QuTiP: Quantum Toolbox in Python

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QuTiP is open-source software for simulating the dynamics of closed and open quantum systems. It uses the excellent Numpy, Scipy, and Cython packages as numerical backends, and graphical output is provided by Matplotlib. QuTiP aims to provide user-friendly and efficient numerical simulations of a wide variety of quantum mechanical problems, including those with Hamiltonians and/or collapse operators with arbitrary time-dependence, commonly found in a wide range of physics applications. QuTiP is freely available for use and/or modification, and it can be used on all Unix-based platforms and on Windows. Being free of any licensing fees, QuTiP is ideal for exploring quantum mechanics in research as well as in the classroom.

Paper references

- J. R. Johansson, P. D. Nation, and F. Nori, *Comp. Phys. Comm.* **183**, 1760 (2012)
- J. R. Johansson, P. D. Nation, and F. Nori, Comp. Phys. Comm. 184, 1234 (2013)

https://qutip.org

Supporting Organizations

QuTiP is currently supported by these organizations:











QuTiP is proud to be affiliated to:





The development of QuTiP was partially supported by the following organizations:

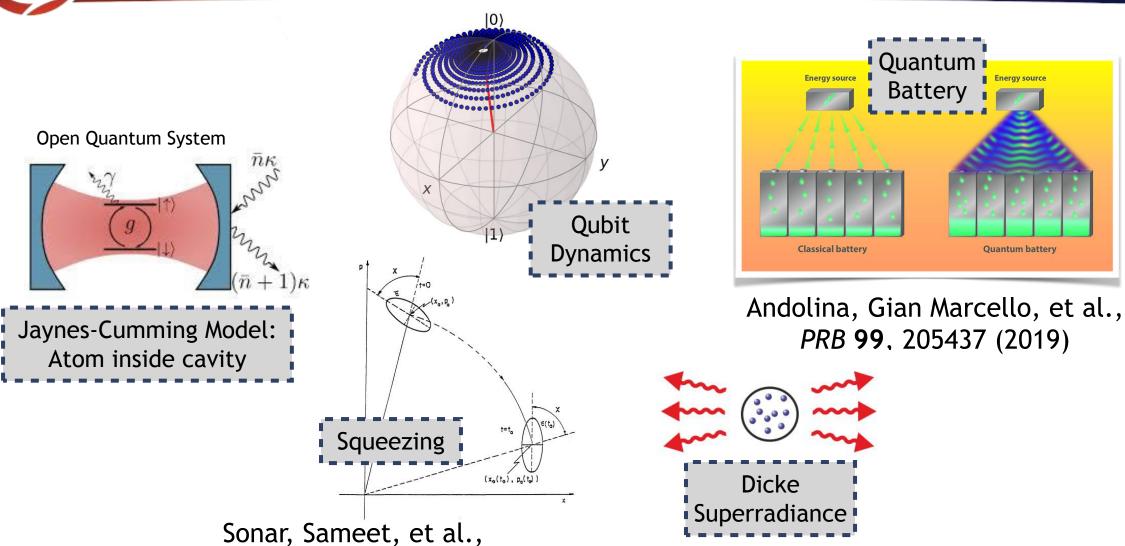






What can be simulated in QuTiP

PRL 120, 163601 (2018)



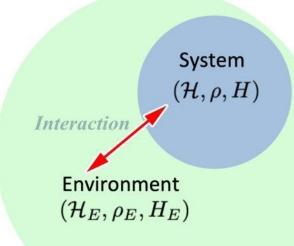


Master equation approach

Open Quantum System

American Journal of Physics

Total System $(\mathcal{H}_T, \rho_T, H_T)$



The evolution of density operator of system ho(t)

BLISH WITH US
$$\frac{i}{h}$$
 [LEGUT, γ) (MORE FROM ARTCY, $\rho(t)C_n^{\dagger} - \rho(t)C_n^{\dagger}C_n^{\dagger} - C_n^{\dagger}C_n^{\dagger}\rho(t)$]

therspoon

updates

288-297 (2002)

Article history @ 1119/1.1445404

Expectation value of the operator

$$\partial_t \rho(t)$$
 $\rho(t)$ $\langle A \rangle = \text{Tr}[A \rho(t)]$

tions of

wed. These are the wavefunction.

ntegral, phase space, density matrix, second quantization, variational, pilot wave, and

cobi formulations. Also mentioned are the many-worlds and transactional interpretations.

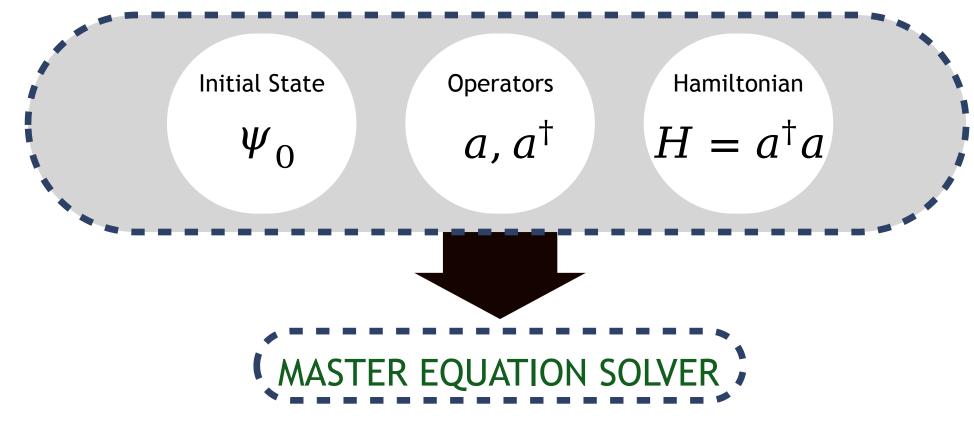
ormulations differ dramatically in mathematical and conceptual overview, yet each one

A total system (belonging to a Hilbert space \mathcal{H}_T , with states described by density matrices ρ_T , and with dynamics determined by a Hamiltonian H_T) divided into the system of interest, "system," and the environment.

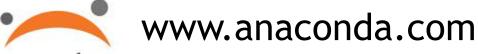
makes identical predictions for all experimental results.



Basic input for QuTiP



$$\dot{\rho}(t) = -\frac{i}{\hbar} [H(t), \rho(t)] + \sum_{n=1}^{\infty} \left[2C_n \rho(t) C_n^{\dagger} - \rho(t) C_n^{\dagger} C_n - C_n^{\dagger} C_n \rho(t) \right]$$

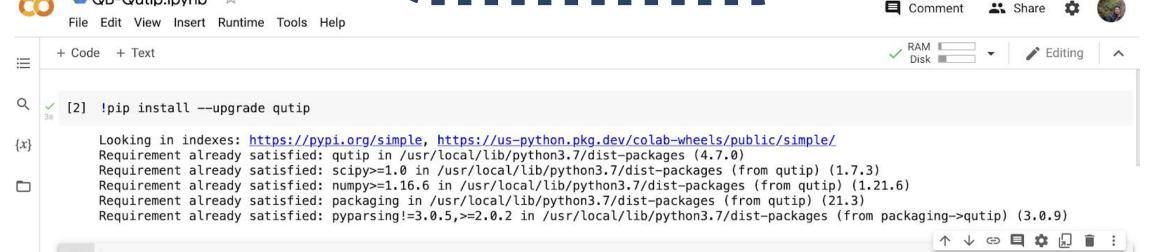




QB-Qutip.ipynb

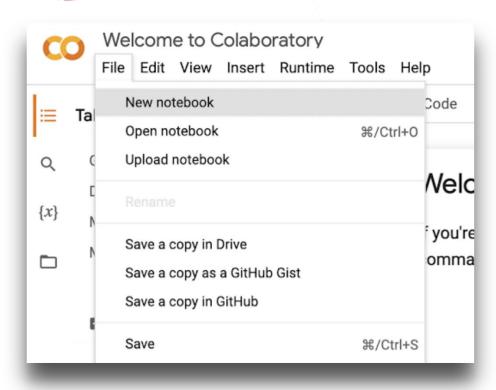


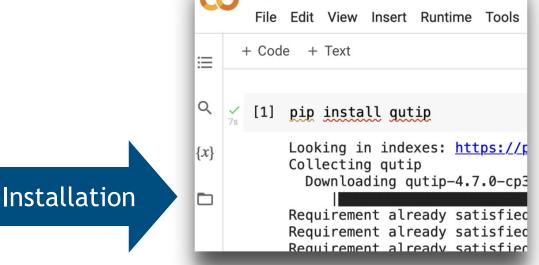
colab.research.google.com



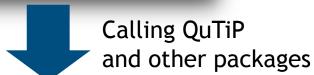


QuTiP with Google Colab





Qutip.ipynb



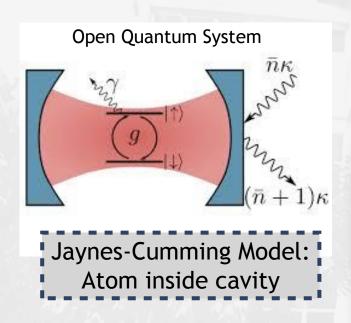


colab.research.google.com

```
[2] %matplotlib inline
  import matplotlib.pyplot as plt
  import numpy as np
  # make qutip available in the rest of the notebook
  from qutip import *
```



Let us simulate a quantum system!



$$H = \underbrace{\omega_0 a^{\dagger} a}_{\text{Cavity}} + \underbrace{\omega_0 \sigma^{+} \sigma^{-}}_{\text{Atom}} + \underbrace{g(a^{\dagger} \sigma^{-} + a \sigma^{+})}_{\text{Interaction}}$$

```
N = 4 #number of bases for cavity photon w0 = 1 g = 0.5 vac = tensor(basis(N,0),basis(2,0))# the vacuum state for the system <math>a = tensor(destroy(N),qeye(2))# the annihilation operator for cavity photon <math>sm = tensor(qeye(N),destroy(2))# the annihilation operator for atom (2 levels system)
```

Since our system is a composite system made of **cavity photon** and atom, the operators and state are given by tensor product.

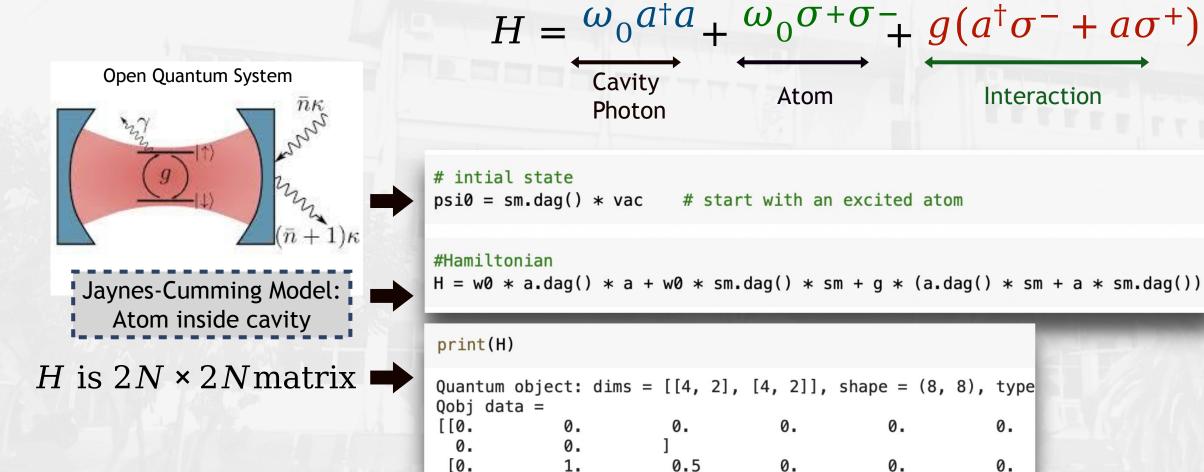


Let us simulate a quantum system! (2)

0.

0.

0.



0.5

[0.



Let us simulate a quantum system! (3)

H.eigenstates()
gives the energy
and wave function



Let us simulate a quantum system! (4)

- expect(a.dag()*a,psi0),expect(sm.dag()*sm,psi0)
 (0.0, 1.0)
- expect(a.dag()*a,state)
 array([0., 0.5, 1.5, 0.5, 2.5, 1.5, 2.5, 3.])
- expect(sm.dag()*sm,state)
 array([0., 0.5, 0.5, 0.5, 0.5, 0.5, 1.])

Expect (O, ψ) gives expectation value of operator O for state ψ

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle$$

Let us evolve the system with time!

$$\dot{\rho}(t) = -\frac{i}{\hbar} [H(t), \rho(t)]$$

$$\langle \hat{O} \rangle = \text{Tr} \left(\hat{O} \rho(t) \right)$$

tlist = np.linspace(0,25,101)

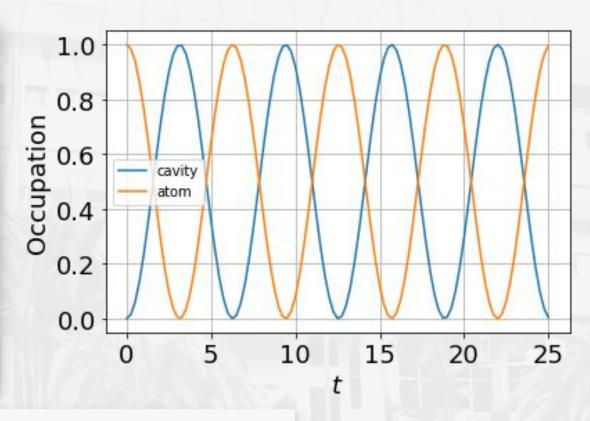
Operators whose expectation values we want to consider

```
output = sesolve(H, psi0, tlist, [a.dag() * a, sm.dag() * sm])
```



Let us simulate a quantum system! (5)

```
n_c = output.expect[0]
n_a = output.expect[1]
fig = plt.figure()
axes = fig.add_subplot(111)
axes.plot(tlist, n_c ,label='cavity')
axes.plot(tlist, n_a, label='atom')
axes.legend(loc=0)
plt.xlabel('$t$',size = 18)
plt.ylabel( 'Occupation', size = 18)
plt.tick_params( labelsize = 18 )
plt.grid()
plt.show()
```



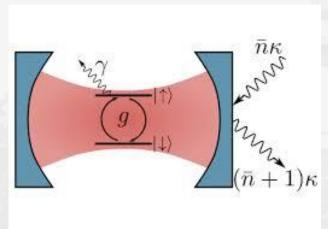
```
output = sesolve(H, psi0, tlist, [a.dag() * a, sm.dag() * sm])
```

output.expect gives an array of expectation values



Let us simulate a quantum system! (6)

Let us add environment!



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

Interaction with environment appears in the collapse operator C_n To decay to the environment, collapse operators are $\sqrt{\kappa}a$ and $\sqrt{\gamma}\sigma^-$

```
kappa = 0.005  # cavity dissipation rate
gamma = 0.05  # atom dissipation rate

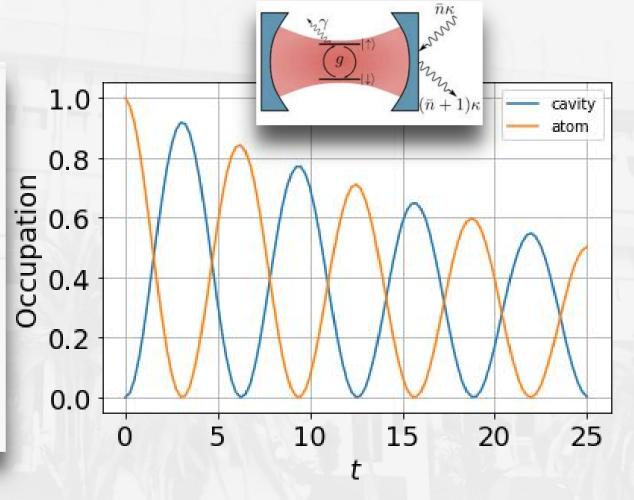
c_ops = [np.sqrt(kappa)*a,np.sqrt(gamma)*sm] #consider only decay in both atom and cavity
outputdecay = mesolve(H, psi0, tlist, c_ops, [a.dag() * a, sm.dag() * sm])
```

Here, we use mesolve, instead of sesolve



Let us simulate a quantum system! (7)

```
n_ce = outputdecay.expect[0]
n_ae = outputdecay.expect[1]
fig = plt.figure()
axes = fig.add_subplot(111)
axes.plot(tlist, n_ce ,label='cavity')
axes.plot(tlist, n_ae, label='atom')
axes.legend(loc=0)
plt.xlabel('$t$',size = 18)
plt.ylabel( 'Occupation', size = 18)
plt.tick_params( labelsize = 18 )
plt.grid()
plt.show()
```





Let us simulate a quantum system! (8)

Can we obtain the density matrix $\rho(t)$? Yes!

```
vac = tensor(basis(N,0),basis(2,0));
a = tensor(destroy(N),qeye(2))#the ;
sm = tensor(qeye(N),destroy(2))#the
```

We can do partial trace

```
(outputdensity.states[100]).ptrace(0)#partial trace for rho_cavity
(outputdensity.states[100]).ptrace(0)#partial trace for rho_atom
```

$$ho_{\text{cav}} = \text{Tr}_{\text{atom}}[\rho(t)]$$

$$ho_{\text{atom}} = \text{Tr}_{\text{cav}}[\rho(t)]$$



Plotting energy levels

Jaynes-Cumming Model:
Atom inside cavity

$$H = \omega_0 a^{\dagger} a + \omega_0 \sigma^{+} \sigma^{-} + g(a^{\dagger} \sigma^{-} + a \sigma^{+})$$

```
def energy(gg):
    i = 0
    en = np.zeros((len(gg),N*2))
    for k in gg:
        # evaluate the Hamiltonian
        H = w0 * a.dag() * a + w0 * sm.dag() * sm + k * (a.dag() * sm + a * sm.dag())
        ener, ekets = H.eigenstates()
        en[i,:] = np.real(ener)
        i += 1

return en

fig = plt.figure()
```

plt.grid()

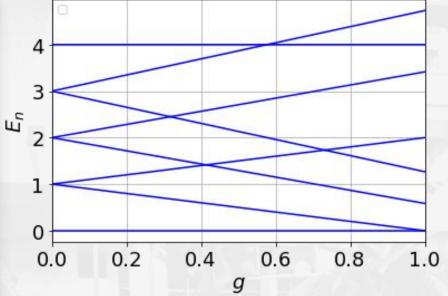
plt.show()

plt.xlim([0,1])

plt.ylabel('\$E_n\$',size = 18)
plt.tick_params(labelsize = 18)

```
axes = fig.add_subplot(111)
for n in [0,1,2,3,4,5,6,7]:
    axes.plot(gg, output_energy[:,n] , 'b')
axes.legend(loc=0)
plt.xlabel('$g$',size = 18)
```



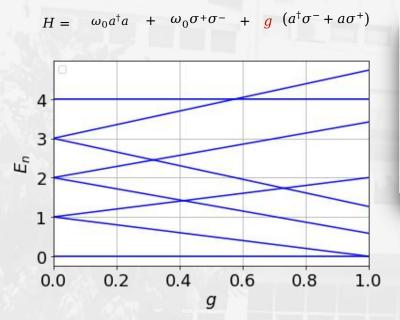




Plotting energy levels (2)



How to understand the eigenstate of each level?



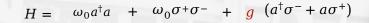
```
g = 0
   Takes first
H = w0 * a.dag() * a + 1*w0 * sm.dag() * sm + 0 * (a.dag() * sm + a * sm.dag())
ener, ekets = H.eigenstates()
ener
array([0., 1., 1., 2., 2., 3., 3., 4.])
                                                   print(ekets[4])
            print(ekets[0])
                                 print(ekets[1])
                                Quantum object:
                                                   Quantum object:
            Quantum object:
                                                    Qobj data =
            Qobi data =
                                Qobj data =
                                                    [[0.]
                                 [[0.]
            [[1.]
                      |0,g\rangle
 n = 0
                                                     [0.]
             [0.]
                      |0,e\rangle
                                  [1.]
                                  [0.]
                                                     [0.]
             [0.]
                                                     [0.]
                                  [0.]
             [0.]
                                                     [1.]
             [0.]
                                  [0.]
                                                     [0.]
                                  [0.]
             [0.]
             [0.]
[0.]]
                      |3,g\rangle
                                  [0.]
                                                     [0.]
 n = 3
                      |3,e\rangle
                                  [0.]]
                                                     [0.]]
                                   |0,e\rangle
               |0,g\rangle
                                                        |2,g\rangle
```

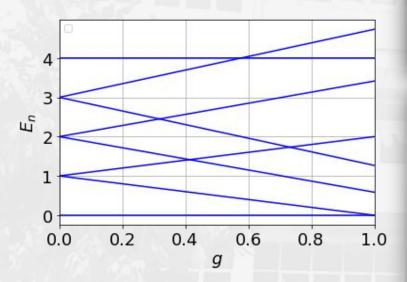


Plotting energy levels (3)



How to understand the eigenstate of each level?





Now, we q = 1

ener

array([0.00000000e+00, 1.11022302e-15, 5.85786438e-01, 1.26794919e+00, 2.00000000e+00, 3.41421356e+00, 4.00000000e+00, 4.73205081e+00])

print(ekets[1])

[0.

print(ekets[3])

print(ekets[6])

Quantum object:

Qobj data =

[[0.]

[0.]

[0.]

[0.]

[0.]

[0.]

[0.]

[1.]

$$\frac{1}{\sqrt{2}}(|0,e\rangle - |1,g\rangle) \quad \frac{1}{\sqrt{2}}(|2,e\rangle - |3,g\rangle)$$

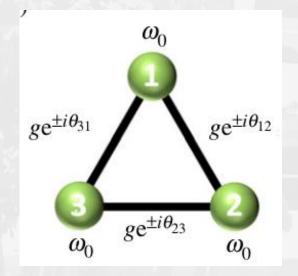
$$|3,e\rangle$$



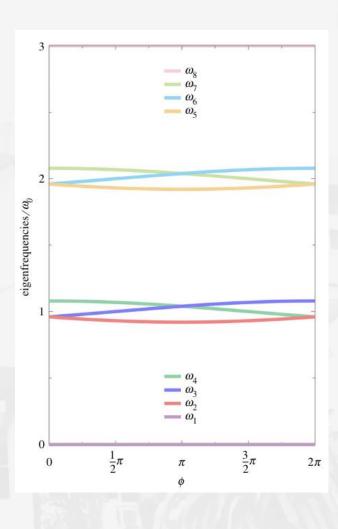
Exercise (1)

Two level system in triangular structure

$$\begin{split} H &= \omega_0 \big(\sigma_1^{\dagger} \sigma_1 + \sigma_2^{\dagger} \sigma_2 + \sigma_3^{\dagger} \sigma_3 \big) \\ &+ g \big(e^{i\theta_{12}} \sigma_1^{\dagger} \sigma_2 + e^{i\theta_{23}} \sigma_2^{\dagger} \sigma_3 + e^{i\theta_{31}} \sigma_3^{\dagger} \sigma_1 + h. \, c. \big) \end{split}$$



$$\phi = \theta_{12} + \theta_{23} + \theta_{31}$$
$$g = \frac{\omega_0}{25}$$

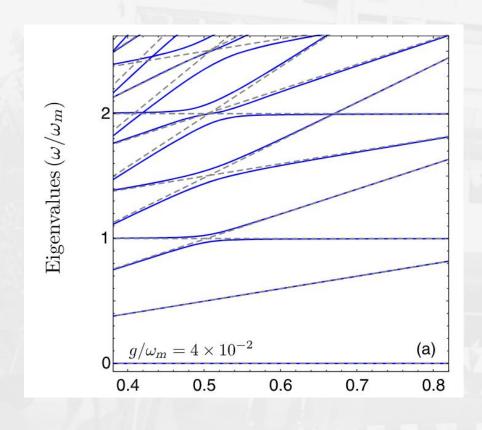


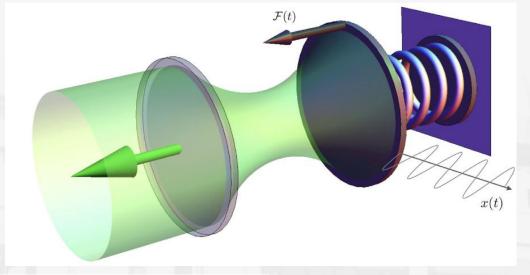
Downing, C. A., & Zueco, D. (2021). Non-reciprocal population dynamics in a quantum trimer. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **477**(2255).

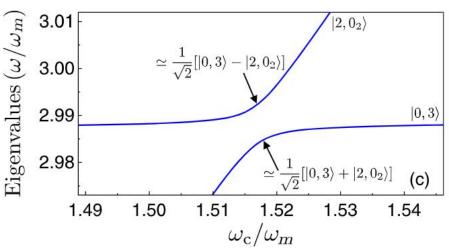


Exercise (2)

Dynamical Casimir effect





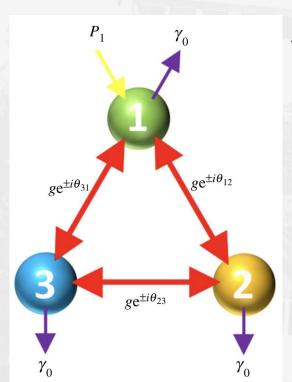


Macrì, V., Ridolfo, A., di Stefano, O., Kockum, A. F., Nori, F., & Savasta, S. (2018). Nonperturbative Dynamical Casimir Effect in Optomechanical Systems: Vacuum Casimir-Rabi Splittings. *Physical Review X*, 8(1), 11031

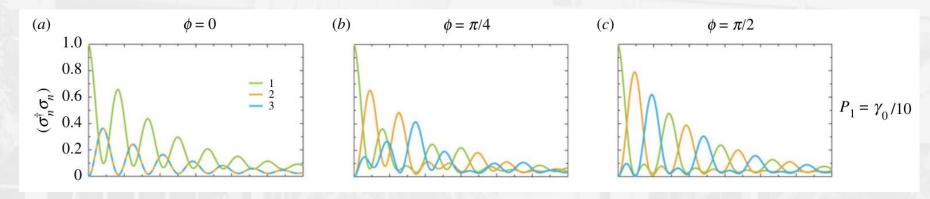


Exercise (3)

Two level system in triangular structure



$$\begin{split} H &= \omega_0 \big(\sigma_1{}^\dagger \sigma_1 + \sigma_2{}^\dagger \sigma_2 + \sigma_3{}^\dagger \sigma_3 \big) \\ &+ g \big(e^{i\theta_{12}} \sigma_1{}^\dagger \sigma_2 + e^{i\theta_{23}} \sigma_2{}^\dagger \sigma_3 + e^{i\theta_{31}} \sigma_3{}^\dagger \sigma_1 + h.c. \big) \end{split}$$



 $g = 5\gamma_0$ Initial state: Particle 1 is excited

Downing, C. A., & Zueco, D. (2021). Non-reciprocal population dynamics in a quantum trimer. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **477**(2255).



Quantum Battery

"Quantum-mechanical systems that can store energy"

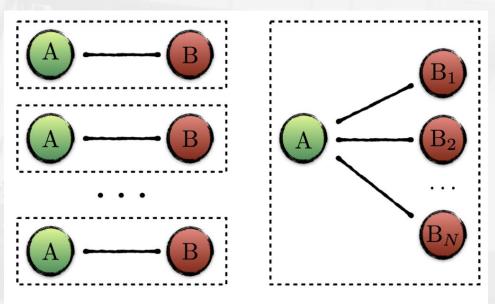


FIG. 1. A sketch of the parallel (left) versus collective (right) charging schemes.

Collective charging gives faster charging which scales with number of B

Andolina, G. M, et al. (2019). Quantum versus classical many-body batteries. Phys. Rev. B, 99(20), 1-7.



Quantum Battery: Spin Battery



N-Qubits of charger
$$H_A = \omega_0 \left(J_z^{(a)} + \frac{N}{2} \right)$$

$$Interaction between A and B$$

$$H_1 = 4g \left(J_x^{(a)} J_x^{(b)} + J_y^{(a)} J_y^{(b)} \right)$$

Interaction

$$H_1 = 4g \left(J_x^{(a)} J_x^{(b)} + J_y^{(a)} J_y^{(b)} \right)$$



N-Qubits of battery
$$H_B = \omega_0 \left(J_z^{(b)} + \frac{N}{2} \right)$$

Collective spin operator with length N/2

$$J_z = \sum_{i=1}^{N} \sigma_z^{(i)}$$

Spin of each qubit

Figure of merit:

$$E_{\rm B}^{(N)}(\tau)\!\equiv\!{\rm Tr}[H_{\rm B}\rho_{\rm B}(\tau)]$$

$$P_{\mathrm{B}}^{(N)}(\tau) = \frac{E_{\mathrm{B}}^{(N)}}{\tau}$$

Total energy stored at batteries

Charging power

Let us simulate it with QuTiP!

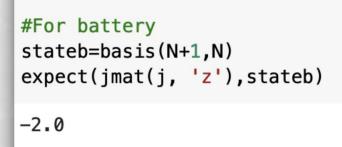


Quantum Battery: Spin Battery (2)

State	Real	In QuTiP
	All chargers are excited states	All spins in A are spin-up
	All batteries are ground states	All spins in B are spin-down

#For charger statea=basis(N+1,0) expect(jmat(j, 'z'),statea)

2.0







Collective spin operator with length N/2

$$J_z = \sum_{i=1}^{N} \sigma_z^{(i)}$$

$$\bot Spin of each qubit$$

jmat(N/2, 'z')
psi0=tensor(basis(N+1,0),basis(N+1,N))
the initial state for the system



Quantum Battery: Spin Battery (3)

```
N = 4 #number of qubits
w0 = 1
j = N/2.0 #length of the collective spin
g = 0.5

psi0 = tensor(basis(N+1,0), basis(N+1,N))# the initial state for the system
Jza = tensor(jmat(j, 'z'), qeye(N+1))
Jzb = tensor(qeye(N+1), jmat(j, 'z'))
Jxa = tensor(jmat(j, 'x'), qeye(N+1))
Jxb = tensor(qeye(N+1), jmat(j, 'x'))
Jya = tensor(jmat(j, 'y'), qeye(N+1))
Jyb = tensor(qeye(N+1), jmat(j, 'y'))
Jpa = tensor(jmat(j, '+'), qeye(N+1))
```

```
HA = w0 * (Jza+N/2)

HB = w0 * (Jzb+N/2)

HI = 4 * g * (Jxa*Jxb +Jya*Jyb)

H = HA + HB + HI
```

$$\omega_0 = 1$$

```
tlist = np.linspace(1e-5,20,301)

output = sesolve(H, psi0, tlist, e_ops=[HB])
```

$$E_{\rm B}^{(N)}(au)\!\equiv\!{
m Tr}[H_{\rm B}
ho_{\rm B}(au)]$$
 Total Energy at B



Quantum Battery: Spin Battery (4)

