QuTiP: Quantum Toolbox in Python

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What is QuTiP?

- Framework for computational quantum dynamics
  - Efficient and easy to use for quantum physicists
  - Thoroughly tested (100+ unit tests)
  - Well documented (200+ pages, 50+ examples)
- Suitable for
  - theoretical work
  - modeling experiments on engineered quantum systems
- 100% open source
- Implemented in Python/Cython using SciPy, Numpy, and matplotlib

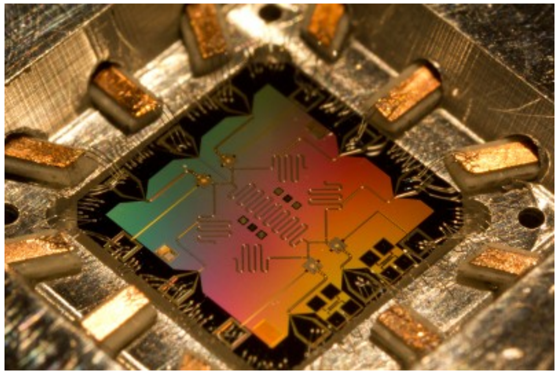
Project information

Authors:	Paul Nation and Robert Johansson
Web site:	http://qutip.googlecode.com
Discussion:	Google group “qutip”
Blog:	http://qutip.blogspot.com
Platforms:	Linux and Mac
License:	GPLv3
Download:	http://code.google.com/p/qutip/downloads
SVN Repository:	https://qutip.googlecode.com/svn/
Publication:	Comp. Phys. Comm. **183**, 1760 (2012)

What can QuTiP be used for?

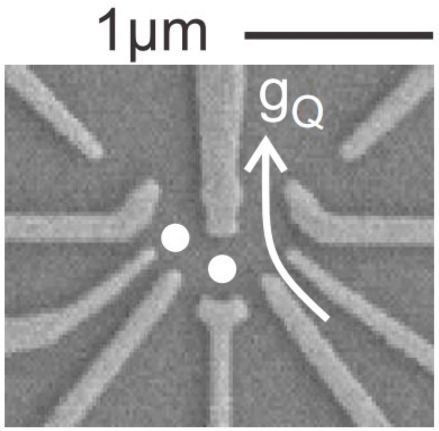
Simulate engineered quantum devices

Superconducting circuits



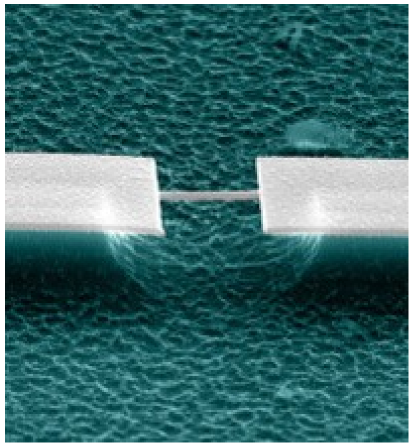
Martinis group at UCSB

Semiconducting circuits



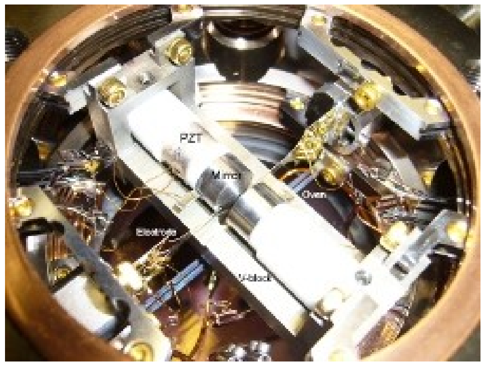
Petta group at at Princeton

Nanomechanical devices



Roukes group at Caltech

Ion traps



Monroe group at Maryland

Quantum mechanics in one slide …

… not as difficult as one might think: It's only linear algebra !

Key concepts	Practical representation
Wavefunction / state: Probability amplitude describing the state of a quantum system.	**Vectors or matrices:** Complex elements, unitary norm/trace.
Hamiltonian / operators: The Hamiltonian is the total energy function of a system, describes the energies of the possible states. Operators represents physical observables, and are used to construct Hamiltonians.	**Matrices:** Hermitian, complex elements, usually sparse.
Equation of motion: Describes how the ***states*** of a system evolve in time for a given ***Hamiltonian.*** Examples: Schrödinger equation, Master equations and Monte-Carlo.	**Ordinary differential equations (ODEs)** Systems of coupled ODEs in matrix form. In general time-dependent. Sometimes including stochastic processes.
Observables and expectation values: Observable physical quantities correspond to operators. Measurement outcomes are "stochastic", expectation values calculated using the wavefunction.	**Inner product** Measurement outcomes are calculated as inner product between state vectors and operator matrices, resulting in a real number for physical observables.

What we want to accomplish with QuTiP

Objectives

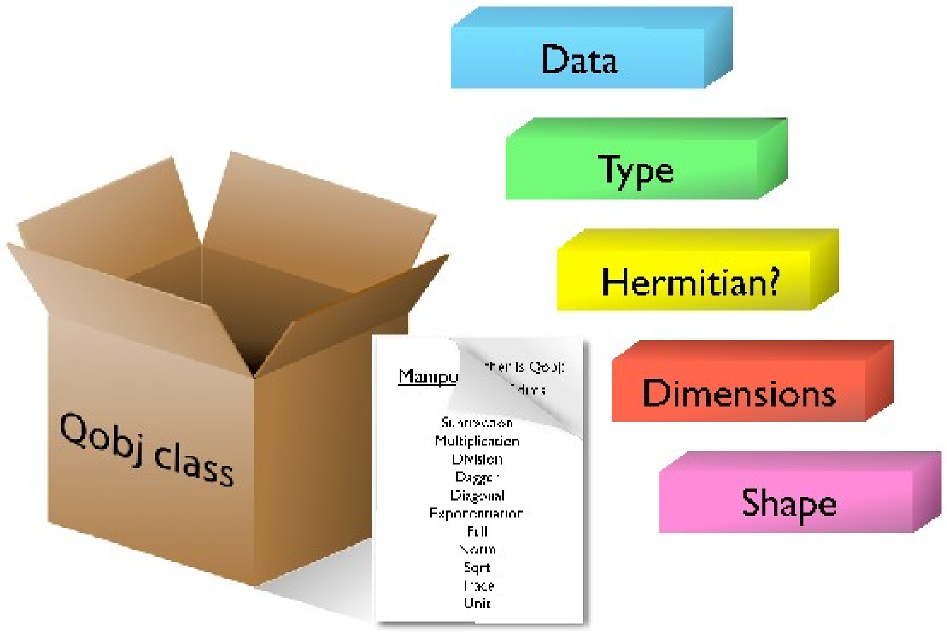
To provide a powerful framework for quantum mechanics that closely resembles the standard mathematical formulation

- Efficient and easy to use
- General framework, able to handle a wide range of different problems

Design and implementation

- Object-oriented design
- Qobj class used to represent quantum objects
  - Operators
  - State vectors
  - Density matrices
- Library of utility functions that operate on Qobj instances

QuTiP core class: Qobj



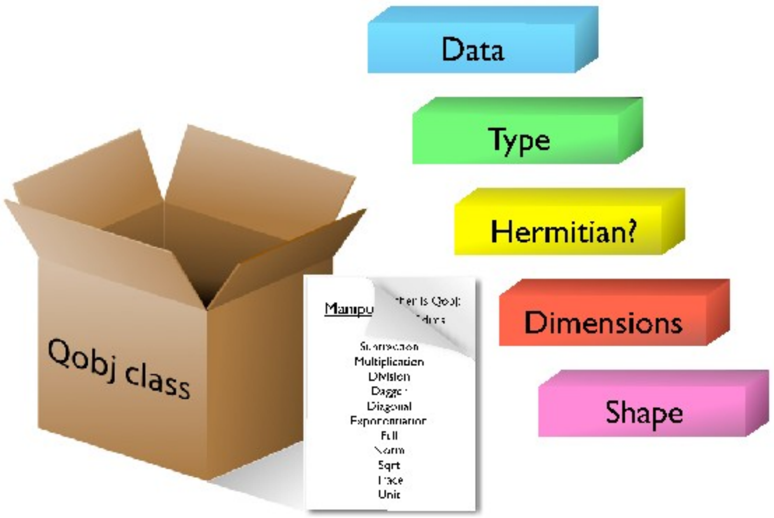
Quantum object class: `Qobj`

Abstract representation of quantum states and operators

- Matrix representation of the object
- Structure of the underlaying state space, Hermiticity, type, etc.
- Methods for performing all common operations on quantum objects:

  `eigs(),dag(),norm(),unit(),expm(),sqrt(),tr(), ...`

- Operator arithmetic with implementations of: +. -, *, ...



Example: built-in operator $\hat{\sigma}_x$

```
>>> sigmax()

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

Example: built-in state $|\alpha = 0.5\rangle$

```
>>> coherent(5, 0.5)

Quantum object: dims = [[5], [1]], shape = [5, 1], type = ket
Qobj data =
[[ 0.88249693]
 [ 0.44124785]
 [ 0.15601245]
 [ 0.04496584]
 [ 0.01173405]]
```

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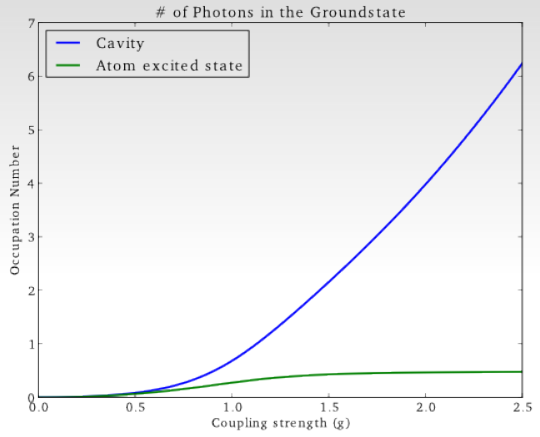

Calculating using Qobj instances

Basic operations

```
# operator arithmetic
>> H = 2 * sigmaz() + 0.5 * sigmax()

Quantum object: dims = [[2], [2]],
shape = [2, 2], type = oper, isHerm = True
Qobj data =
[[ 2.   0.5]
 [ 0.5 -2. ]]

# superposition states
>> psi = (basis(2,0) + basis(2,1))/sqrt(2)

Quantum object: dims = [[2], [1]],
shape = [2, 1], type = ket
Qobj data =
[[ 0.70710678]
 [ 0.70710678]]


# expectation values
>> expect(num(2), psi)

0.4999999999999999

>> N = 25
>> psi = (coherent(N,1) + coherent(N,3)).unit()
>> expect(num(N), psi)

4.761589143572134
```

Composite systems

```
# operators
>> sx = sigmax()
Quantum object: dims = [[2], [2]],
shape = [2, 2], type = oper, isHerm = True
Qobj data =
[[ 0.  1.]
 [ 1.  0.]]

>> sxsx = tensor([sx,sx])
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.]]

# states
>> psi_a = fock(2,1); psi_b = fock(2,0)
>> psi = tensor([psi_a, psi_b])
Quantum object: dims = [[2, 2], [1, 1]],
shape = [4, 1], type = ket
Qobj data =
[[ 0.]
 [ 1.]
 [ 0.]
 [ 0.]]

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

Basis transformations

```
# eigenstates and values for a Hamiltonian
>> H = sigmax()
>> evals, evecs = H.eigenstates()
>> evals

array([-1.,  1.])

>> evecs

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)

# transform an operator to the eigenbasis of H
>> sx_eb = sigmax().transform(evecs)

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

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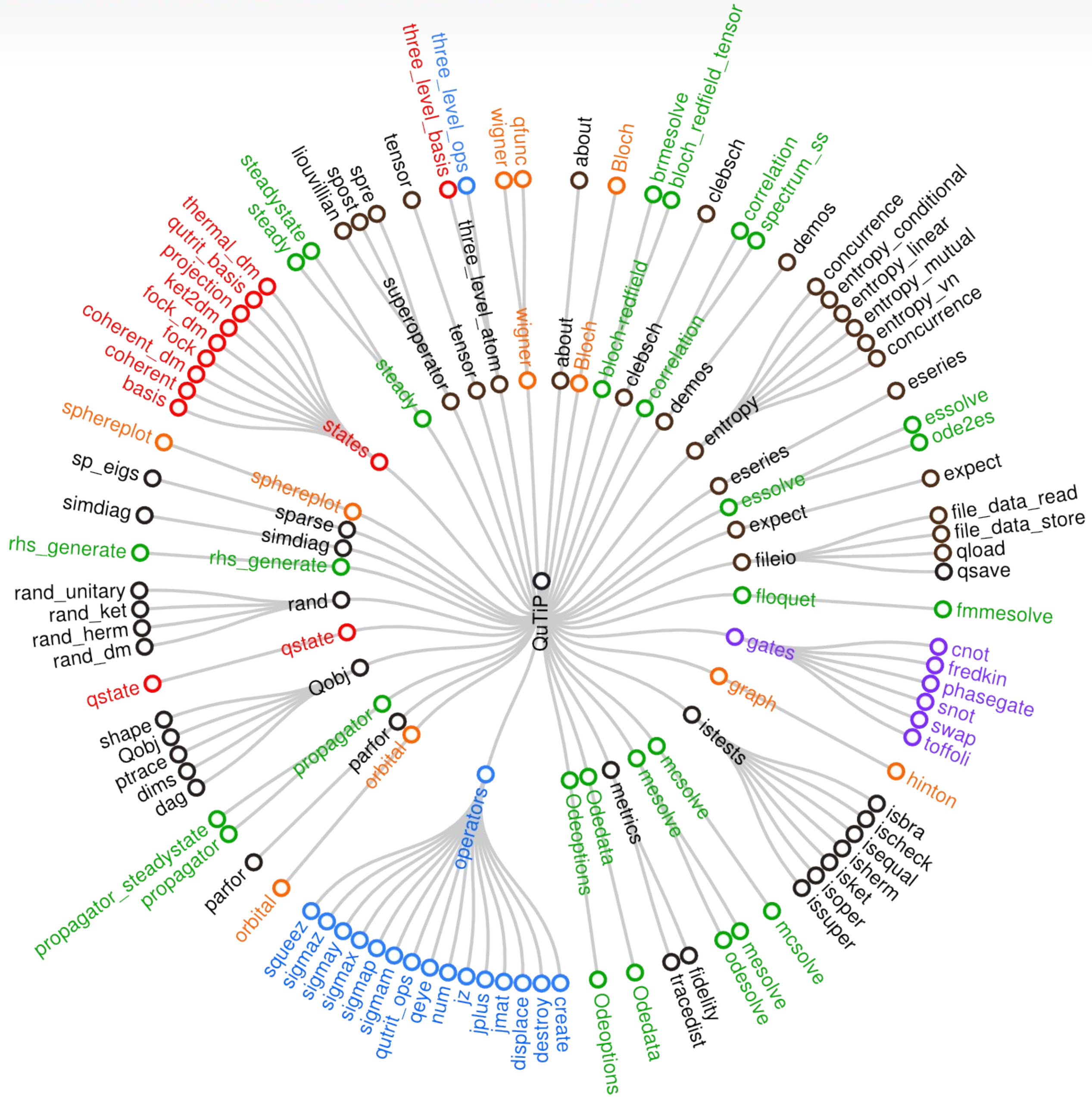
The Quantum Toolbox in Python

Organization

- States
- Operators
- Time evolution
- Visualization
- Gates
- Core/Utility functions



Evolution of quantum systems

The main use of QuTiP is quantum evolution. A number of solvers are available.

Typical simulation workflow:

i. Define parameters that characterize the system

ii. Create Qobj instances for operators and states

iii. Create Hamiltonian, initial state and collapse operators, if any

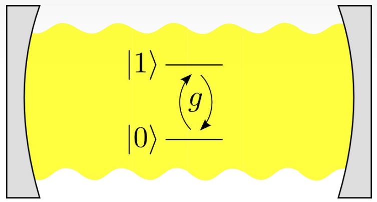
iv. Choose a solver and evolve the system

v. Post-process, visualize the data, etc.

Available evolution solvers:

- Unitary evolution: Schrödinger and von Neumann equations
- Lindblad master equations
- Monte-Carlo quantum trajectory method
- Bloch-Redfield master equation
- Floquet-Markov master equation
- Propagators

Example: Jaynes-Cummings model



(a two-level atom in a cavity)

Mathematical formulation:

Hamiltonian

$$\hat{H} = \hbar\omega_c \hat{a}^\dagger \hat{a} - \frac{\hbar\omega_q}{2}\hat{\sigma}_z + \frac{\hbar g}{2}\left(\hat{a}\hat{\sigma}_+ + \hat{a}^\dagger\hat{\sigma}_-\right)$$

Initial state

$$|\psi(t=0)\rangle = |1\rangle_c \otimes |0\rangle_q$$

Time evolution

$$\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

Expectation values

$$\langle \hat{a}^\dagger \hat{a}\rangle = \langle\psi(t)|\,\hat{a}^\dagger\hat{a}\,|\psi(t)\rangle$$

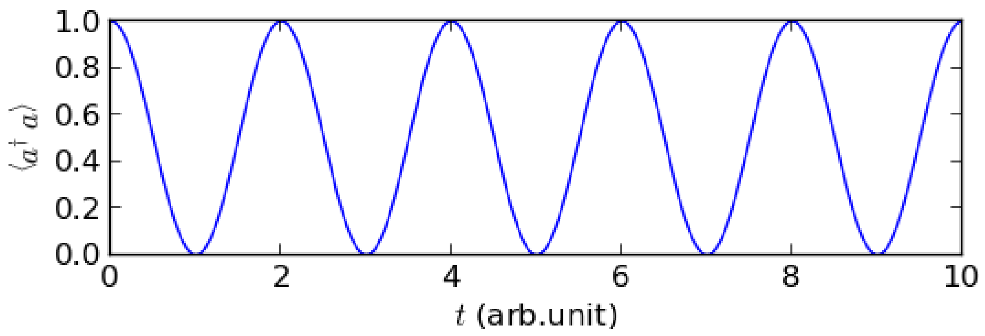
QuTiP code:

```
from qutip import *
N  = 10

a  = tensor(destroy(N),qeye(2))
sz = tensor(qeye(N),sigmaz())
s  = tensor(qeye(N),destroy(2))
wc = wq = 1.0 * 2 * pi
g  = 0.5 * 2 * pi
H  = wc * a.dag() * a - 0.5 * wq * sz + \
     0.5 * g * (a * s.dag() + a.dag() * s)
psi0  = tensor(basis(N,0), basis(2,0))
tlist = linspace(0, 10, 100)
out   = mesolve(H, psi0, tlist, [], [a.dag()*a])

from pylab import *
plot(tlist, out.expect[0])
show()
```

Qobj instances



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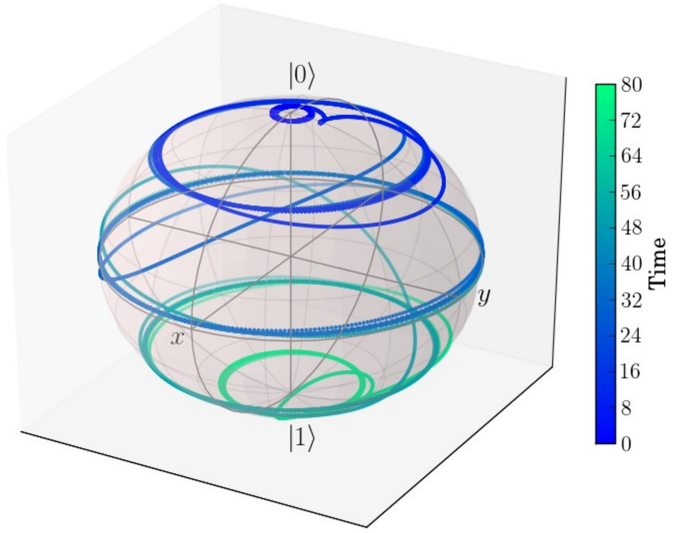
The Quantum Toolbox in Python

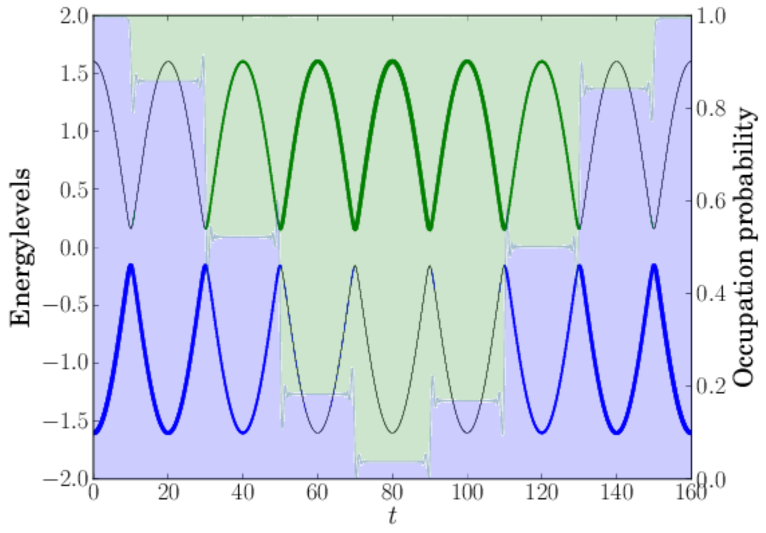
Example: time-dependence

Multiple Landau-Zener transitions

$$\hat{H}(t) = -\frac{\Delta}{2}\hat{\sigma}_z - \frac{\epsilon}{2}\hat{\sigma}_x - A\cos(\omega t)\hat{\sigma}_z$$

```
from qutip import *

# Parameters
epsilon = 0.0
delta = 1.0

# Initial state: start in ground state
psi0 = basis(2,0)

# Hamiltonian
H0 = - delta * sigmaz() - epsilon * sigmax()
H1 = - sigmaz()
h_t = [H0, [H1, 'A * cos(w*t)']]
args = {'A': 10.017, 'w': 0.025*2*pi}

# No dissipation
c_ops = []

# Expectation values
e_ops = [sigmax(), sigmay(), sigmaz()]

# Evolve the system
tlist = linspace(0, 160, 500)
output = mesolve(h_t, psi0, tlist, c_ops, e_ops, args)

# Process and plot result
# ...
```





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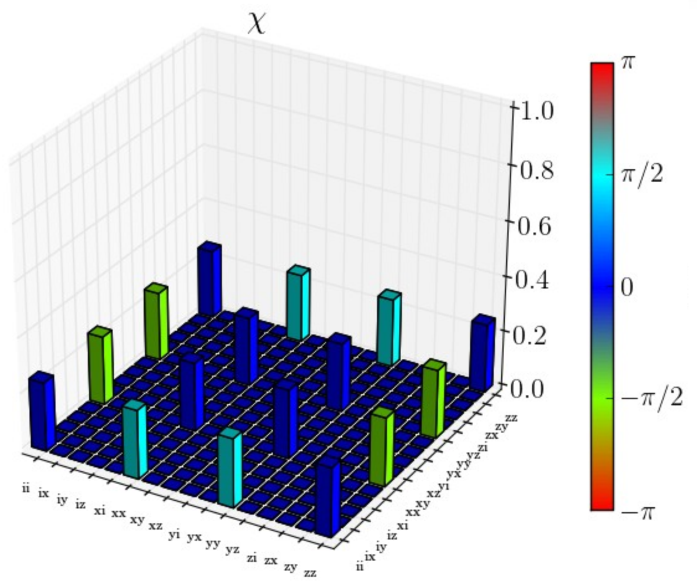
Example: open quantum system

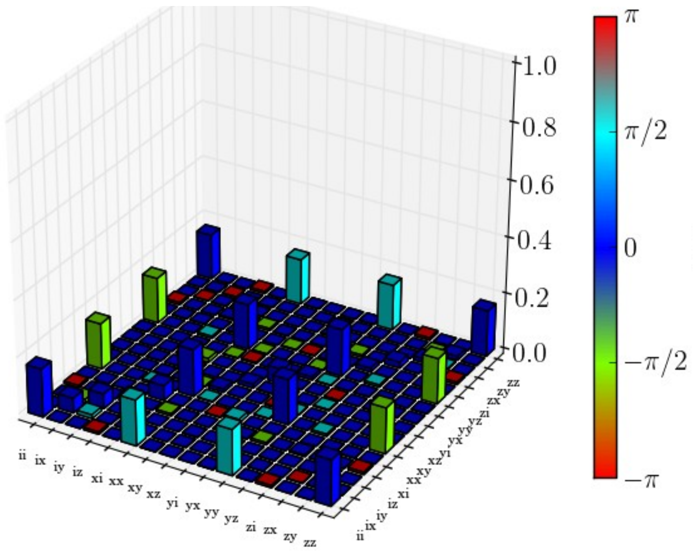
Dissipative two-qubit iSWAP gate

$$\hat{H} = g\left(\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y\right),\ t \in [0, T = \pi/4g]$$

Collapse operators

```
from qutip import *

g = 1.0 * 2 * pi # coupling strength
g1 = 0.75        # relaxation rate
g2 = 0.25        # dephasing rate
n_th = 1.5       # environment temperature
T = pi/(4*g)

H = g * (tensor(sigmax(), sigmax()) + tensor(sigmay(), sigmay()))

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())
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)

U = propagator(H, T, c_ops)

qpt_plot(qpt(U, op_basis), op_labels)
```





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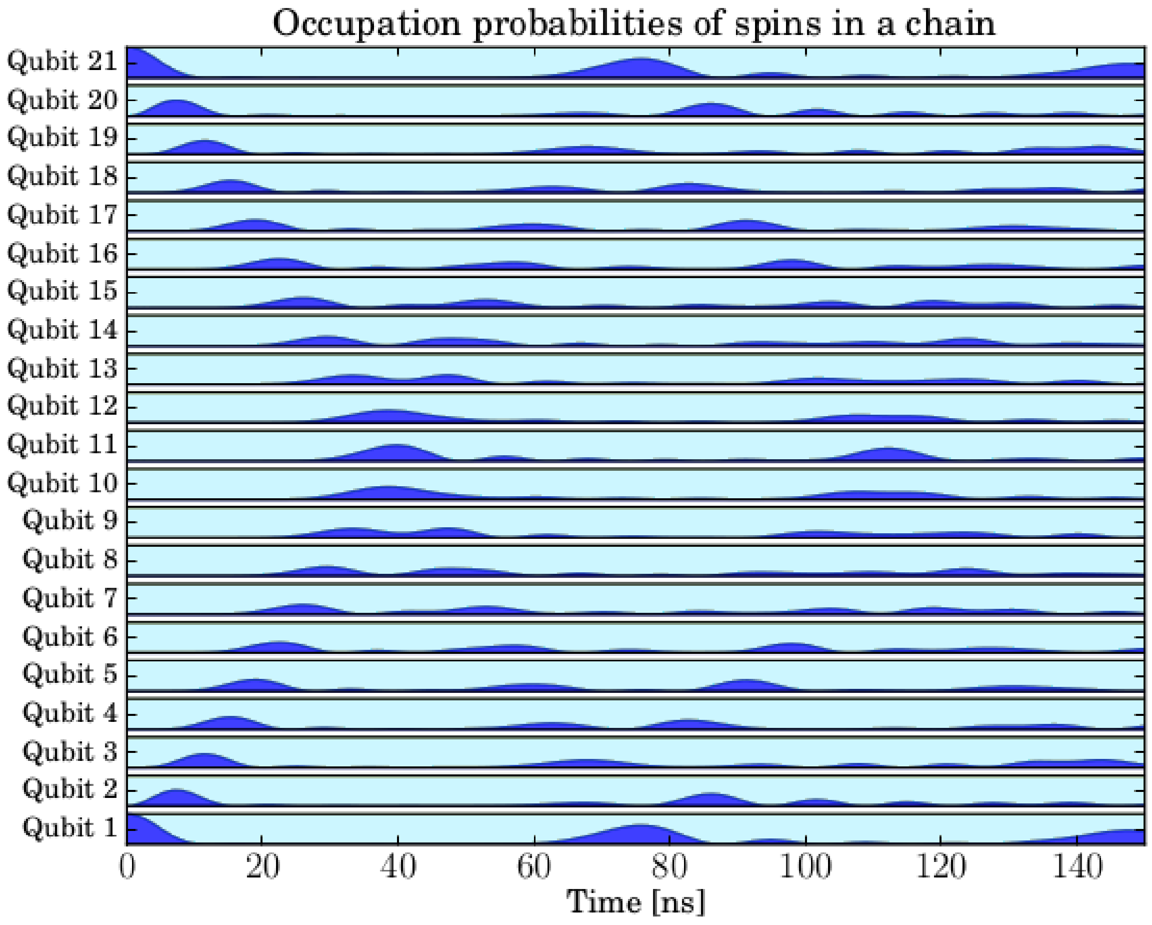
The Quantum Toolbox in Python

Advanced example

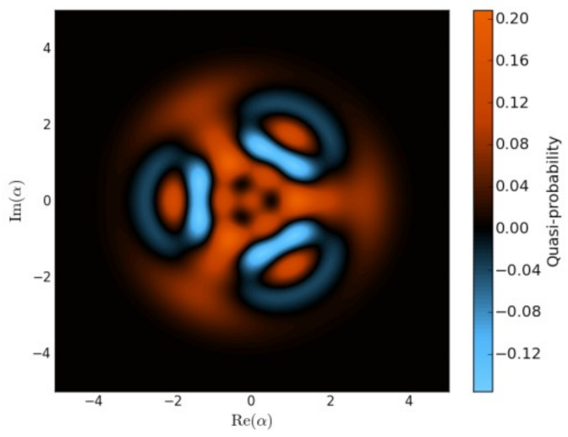
- *21 spin-½ with nearest-neighbor interaction*
- *~40 lines of code*
- *2’097’152 basis states*
- *simulation time: ~7 hours*

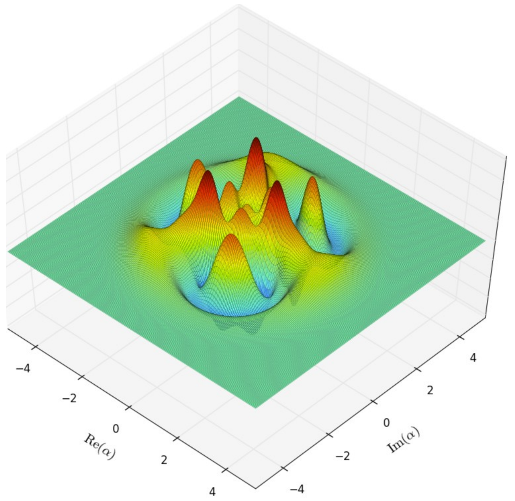


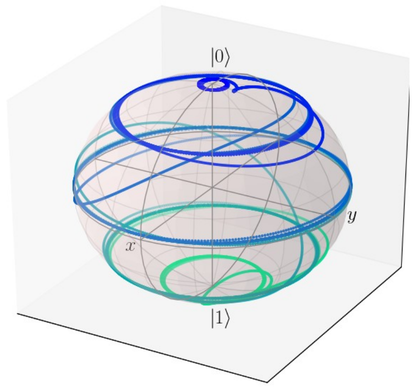
```python
from qutip import *

def system_ops(N, h, J, gamma):
    # pre-compute operators
    si = qeye(2); sx = sigmax(); sz = sigmaz()
    sx_list = []; sz_list = []
    for n in range(N):
        op_list = [si for m in range(N)]
        op_list[n] = sx
        sx_list.append(tensor(op_list))
        op_list[n] = sz
        sz_list.append(tensor(op_list))
    # construct the hamiltonian
    H = 0
    for n in range(N):   # energy splitting terms
        H += - 0.5 * h[n] * sz_list[n]
    for n in range(N-1): # interaction terms
        H += - 0.5 * J[n] * sx_list[n] * sx_list[n+1]

    # collapse operators for spin dephasing
    c_op_list = []
    for n in range(N):
        if gamma[n] > 0.0:
            c_op_list.append(sqrt(gamma[n]) * sz_list[n])

    # initial state
    # first and last spin in state |1>, rest in state |0>
    psi_list = [basis(2,0) for n in range(N-2)]
    psi_list.insert(0, basis(2,1)) # first
    psi_list.append(basis(2,1))    # last
    psi0 = tensor(psi_list)
    return H, c_op_list, sz_list, psi0

N = 21                         # number of spins
h =  1.0 * 2 * pi * ones(N)    # energy splittings
J = 0.05 * 2 * pi * ones(N)    # coupling
gamma = 0.0 * ones(N)          # dephasing rate

# pre-compute operators
H, c_ops, e_ops, psi0 = system_ops(N, h, J, gamma)

# evolve
tlist = linspace(0, 150, 150)
output = mesolve(H, psi0, tlist, c_ops, e_ops)
sn_expt = (1 - array(output.expect))/2.0

# post-process and plot ...
```

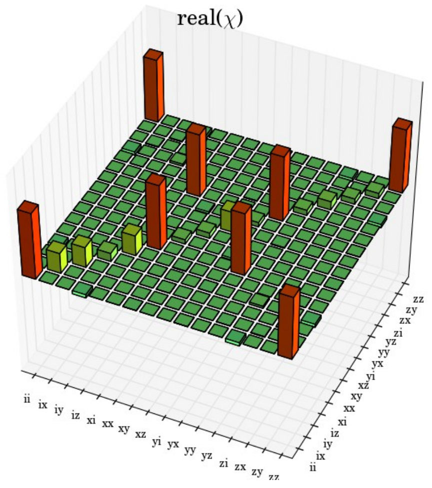
Visualization

- Objectives of visualization in quantum mechanics:
  - Visualize the composition of complex quantum states (superpositions and statistical mixtures).
  - Distinguish between quantum and classical states. Example: Wigner function.
- In QuTiP:
  - Wigner and Q functions, Bloch spheres, process tomography, ...
  - *most common visualization techniques used in quantum mechanics are implemented*









What do we use to implement QuTiP?

- Python core language and the *multiprocessing package*
- *Numpy* and *Scipy*
  - Sparse matrix library in Scipy
  - ODE solve in Scipy
- *Matplotlib*
  - With custom functions for performing many common visualizations for quantum systems, e.g. plotting Wigner distributions, Bloch sphere representations
- *Cython*
  - For various optimizations, most notably for faster sparse-matrix-vector multiplication and for evaluating the derivative callback function for the Scipy ODE solver
  - Dynamic generation and compilation of Cython code using a home-brewed code generator for time-dependent ODE callback functions

QuTiP2

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Parallelization with multiprocessing package

- Many tasks in QuTiP can be parallelized:
  - Quantum Monte-Carlo: solving and averaging over many ODEs for trajectories with stochastic quantum jumps
  - In applications, we typically need to repeat calculations over a range or grid of parameters
- In QuTiP we use a `parfor` function to parallelize such tasks on multicore machines.
  - `parfor` is implemented using the Python multiprocessing standard package
  - Powerful and very easy-to-use interface for parallel computations

```
#
# example use of parfor in QuTiP
#

def task(args):

    rank, param = args
    # compute ...
    return [rank, result]

param_list = linspace(0, 10, 100)
result_list = parfor(task, enumerate(param_list))
```

Optimizations using Cython

- Significant performance gains by replacing our Python callback functions for the SciPy ODE solver with Cython implementations
- Problem with this approach:
  - our ODE callback functions are dynamically generated from our abstract quantum object representation, and can in general be time-dependent.
  - The ODE RHS cannot be represented by a static Cython RHS function for general time-dependent problems

Example use of Cython in QuTiP

```
# ---------------------------------------------------------------------------
# cython code
@cython.boundscheck(False)
@cython.wraparound(False)
def cyq_ode_rhs(double t, np.ndarray[CTYPE_t, ndim=1] rho, np.ndarray[CTYPE_t,
ndim=1] data, np.ndarray[int] idx,np.ndarray[int] ptr):
    cdef int row, jj, row_start, row_end
    cdef int nrows=len(rho)
    cdef CTYPE_t dot
    cdef np.ndarray[CTYPE_t, ndim=2] out = np.zeros((nrows,1),dtype=np.complex)
    for row from 0 <= row < nrows:
        dot = 0.0
        row_start = ptr[row]
        row_end = ptr[row+1]
        for jj from row_start <= jj < row_end:
            dot = dot + data[jj] * rho[idx[jj]]
        out[row,0] = dot
    return out


# ---------------------------------------------------------------------------
# python code: from mesolve function, for time-independent Hamiltonian
...
initial_vector = psi0.full()
r = scipy.integrate.ode(cyq_ode_rhs)
L = -1.0j * H
r.set_f_params(L.data.data, L.data.indices, L.data.indptr)
r.set_integrator('zvode', method=opt.method, order=opt.order, ...)
r.set_initial_value(initial_vector, tlist[0])
...
```

Optimizations using Cython

- Significant performance gains by replacing our Python callback functions for the SciPy ODE solver with Cython implementations
- Solution:
  - Dynamically generate, compile and load Cython code for the ODE RHS

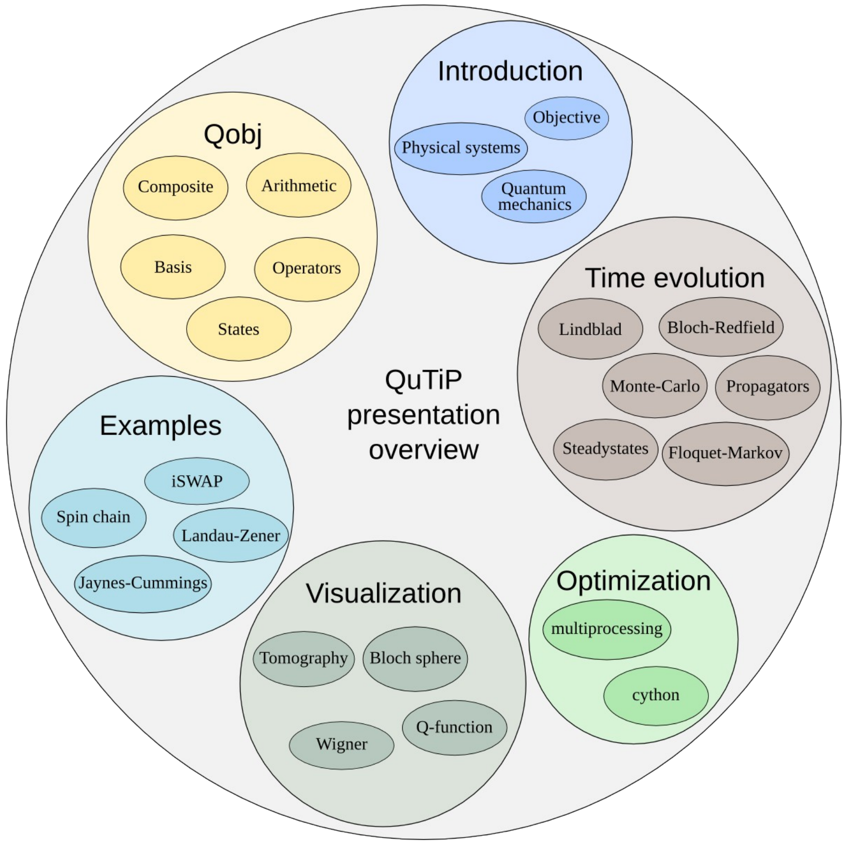
Example use of Cython in QuTiP

```
# --------------------------------------------------------------------------
# python code: from mesolve function, for time-dependent Hamiltonian
...
# code generator
if not opt.rhs_reuse:
    odeconfig.tdname="rhs"+str(odeconfig.cgen_num)
    cgen=Codegen(h_terms=n_L_terms,h_tdterms=Lcoeff, args=args)
    cgen.generate(odeconfig.tdname+".pyx")
    os.environ['CFLAGS'] = '-O3 -w'
    import pyximport
    pyximport.install(setup_args={'include_dirs':[numpy.get_include()]})
    code = compile('from '+odeconfig.tdname+' import cyq_td_ode_rhs', 
'<string>', 'exec')
    exec(code, globals())
    odeconfig.tdfunc=cyq_td_ode_rhs

# setup integrator
initial_vector = mat2vec(rho0.full())
r = scipy.integrate.ode(odeconfig.tdfunc)
r.set_integrator('zvode', method=opt.method, order=opt.order,
                          atol=opt.atol, rtol=opt.rtol, nsteps=opt.nsteps,
                          first_step=opt.first_step, min_step=opt.min_step,
                          max_step=opt.max_step)
r.set_initial_value(initial_vector, tlist[0])
code = compile('r.set_f_params('+string+')', '<string>', 'exec')
exec(code)

r.set_initial_value(initial_vector, tlist[0])
...
```

Summary

More info at:
http://qutip.googlecode.com

- QuTiP: framework for numerical simulations of quantum systems
  - Generic framework for representing quantum states and operators
  - Large number of dynamics solvers
- Main strengths:
  - Ease of use: complex quantum systems can programmed rapidly and intuitively
  - Flexibility: Can be used to solve a wide variety of problems
  - Performance: Near C-code performance due to use of Cython for time-critical functions
- Future developments:
  - OpenCL? Stochastic master equations? Non-markovian master equations?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