QuTiP 2: A Python framework for the dynamics of open quantum systems

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Abstract

We present version 2 of QuTiP, the Quantum Toolbox in Python. Compared to the preceding version [Comput. Phys. Comm. 183 (2012) 1760], we have introduced numerous Application Programming Interface (API) for improved for increased compatibility with existing conventions used in a inficant new features include efficient solvers for arbitrary to for the Floquet formalism, and new solvers for Bloch-Redfie these new features, demonstrate their use, and give a sum introduced in this version.

Keywords: Open quantum systems, Lindblad, Bloch-Redfield, Python
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Program Summary

Manuscript Title: QuTiP 2: A Python framework for the dynamics of open quantum systems

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Program Title: QuTiP: The Quantum Toolbox in Python

Journal Reference:
Catalogue identifier:
Licensing provisions: GPLv3
Programming language: Python

Computer: i386, x86-64
Operating system: Linux, Mac OSX

RAM: 2+ Gigabytes

Number of processors used: 1+

Keywords: Open quantum systems, Lindblad, Bloch-Redfield,
Floquet-Markov, master equation, Quantum Monte Carlo,
Python

Classification: 7 Condensed Matter and Surface Science

External routines/libraries: NumPy, SciPy, Matplotlib,
Cython

Journal reference of previous version: Comput. Phys. Comm.

183 (2012) 1760 Comm. 183 (2012) 1760, we have introduced numerous new features, enhanced performance, made changes in the Application Programming Interface (API) for improved functionality and consistency within the package, as well as increased compatibility with existing conventions used in other scientific software packages for Python. The most significant new features include efficient solvers for arbitrary time-dependent Hamiltonians and collapse operators, support for the Floquet formalism, and new solvers for Bloch-Redfield and Floquet-Markov master equations. Here we introduce these new features, demonstrate their use, and give a summary of the important backward-incompatible API changes

Keywords: Open quantum systems, Lindblad, Bloch-Redfield, Floquet-Markov, master equation, Quantum Monte

Journal reference of previous version: Comput. Phys. Comm. 183 (2012) 1760

Does the new version supersede the previous version?: Yes Nature of problem: Dynamics of open quantum systems Solution method: Numerical solutions to Lindblad, Floquet-Markov, and Bloch-Redfield master equations, as well as the Monte Carlo wave function method.

Restrictions: Problems must meet the criteria for using the master equation in Lindblad, Floquet-Markov, or Bloch-Redfield form.

Running time: A few seconds up to several tens of hours, depending on size of the underlying Hilbert space.

1. Introduction

The Quantum Toolbox in Python (QuTiP), is a generic framework for numerical simulation and computation of the dynamics of both open and closed quantum systems. This framework follows an object-oriented design that makes the programming of a quantum mechanical problem an intuitive process that closely follows the corresponding mathematical formulation. Although implemented in the interpreted programming language Python, the use of the NumPy and SciPy scientific libraries, and selective optimization using Cython, allows QuTiP to achieve performance that matches, or in many cases, exceeds that of natively compiled alternatives. At the same time, QuTiP provides a significantly more convenient and flexible programming environment that is easy to learn, and is well suited for use in the classroom.

Since the first major-version release of QuTiP [1] (the 1.x series), active development of the framework has resulted in a significant number of new features and performance enhancements, that have culminated in the second major-version release. Here we briefly describe the most

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significant changes and additional functionality introduced in this most recent release.

This paper is organized as follows. In Sec. 2 we highlight the important API changes introduced in going from QuTiP 1.x to versions 2.x and higher. Section 3 details the primary new features included in this latest version. To illustrate the new functionality in QuTiP, Sec. 4 contains a selection of examples that highlight how these functions are used in numerical quantum simulations. Finally, a list of all new user-accessible functions, including a brief description, is given in Appendix A.

2. API changes

Here we list the backward-incompatible changes in the API of QuTiP 2 as compared to the previous version (1.1.4) described in Ref. [1]. These changes are important when porting applications and simulations that are developed for QuTiP 1.1.4 to QuTiP 2.0 and higher. For newly developed simulations, we recommend following the documentation and examples for QuTiP 2.1 [2], in which case the following API changes are not relevant. Note that this article covers version 2.1.0 of the QuTiP framework, and incorporates several features added since the initial 2.0 release.

1. All quantum dynamics solvers (mcsolve, mesolve, odesolve, essolve, brmesolve, and fmmesolve) now return an Odedata instance, that contains all information about the solution (as opposed to data lists or Qobjs lists as in QuTiP version 1.1.4). A typical call to a time-evolution solver using the new API is:

```
sol = solver(H, psi0, tlist, c_ops, e_ops)
```

where the sol.expect or sol.states contain the lists of expectation values or Qobj instances, respectively, that would be returned by the same solver in QuTiP 1.1.4. With this new API, each solver can optionally store additional information in the return object such as, for example, the collapse times calculated in the Monte Carlo solver.

- 2. The name of the function for Lindblad master equation solver has been changed from odesolve to mesolve. The odesolve function can still be called, however it is officially deprecated, and will be removed in a future release. Being a QuTiP version 1.x function, odesolve does not return an Odedata object.
- 3. The order of the return values of the method Qobj.eigenstates have been swapped, so that the eigenenergies and eigenstates of a Qobj instance op are now returned in the following order:

```
eigvals, eigkets = op.eigenstates()
```

4. Functions for calculating correlations using different solvers have now been consolidated under the functions correlation and correlation_ss, for transient and steady state correlations respectively. Here, the selection of the underlying dynamics solver now is specified

using the optional keyword argument solve that defaults to the Lindblad master equation (mesolve) if it is not explicitly specified. For example:

3. New features

QuTiP 2 includes a wide variety of new computational functions, as well as utility functions for better handling of data. Here we give a brief description the new major features in QuTiP 2.1. For full documentation of these new features, as well as the rest of the QuTiP package, see the QuTiP 2.1 Documentation [2]. Examples illustrating the usage of these functions can be found in Sec. 4.

- Support for time-dependent collapse operators: We have created a new system for representing time-dependent quantum operators used in defining system Hamiltonians and collapse operators for the Lindblad master equation and the Monte Carlo This allows support for arbitrary timedependent collapse operators (the new method is still backwards compatible with the python function callback method used for time-dependent Hamiltonians in QuTiP version 1.1.4). This new method of defining arbitrary time-dependencies is both more efficient and more flexible, allowing for high performance simulations of arbitrary time-dependent quantum systems. In particular, many problems of interest may be compiled at runtime into C code via Cython [3]. This particular feature, and its implementation, will be discussed elsewhere [4].
- Floquet formalism, Floquet-Markov master equation: For periodic time-dependent systems, the Floquet formalism can be a useful technique where the original time-dependent problem is transformed into a time-independent problem using the time-dependent Floquet-modes as the basis set. In QuTiP 2.0 we added a new module for the Floquet-related decomposition of time-dependent problems, and the evolution of unitary and dissipative dynamics using equations of motion and master equations in the Floquet formalism.
- Bloch-Redfield master equation solver: A new quantum dynamics solver for the time evolution according to the Bloch-Redfield master equation is now included in QuTiP. While not as efficient as the Lindblad master equation solver, in situations where the environment is expressed in terms of its noise power spectrum, rather than phenomenological decay and dephasing rates used in the Lindblad formalism, the Bloch-Redfield master equation has significant advantages.

- Quantum Process Tomography: Quantum process tomography (QPT) [5] 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 gives insight into how a given process transforms density matrices, and can be used, for example, to study how noise or other imperfections deteriorate quantum gate operations. Unlike the fidelity or trace distance, that give a single number indicating how far from ideal a gate is, quantum process tomography gives detailed information as to exactly what kind of errors various imperfections and losses introduce.
- Functions for generating random states and matrices: It is now possible to generate random kets, density matrices, Hamiltonians, and Unitary operators. This includes the ability to set the sparsity (density) of the resultant quantum object.
- Support for sparse eigensolvers: The quantum object (Qobj) methods eigenstates, eigenenergies, and groundstate can now use sparse eigensolvers for systems with large Hilbert spaces. This option is not enabled by default, and must be set with the keyword argument sparse.
- New entropy and entanglement functions: Functions for calculating the concurrence, mutual information, and conditional entropy have been added.
- New operator norms: When calculating operator norms, one can now select between the following norms: trace, Frobius, one, and max. The trace norm is chosen by default. For ket and bra vectors, only the L2-norm is available.
- Saving and loading data: Saving and loading of quantum objects and array data is now internally supported by QuTiP. The storage and retrieval of all quantum objects and Odedata objects can be accomplished via the qsave and qload functions, respectively. In order to facilitate the export of QuTiP data to other programs, the file_data_store and file_data_read allow the user to read and write array data, both real and complex, into text files with a wide variety of formatting options.
- Performance improvements: In QuTiP 2.1, numerous performance optimizations have been implemented, including more efficient quantum object creation, significantly faster ptrace implementation, and an improved steadystate solver.
- Unit tests for verification of installation: The installation of QuTiP 2.1 comes with a set of unit tests that can be used to verify that the installation was successful, and that the underlying routines are functioning as expected.

4. Example scripts featuring new functionality

In this section we highlight, via examples, several of the main features added in QuTiP 2.1 and listed in Sec. 3. Although we will demonstrate the use of the new time-dependent evolution framework, a full discussion of this feature is presented elsewhere [4]. The examples listed below, as well as a growing collection of additional demonstrations, can be found on the QuTiP website [2], or run after installing QuTiP using the demos function. For brevity, we do not include the portions of code related to figure generation using the matplotlib framework [6].

4.1. API changes to dynamics solvers

Here we demonstrate using the new Odedata class that is returned by the mcsolve, mesolve, brmesolve, and fmmesolve evolution solvers in QuTiP version 2.1. To better illustrate the API changes, we have recoded the two-qubit gate example from Ref. [1] Sec. (4.1) that is written using the older QuTiP 1.x API. The sections of the script featuring the new API are indicated below:

```
from qutip import *
  = 1.0 * 2 * pi
                    # coupling strength
g1 = 0.75
                    # relaxation rate
g2 = 0.05
                    # dephasing rate
n_{th} = 0.75
                    # bath avg. thermal excitations
T = pi/(4*g)
                    # gate period
# construct Hamiltonian
H = g * (tensor(sigmax(), sigmax()) +
         tensor(sigmay(), sigmay()))
# construct inital state
psi0 = tensor(basis(2,1), basis(2,0))
# construct collapse operators
c_{ops} = []
## qubit 1 collapse operators
sm1 = tensor(sigmam(), qeye(2))
sz1 = tensor(sigmaz(), qeye(2))
c_ops.append(sqrt(g1 * (1+n_th)) * sm1)
{\tt c\_ops.append(sqrt(g1*n\_th)*sm1.dag())}
c_ops.append(sqrt(g2) * sz1)
## qubit 2 collapse operators
sm2 = tensor(qeye(2), sigmam())
sz2 = tensor(qeye(2), sigmaz())
c_{ops.append}(sqrt(g1 * (1+n_th)) * sm2)
c_ops.append(sqrt(g1 * n_th) * sm2.dag())
c_ops.append(sqrt(g2) * sz2)
# evolve the dissipative system
tlist = linspace(0, T, 100)
medata = mesolve(H, psi0, tlist, c_ops, [])
## NEW API CALL ##
# extract density matrices from Odedata object
rho_list = medata.states
# get final density matrix for fidelity comparison
rho_final = rho_list[-1]
# calculate expectation values
n1 = expect(sm1.dag() * sm1, rho_list)
n2 = expect(sm2.dag() * sm2, rho_list)
# calculate the ideal evolution
medata_ideal = mesolve(H, psi0, tlist, [], [])
```

```
## NEW API CALL ##
# extract states from Odedata object
psi_list = medata_ideal.states

# calculate expecttation values
n1_ideal = expect(sm1.dag() * sm1, psi_list)
n2_ideal = expect(sm2.dag() * sm2, psi_list)
# get last ket vector for comparison
psi_ideal = psi_list[-1]
# output is ket since no collapse operators.
rho_ideal = ket2dm(psi_ideal)

# calculate the fidelity of final states
F = fidelity(rho_ideal, rho_final)
```

4.2. Floquet modes of a driven two-level system

Following the example in Ref. [7], here we calculate the quasienergies for the time-dependent Floquet basis vectors of a sinusoidally driven two-level system [8] with Hamiltonian

$$H = \frac{\Delta}{2}\sigma_z + \frac{E}{2}\cos(\omega t)\,\sigma_x,\tag{1}$$

where Δ is the qubit energy splitting and ω is the driving frequency, for different values of the driving amplitude E. The results of the simulation are presented in Fig. 1 .

```
from qutip import *
```

```
delta = 1.0 * 2 * pi # bare qubit sigma_z coefficient
omega = 8.0 * 2 * pi # driving frequency
      = (2*pi)/omega # driving period
# vector of driving amplitudes
E_{vec} = linspace(0.0, 12.0, 100) * omega
# generate spin operators
sx = sigmax()
sz = sigmaz()
# create array for storing energy values
q_energies = zeros((len(E_vec), 2))
# define time-independent Hamiltonian term
HO = delta/2.0 * sz
args = {'w': omega}
# loop over driving amplitudes
for idx. E in enumerate(E vec):
    # amplitude-dependent Hamiltonian term
   H1 = E/2.0 * sx
   # H = H0 + H1 * cos(w * t) in 'list-string' format
   H = [H0, [H1, 'cos(w * t)']]
   # find the Floquet modes
   f_modes, f_energies = floquet_modes(H, T, args)
   # record quasi-energies
    q_energies[idx,:] = f_energies
```

4.3. Floquet Evolution

A driven system that is interacting with its environment is not necessarily well described by the standard Lindblad master equation as its dissipation process could be timedependent due to the driving. In such cases a rigorous

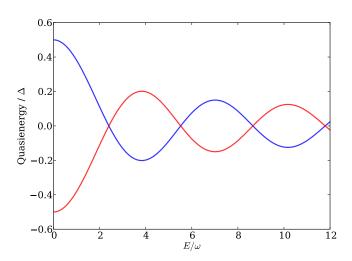


Figure 1: (Color) Quasienergies corresponding to the two Floquet basis states of a driven two-level system as the driving strength is increased. Here the quasienergy and driving amplitude are expressed in units of the qubit energy splitting and driving frequency ($\hbar=1$), respectively. In this simulation, $\Delta=1\times 2\pi$ and $\omega=8\times 2\pi$.

approach would be to take the driving into account when deriving the master equation. This can be done in many different ways, but one common approach is to derive the master equation in the Floquet basis, the Floquet-Markov master equation [9]. In QuTiP, this Floquet-Markov master equation is implemented in the fmmesolve function. As this approach is for time-dependent systems, here we model a sinusoidally driven qubit with Hamiltonian

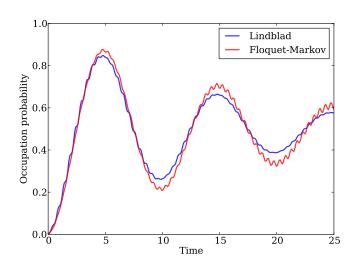
$$H = -\frac{\Delta}{2}\sigma_x - \frac{\epsilon}{2}\sigma_z - A\sigma_x \sin \omega t \tag{2}$$

where Δ and ϵ are the coupling and energy splitting constants, while A and ω are the driving strength and frequency, respectively. In addition, we define the spectral density of the environmental noise to be Ohmic. In Fig. 2 we plot the occupation probability of the qubit for both the Lindblad and Floquet-Markov master equations as a function of time.

from qutip import *

```
gamma1 = 0.05
                      # relaxation rate
gamma2 = 0.0
                      # dephasing rate
delta = 0.0 * 2 * pi # qubit sigma_x coefficient
eps0 = 1.0 * 2 * pi
                      # qubit sigma_z coefficient
      = 0.1 * 2 * pi # driving amplitude
Α
      = 1.0 * 2 * pi # driving frequency
                      # driving period
Т
      = 2*pi / w
psi0 = basis(2,0)
                      # initial state
tlist = linspace(0, 25.0, 250)
def J_cb(omega):
    """ Noise spectral density """
    return 0.5 * gamma1 * omega/(2*pi)
# Hamiltonian in list-string format
args = {'w': w}
```

```
HO = - delta/2.0 * sigmax() - eps0/2.0 * sigmaz()
H1 = - A * sigmax()
H = [H0, [H1, 'sin(w * t)']]
# Lindblad equation with time-dependent Hamiltonian
     = [sqrt(gamma1) * sigmax(),
         sqrt(gamma2) * sigmaz()]
p_ex_me = mesolve(H, psi0, tlist, c_ops,
                  [num(2)], args=args).expect[0]
# Floquet-Markov master equation dynamics
rhs_clear() # clears previous time-dependent Hamiltonian
# find initial Floquet modes and quasienergies
f_modes_0, f_energies = floquet_modes(H, T, args, False)
# precalculate Floquet modes for the first driving period
f_modes_table = floquet_modes_table(f_modes_0, f_energies,
                    linspace(0, T, 500+1), H, T, args)
# solve the Floquet-Markov master equation
rho_list = fmmesolve(H, psi0, tlist, [sigmax()]
                     [], [J_cb], T, args).states
# calculate expectation values in the computational basis
p_ex_fmme = zeros(shape(p_ex_me))
for idx, t in enumerate(tlist):
    f_modes_t = floquet_modes_t_lookup(f_modes_table, t, T)
    p_ex_fmme[idx] = expect(num(2),
```



rho_list[idx].transform(f_modes_t, False))

Figure 2: (Color) Occupation probability of a sinusoidally driven qubit, initially in its ground state, under both Lindblad and Floquet-Markov master equation evolution, where the qubit parameters are $\Delta=0,\,\epsilon=1.0\times 2\pi,$ and the relaxation and dephasing rates are given by $\gamma_1=0.05,\,\gamma_2=0.$ The driving term has amplitude $A=0.1\times 2\pi$ and frequency $\omega=1.0\times 2\pi.$ Here, the spectral noise density of the environment is assumed to be Ohmic.

4.4. Bloch-Redfield master equation

The Lindblad master equation 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. However, a microscopic model can in some cases be advantagous, as for example in systems with varying energy biases and eigenstates that couple to an environment in some well-defined manner, through a physically motivated system-environment interaction operator that can be related to a noise-power spectrum. The Bloch-Redfield formalism is one such approach to derive a master equation from the underlying microscopic physics of the systembath coupling. To highlight the differences inherent in these two approaches, in Fig. 3 we plot the expectation values for the spin-operators of the first qubit in a coupled qubit system given by the Hamiltonian

$$H = \omega_1 \left[\cos \theta_1 \sigma_z^{(1)} + \sin \theta_1 \sigma_x^{(1)} \right]$$

$$+ \omega_2 \left[\cos \theta_2 \sigma_z^{(2)} + \sin \theta_2 \sigma_x^{(2)} \right] + g \sigma_x^{(1)} \sigma_x^{(2)}$$
(3)

with the initial state $|\phi\rangle = |\psi_1\rangle |\psi_2\rangle$ with

$$\begin{aligned} |\psi_1\rangle &= \frac{5}{\sqrt{17}} \left[0.8 \, |0\rangle_{(1)} + (1 - 0.8) \, |1\rangle_{(1)} \right] \\ |\psi_2\rangle &= \frac{5}{\sqrt{17}} \left[(1 - 0.8) \, |0\rangle_{(2)} + 0.8 \, |1\rangle_{(2)} \right]. \end{aligned}$$

where the subscripts indicate which qubit the state belongs to. In Eq. (3), g is the qubit coupling, ω_1 and ω_2 are the qubit frequencies, and finally θ_1 and θ_2 represent the angles of each qubit with respect to the σ_z direction. In this example, the qubit environments in the Bloch-Redfield simulation are assumed to have Ohmic spectrum. The code for the corresponding simulation is given below:

from qutip import *

```
= array([1.0,1.0])*2*pi
                                 # qubit angular frequency
theta = array([0.025,0.0])*2*pi
                                 # angle from sigma_z axis
                                  # qubit relaxation rate
gamma1 = [0.25, 0.35]
gamma2 = [0.0, 0.0]
                                 # qubit dephasing rate
       = 0.1 * 2 * pi
                                  # coupling strength
a = 0.8
psi1 = (a*basis(2,0)+(1-a)*basis(2,1)).unit()
psi2 = ((1-a)*basis(2,0)+a*basis(2,1)).unit()
psi0 = tensor(psi1, psi2)
# times at which to evaluate expectation values
tlist = linspace(0, 15, 500)
# operators for qubit 1
sx1 = tensor(sigmax(), qeye(2))
sy1 = tensor(sigmay(), qeye(2))
sz1 = tensor(sigmaz(), qeye(2))
sm1 = tensor(sigmam(), qeye(2))
# operators for qubit 2
sx2 = tensor(qeye(2), sigmax())
sy2 = tensor(qeye(2), sigmay())
sz2 = tensor(qeye(2), sigmaz())
sm2 = tensor(qeye(2), sigmam())
# Hamiltonian
# qubit 1
H = w[0] * (cos(theta[0]) * sz1 + sin(theta[0]) * sx1)
# qubit 2
H += w[1] * (cos(theta[1]) * sz2 + sin(theta[1]) * sx2)
```

```
# interaction term
H += g * sx1 * sx2
# Lindblad master equation
c_{ops} = []
c_ops.append(sqrt(gamma1[0]) * sm1)
c_ops.append(sqrt(gamma1[1]) * sm2)
lme_results = mesolve(H, psi0, tlist, c_ops,
                      [sx1, sy1, sz1])
# Bloch-Redfield master equation
#
def ohmic_spectrum1(w):
    if w == 0.0:
        # dephasing inducing noise
        return 0.5 * gamma2[0]
        # relaxation inducing noise
        return 0.5 * gamma1[0]*w/(2*pi)*(w > 0.0)
def ohmic_spectrum2(w):
    if w == 0.0:
        # dephasing inducing noise
        return 0.5 * gamma2[1]
        # relaxation inducing noise
        return 0.5 * gamma1[1]*w/(2*pi)*(w > 0.0)
brme_results = brmesolve(H, psi0, tlist, [sx1, sx2],
                 [sx1, sy1, sz1], [ohmic_spectrum1,
                 ohmic_spectrum2])
```

4.5. Quantum process tomography

To demonstrate quantum process tomography, here we simulate the effects of relaxation and dephasing on the two-qubit iSWAP gate [10] when the qubits are coupled to a thermal environment with on average $\langle n \rangle = 1.5$ excitations. The χ -matrix obtained from QPT contains all the information about the dynamics of this open quantum system. In Fig. 4 we plot the χ -matrix for both the dissipative and corresponding ideal (unitary) iSWAP gate dynamics.

```
from qutip import *
g = 1.0 * 2 * pi # coupling strength
g1 = 0.75
                  # relaxation rate
g2 = 0.25
                  # dephasing rate
n_{th} = 1.5
                  # bath avg. thermal excitations
T = pi/(4*g)
                  # gate period
H = g*(tensor(sigmax(),sigmax())+tensor(sigmay(),sigmay()))
psi0 = tensor(basis(2,1), basis(2,0))
c_{ops} = []
# qubit 1 collapse operators
sm1 = tensor(sigmam(), qeye(2))
sz1 = tensor(sigmaz(), qeye(2))
c_ops.append(sqrt(g1 * (1+n_th)) * sm1)
c_ops.append(sqrt(g1 * n_th) * sm1.dag())
c_ops.append(sqrt(g2) * sz1)
# qubit 2 collapse operators
sm2 = tensor(qeye(2), sigmam())
```

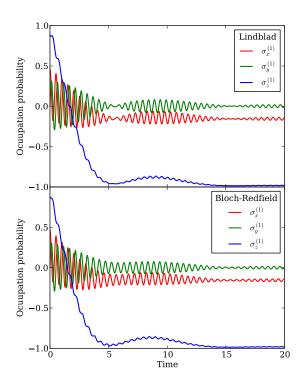


Figure 3: (Color) Expectation values for the spin operators of qubit #1, for both the Lindblad master equation (top) and the Bloch-Redfield master equation (bottom), where the qubit environment in the latter case is assumed to have an Ohmic spectrum. Here, $\omega_1=\omega_2=1.0\times 2\pi, \theta_1=0.025\times 2\pi, \theta_2=0$, and the qubit relaxation terms for qubit #1 and qubit #2 are give by $\gamma_1^{(1)}=0.25$ and $\gamma_1^{(2)}=0.35$, respectively. The qubit coupling is $g=0.05\times 2\pi$. In this simulation, the dephasing terms are assumed to be zero.

```
sz2 = tensor(qeye(2), sigmaz())
c_ops.append(sqrt(g1 * (1+n_th)) * sm2)
c_ops.append(sqrt(g1 * n_th) * sm2.dag())
c_ops.append(sqrt(g2) * sz2)

# process tomography basis
op_basis = [[qeye(2), sigmax(), sigmay(), sigmaz()]] * 2
op_label = [["i", "x", "y", "z"]] * 2

# dissipative gate
U_diss = propagator(H, T, c_ops)
chi = qpt(U_diss, op_basis)
qpt_plot_combined(chi, op_label)

# ideal gate
U_psi = (-1j * H * T).expm()
U_ideal = spre(U_psi) * spost(U_psi.dag())
chi = qpt(U_ideal, op_basis)
qpt_plot_combined(chi, op_label)
```

4.6. Exporting QuTiP data

Finally, we demonstrate the exporting of data generated in QuTiP to an external plotting program using the file_data_store and file_data_read to save and load

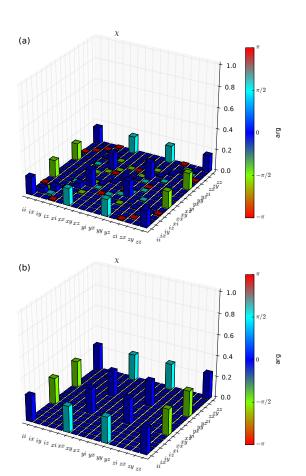


Figure 4: (Color) (a) The QPT process χ -matrix for the dissipative iSWAP gate between two-qubits. Here the color indicates the phase of each matrix element. The qubit-qubit coupling strength is $g=1.0\times 2\pi$, whereas the relaxation and dephasing rates are g1=0.75 and g2=0.25, respectively. (b) The ideal iSWAP gate χ -matrix when the qubit dissipation and dephasing are not present.

the data, respectively. To keep the example completely in Python, we have chosen to use Mayavi [11] to plot a Wigner function in Fig. 5 generated in QuTiP corresponding to the state $|\Psi\rangle = |\alpha\rangle + |-\alpha\rangle + |\tilde{\phi}\rangle$ that is a Schrödinger cat state consisting of two coherent states with complex amplitude α , with an additional random ket vector $|\tilde{\phi}\rangle$ created using QuTiP's random state generator:

```
from qutip import *
# Number of basis states
N = 20
# amplitude of coherent states
alpha = 2.0 + 2.0j
# define ladder operators
a = destroy(N)
# define displacement operators
D1 = displace(N, alpha)
D2 = displace(N, -alpha)
# create superposition of coherent states + random ket
psi = (D1 + D2) * basis(N,0) + 0.5 * rand_ket(N)
psi = psi.unit() # normalize
# calculate Wigner function
xvec = linspace(-5, 5, 500)
vvec = xvec
```

```
W = wigner(psi, xvec, yvec)
## new function calls ##
# store Wigner function to file
file_data_store("wigner.dat", W, numtype='real')
# load input data from file
input_data = file_data_read('wigner.dat')

# plot using mayavi
from mayavi.mlab import *
X,Y = meshgrid(xvec, yvec)
surf(xvec, yvec, input_data, warp_scale='auto')
view(0, 45)
show()
```

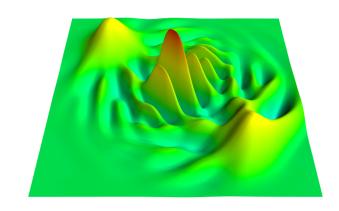


Figure 5: (Color) Wigner function for the state $|\Psi\rangle = |\alpha\rangle + |-\alpha\rangle + |\tilde{\phi}\rangle$ where $\alpha=2+2j$ is the coherent state amplitude, and $|\tilde{\phi}\rangle$ is a randomly generated state vector. This plot is generated in Mayavi using data from the QuTiP wigner function.

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Appendix A. New functions in QuTiP 2.1

Quantum Object Methods

conj Conjugate of quantum object.

eigenenergies Calculates the eigenvalues (eigenenergies if the operator is a Hamiltonian) for a quantum operator. Returns the eigenvalue and eigenstate corresponding to the ground state of the quantum operator. Gives the matrix element $Q_{nm} = \langle \psi_n | \hat{Q} | \psi_m \rangle$ for the given operator and states ψ_n and ψ_m .

tidyup Removes the small elements from a quantum object.

trans Transpose of a quantum object.

Bloch-Redfield Functions

bloch.redfield_solve Evolve the ODEs defined by the Bloch-Redfield tensor.

bloch_redfield_tensor Bloch-Redfield tensor for a set of system-bath operators and corresponding spectral functions.

Floquet Functions

floquet_modes Calculate the initial Floquet modes given a periodic time-dependent Hamiltonian.

floquet_modes_t Calculate the Floquet modes at a time t.

floquet_modes_table Calculate a table of Floquet modes for an interval of times.

floquet_modes_t_lookup Look up the Floquet modes at an arbitrary time t given a pre-computed Floquet-mode table.

floquet_states Calculate the initial Floquet states given a set of Floquet modes.

floquet_states_t

Calculate the Floquet states for an arbitrary time t given a set of Floquet modes.

Decompose an arbitrary state vector in the basis of the given Floquet modes.

 $floquet_wavefunction_t$ Calculate the wavefunction for an arbitrary time t given a Floquet-state decomposition and modes.

Evolution Solvers

brmesolve Bloch-Redfield master equation solver.

fmmesolve Floquet-Markov master equation solver.

Correlation Functions

correlationTransient two-time correlation function.correlation_ssSteady-state two-time correlation function.

Entropy/Entanglement Functions

concurrence Calculate the concurrence entanglement measure for a two-qubit state.

entropy_conditional The conditional entropy S(A|B) = S(A,B) - S(B) of a selected density matrix component. entropy_mutual Mutual information S(A:B) between selection components of a system density matrix.

Quantum Process Tomography

qpt Quantum process tomography χ -matrix for a given (possibly non-unitary) transformation matrix U. qpt-plot Visualize the quantum process tomography χ -matrix. Plot the real and imaginary parts separately.

 χ -matrix plot with height and color corresponding to the absolute value and phase, respectively.

Random State/Operator Generation

Gates

iswap Quantum object representing the iSWAP gate.

 ${\tt sqrtiswap} \qquad \qquad {\tt Quantum\ object\ representing\ the\ square\ root\ } i {\tt SWAP\ gate}.$

 $Utility\ Functions$

qpt_plot_combined

file_data_read Retrieves an array of data from the requested file

file_data_store

qload

Stores a matrix of data to a file to be read by an external program.

Loads quantum object or array data contained from given file.

Saves any quantum object or array data to the specified file.

rhs_generate Pre-compiles the Cython code for time-dependent mesolve problems run inside a parfor loop.

rhs_clear Clears string-format time-dependent Hamiltonian data.

Table A.1: List of new user-accessible functions available in QuTiP 2.1. Additional information about each function may be obtained by calling help(function_name) from the Python command line, or at the QuTiP website [2].

References

- [1] J. R. Johansson, P. D. Nation, F. Nori, Comput. Phys. Commun. 183 (2012) 1760.
- [2] P. D. Nation, J. R. Johansson, QuTiP: Quantum Toolbox in Python, http://code.google.com/p/qutip/, 2011-2012.
- [3] S. Behnel, R. Bradshaw, C. Citro, L. Dalcin, D. Seljebotn, K. Smith, Computing in Science & Engineering 13 (2011) 31.
- J. R. Johansson, P. D. Nation, F. Nori (2013) unpublished.
- [5] M. Mohseni, A. T. Rezakhani, D. A. Lidar, Phys. Rev. A 77 (2008) 032322.
- J. D. Hunter, Computing in Science & Engineering 9 (2007) 90.
- C. E. Creffield, Phys. Rev. B 67 (2003) 165301.
- [8] S. N. Shevchenko, S. Ashhab, F. Nori, Phy. Rep. 492 (2010) 1.
- [9] M. Grifoni, P. Hänggi, Phys. Rep. 304 (1998) 229.
- [10] N. Schuch, J. Siewert, Phys. Rev. A 67 (2003) 032301.
 [11] P. Ramachandran, G. Varoquaux, Computing in Science & Engineering 13 (2011) 40.