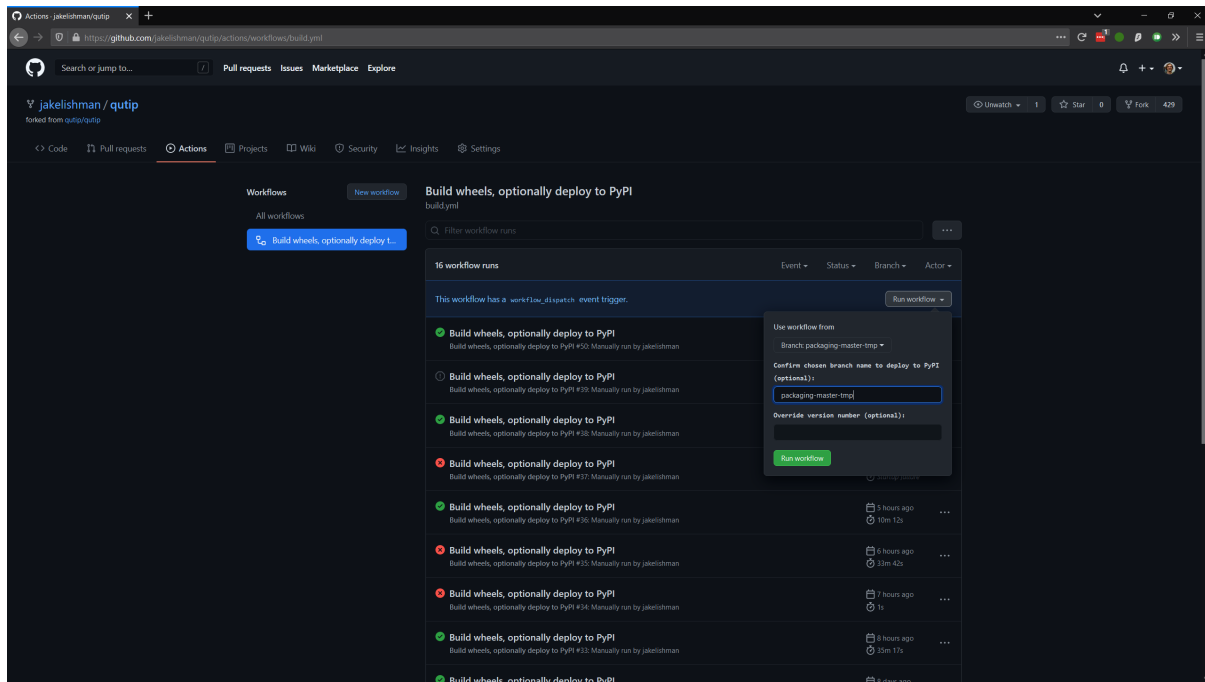
You are now ready to actually perform the release. Go to [deploy](#).

### 8.5.3 Build Release Distribution and Deploy

This step builds the source (sdist) and binary (wheel) distributions, and uploads them to PyPI (pip). You will also be able to download the built files yourself in order to upload them to the QuTiP website.

#### Build and Deploy

This is handled entirely by a GitHub Action. Go to the “Actions” tab at the top of the QuTiP code repository. Click on the “Build wheels, optionally deploy to PyPI” action in the left-hand sidebar. Click the “Run workflow” dropdown in the header notification; it should look like the image below.

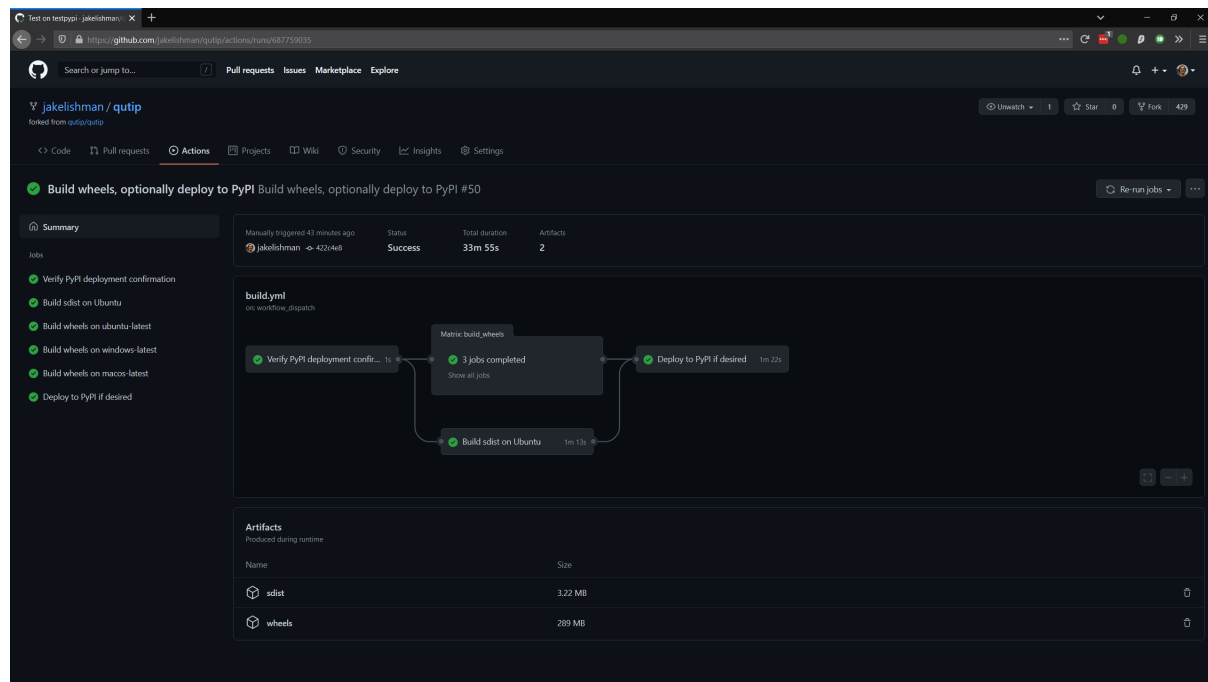


- Use the drop-down menu to choose the branch or tag you want to release from. This should be called `quTip-4.5.X` or similar, depending on what you made earlier. This must *never* be `master`.
- To make the release to PyPI, type the branch name (e.g. `quTip-4.5.X`) into the “Confirm chosen branch name [...]” field. You *may* leave this field blank to skip the deployment and only build the package.
- (Special circumstances) If for some reason you need to override the version number (for example if the previous deployment to PyPI only partially succeeded), you can type a valid Python version identifier into the “Override version number” field. You probably do not need to do this. The mechanism is designed to make alpha-testing major upgrades with nightly releases easier. For even a bugfix release, you should commit the change to the `VERSION` file.
- Click the lower “Run workflow” to perform the build and deployment.

At this point, the deployment will take care of itself. It should take between 30 minutes and an hour, after which the new version will be available for install by `pip install quTip`. You should see the new version appear on QuTiP’s PyPI page.

### Download Built Files

When the build is complete, click into its summary screen. This is the main screen used to both monitor the build and see its output, and should look like the below image on a success.



The built binary wheels and the source distribution are the “build artifacts” at the bottom. You need to download both the wheels and the source distribution. Save them on your computer, and unzip both files; you should have many wheel `qutip-*.whl` files, and two sdist files: `qutip-*.tar.gz` and `qutip-*.zip`. These are the same files that have just been uploaded to PyPI.

### Monitoring Progress (optional)

While the build is in progress, you can monitor its progress by clicking on its entry in the list below the “Run workflow” button. You should see several subjobs, like the completed screen, except they might not yet be completed.

The “Verify PyPI deployment confirmation” should get ticked, no matter what. If it fails, you have forgotten to choose the correct branch in the drop-down menu or you made a typo when confirming the correct branch, and you will need to restart this step. You can check that the deployment instruction has been understood by clicking the “Verify PyPI deployment confirmation” job, and opening the “Compare confirmation to current reference” subjob. You will see a message saying “Built wheels will be deployed” if you typed in the confirmation, or “Only building wheels” if you did not. If you see “Only building wheels” but you meant to deploy the release to PyPI, you can cancel the workflow and re-run it after typing the confirmation.

### 8.5.4 Getting the Built Documentation

The documentation will have been built automatically for you by a GitHub Action when you merged the final pull request into the release branch before building the wheels. You do not need to re-release the documentation on either GitHub or the website if this is a patch release, unless there were changes within it.

Go to the “Actions” tab at the top of the `qutip/qutip` repository, and click the “Build HTML documentation” heading in the left column. You should see a list of times this action has run; click the most recent one whose name is exactly “Build HTML documentation”, with the release branch name next to it (e.g. `qutip-4.6.X`). Download the `qutip_html_docs` artifact to your local machine and unzip it somewhere safe. These are all the HTML files for the built documentation; you should be able to open `index.html` in your own web browser and check that everything is working.



### 8.5.5 Making a Release on GitHub

This is all done through the “Releases” section of the qutip/qutip repository on GitHub.

- Click the “Draft a new release” button.
- Choose the correct branch for your release (e.g. qutip-4.5.X) in the drop-down.
- For the tag name, use v<your-version>, where the version matches the contents of the VERSION file. In other words, if you are releasing a micro version 4.5.3, use v4.5.3 as the tag, or if you are releasing major version 5.0.0, use v5.0.0.
- The title is “QuTiP <your-version>”, e.g. “QuTiP 4.6.0”.
- For the description, write a short (~two-line for a patch release) summary of the reason for this release, and note down any particular user-facing changes that need special attention. Underneath, put the changelog you wrote when you did the documentation release. Note that there may be some syntax differences between the .rst file of the changelog and the Markdown of this description field (for example, GitHub’s markdown typically maintains hard-wrap linebreaks, which is probably not what you wanted).
- Drag-and-drop all the qutip-\*.whl, qutip-\*.tar.gz and qutip-\*.zip files you got after the build step into the assets box. You may need to unzip the files wheels.zip and sdist.zip to find them if you haven’t already; **don’t** upload those two zip files.

Click on the “Publish release” button to finalise.

### 8.5.6 Website

This assumes that qutip.github.io has already been forked and familiarity with the website updating workflow. The documentation need not be updated for every patch release.

#### Copying New Files

You only need to copy in new documentation to the website repository. Do not copy the .whl, .tar.gz or .zip files into the git repository, because we can access the public links from the GitHub release stage, and this keeps the website .git folder a reasonable size.

For all releases move (no new docs) or copy (for new docs) the qutip-doc-<MAJOR>.<MINOR>.pdf into the folder downloads/<MAJOR>.<MINOR>.<MICRO>.

The legacy html documentation should be in a subfolder like

```
docs/<MAJOR>.<MINOR>
```

For a major or minor release the previous version documentation should be moved into this folder.

The latest version HTML documentation should be the folder

```
docs/latest
```

For any release which new documentation is included - copy the contents qutip/doc/\_build/html into this folder. **Note that the underscores at start of the subfolder names will need to be removed, otherwise Jekyll will ignore the folders.** There is a script in the docs folder for this. [https://github.com/qutip/qutip.github.io/blob/master/docs/remove\\_leading\\_underscores.py](https://github.com/qutip/qutip.github.io/blob/master/docs/remove_leading_underscores.py)

## HTML File Updates

- Edit `download.html`
  - The ‘Latest release’ version and date should be updated.
  - The `tar.gz` and `zip` links need to have their micro release numbers updated in their filenames, labels and `trackEvent` javascript. These links should point to the “Source code” links that appeared when you made in the GitHub Releases section. They should look something like `https://github.com/qutip/qutip/archive/refs/tags/v4.6.0.tar.gz`.
  - For a minor or major release links to the last micro release of the previous version will need to be moved (copied) to the ‘Previous releases’ section.
- Edit `_includes/sidebar.html`
  - The ‘Latest release’ version should be updated. The `gz` and `zip` file links will need the micro release number updating in the `trackEvent` and file name.
  - The link to the documentation folder and PDF file (if created) should be updated.
- Edit `documentation.html`
  - The previous release tags should be moved (copied) to the ‘Previous releases’ section.

## 8.5.7 Conda Forge

If not done previously then fork the [qutip-feedstock](#).

Checkout a new branch on your fork, e.g.

```
$ git checkout -b version-4.0.2
```

Find the sha256 checksum for the tarball that the GitHub web interface generated when you produced the release called “Source code”. This is *not* the sdist that you downloaded earlier, it’s a new file that GitHub labels “Source code”. When you download it, though, it will have a name that *looks* like it’s the sdist

```
$ openssl sha256 qutip-4.0.2.tar.gz
```

Edit the `recipe/meta.yaml` file. Change the version at the top of the file, and update the sha256 checksum. Check that the recipe package version requirements at least match those in `setup.cfg`, and that any changes to the build process are reflected in `meta.yaml`. Also ensure that the build number is reset

```
build:  
  number: 0
```

Push changes to your fork, e.g.

```
$ git push --set-upstream origin version-4.0.2
```

Make a Pull Request. This will trigger tests of the package build process.

If (when) the tests pass, the PR can be merged, which will trigger the upload of the packages to the conda-forge channel. To test the packages, add the conda-forge channel with lowest priority

```
$ conda config --append channels conda-forge
```

This should mean that the prerequisites come from the default channel, but the qutip packages are found in conda-forge.

## **Chapter 9**

# **Bibliography**



# Chapter 10

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