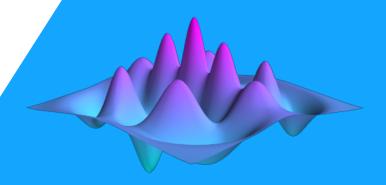
### Make your code count

Quantum simulations and collaborative code

Shahnawaz Ahmed



QuTiP:
The Quantum Toolbox in
Python

#### About me

2016

### sahmed.in

2019	PhD @Applied Quantum Physics, Chalmers University of Technology, Sweden Anton Fisk Kockum, Prof. Göran Johansson	Quantum simulations, Machine Learning
2018	Master's thesis @Theoretical Quantum Physics Lab Riken, Japan Mauro Cirio, Neill Lambert, Prof. Franco Nori	Spin-boson model Ultrastrong coupling
2017	Intern @Theoretical Quantum Physics Lab Riken, Japan Nathan Shammah, Clemens Gneiting, Prof. Franco Nori	Deep Learning  Collective effects in large spin systems
2016	Intern @Google Summer of Code	Diffusion Imaging

Ariel Rokem, Eric Peterson, Rafael Henriques

Diffusion Imaging



## Do you guys put "Quantum" in everything?

- Ant-man and the Wasp (2018)

- Quantum Machine Learning
- Quantum Big Data
- Quantum Neural Networks
- Quantum Cryptography
- Quantum Sensing (GPS)
- Quantum Internet





Wallenberg
Center for
Quantum
Technologies





quantumcomputingreport.com

#### Interests @ FOSDEM19

Photonic quantum computing

Standardization and availability of code

Spin systems, quantum annealing

Hybrid quantum classical algorithms

Optimization and control

NISQ - Noisy intermediate scale quantum

Quantum circuits

Cloud quantum computing

### Quantum physics simulator

Photonic quantum computing

Standardization and availability of code



Spin systems, quantum annealing

Hybrid quantum classical algorithms



Optimization and control

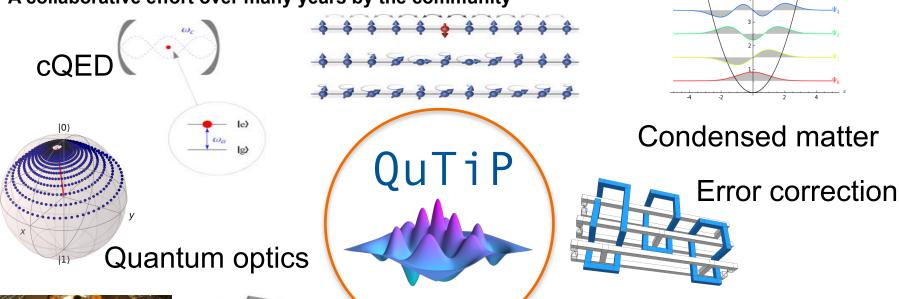
NISQ - Noisy intermediate scale quantum

Quantum circuits

Cloud quantum computing

### Quantum physics simulator

A collaborative effort over many years by the community







 $\hat{b}, \omega_{\mathrm{m}}, \Gamma_{\mathrm{m}}$   $\hat{a}, \omega_{\mathrm{c}}$ 

and more ...

Optomechanics

Superconducting circuits

### QuTiP: features at a glance

#### The Quantum Toolbox in Python



#### **Built with Python**

Python's **straightforward syntax** allows for constructing, manipulating, and evolving quantum objects using QuTiP with just a few lines of code. QuTiP is the ideal toolbox for research or the classroom.



#### **Built-in solvers**

A variety of built-in solvers allow the study of **dynamical simulations** and steady-state analysis. In addition to Lindblad and Monte Carlo solvers, QuTiP offers advanced routines for Bloch-Redfield and Floquet formalism, and non-Markovian systems.



#### Ad-hoc visualization tools

From Bloch spheres to nonlinear colormaps for Wigner functions, QuTIP includes a host of **built-in visualization** routines that help bring data to life, including through animations and 3D graphics.



#### **Custom algorithms**

QuTiP can determine if an operator is Hermitian without performing the conjugate transpose. This is just one of many custom algorithms devised to **maximize performance**. Sparse matrices deployment efficiently manipulates large datasets.



#### C++ performance

A wide range of time-dependent evolution simulations can be runtime compiled into C++ behind the scenes using Cython. The ease of use of Python is boosted by **compiled code**.



#### Independent testing

QuTiP is thoroughly tested, both by its thousands of users, and by a large collection of **built-in test scripts** independently run by Travis Cl. Over a thousand such tests help cover nearly all of the built-in functions, continuously running in development.



#### Fast

QuTiP is capable of leveraging the multiprocessing power inside every modern computer. QuTiP can take advantage of the Python multiprocessing library, OPENMP, SSE3 processor extensions, and Intel MKL.



#### **Experimental Data**

If you need to construct a function from a data set, QuTiP allows for passing interpolating functions as time-dependent arguments to the evolution solvers, also runtime compiling into C++.



#### User friendly

No software should be a black box to the user, especially in science. Qu'TiP includes hundreds of pages of **documentation**, a multitude of **tutorial** Jupyter notebooks, and a friendly community of users who help answer questions.

### Open source quantum (2016 - )

2016 2016 2016 2016 2016	QETLAB Liquil> Quantum Fog Qubiter IBM Q Experience	Matlab F# Python Python	University of Waterloo, Canada Microsoft Artiste-qb Artiste-qb IBM
2017 2017 2017 2017 2017	ProjectQ Forest (QUIL) QISKit Quantum Optics.jl PsiQuaSP	Python Python Python Julia C++.	ETH Zurich Rigetti IBM Universität Innsbruck Gegg M, Richter M
2018 2018 2018 2018 2018	Strawberry Fields Quantum Dev Kit QCGPU NetKet OpenFermion	Python Q#. Rust, OpenCl C++ Python	Xanadu, Canada Microsoft Adam Kelly The Simons Foundation Google, Harvard, UMich, ETH

https://github.com/markf94/os\_quantum\_software

#### **QuTiP - IMPACT**





Modern Optics

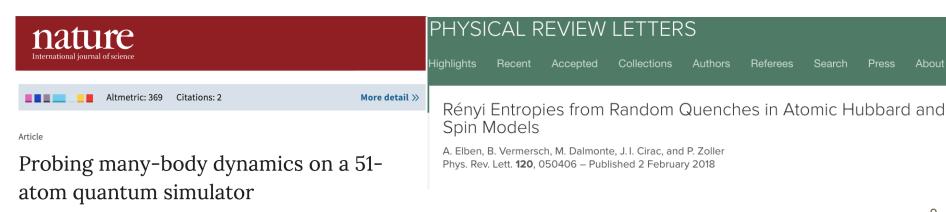




**Economist** 



#### **EDUCATION • INDUSTRY** RESEARCH



About

#### Open source

**Impact** 

Easier to understand and develop an idea with good code and implementation, wider visibility and impact. (eg., PIQS)

Reproducibility

Faster reproduction of results and application to new problems, data and ideas. (eg., SciNet, Neural ODE, QGAN)

Collaborations and feedback

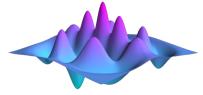
Combine efforts and expertise of a wide range of people without barriers. Get feedback, bug reports, suggestions from users.

Paper to production

Stable software implementations can be converted to applications faster. (eg., Tensor Flow, PyTorch, Scikit-learn)

#### Talk outline





### Open source

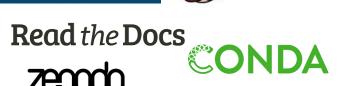






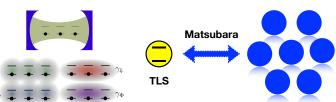


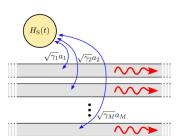






- Open source?
- **GSoC 2019**

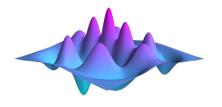






- Quantum
- QuTiP intro
- Whats new?

### Quantum physics A brief introduction

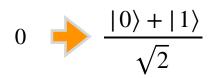


#### **QuBits**

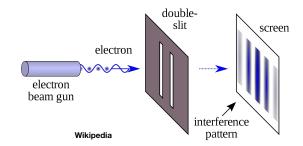
### Superposition

Why?

Quantum mechanics describes realities in terms of probability wave functions.



**Double slit (electrons)** 



Associate wave-like nature to electrons.

Probability wave function to describe states.



**Waves interfere** 

### **QuBits**

### Superposition

Why?

$$0 \quad \stackrel{|0\rangle + |1\rangle}{\sqrt{2}}$$

Quantum mechanics describes realities in terms of probability wave functions.

Wave amplitudes add up

One of the most successful theories out there.

The experiments!

Shut up and calculate

Dr. Dan Russell, Grad. Prog. Acoustics, Penn State

#### QuBits

### **Exponential power of** quantum superpositions!(?)

Three qubits can be a superposition of all eight possibilities



One shot application of a function to all possible data. Seemingly massive parallelization!

Explore all possibilities simultaneously.

$$N \sim 2^N$$

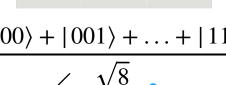
 $|000\rangle + |001\rangle + ... + |111\rangle$ 

0

0

But we see only 1s and 0s when we look!

The measurement problem.



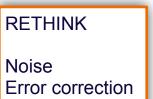
#### Measurement and reality

Measurement can change a quantum state, collapse it to one of the possibilities.

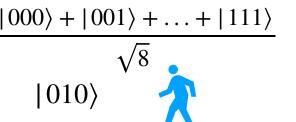
Copenhagen interpretation

- Determining an unknown quantum state is tricky. Measurement collapses wave function. Only a probable answer to the computation.
- Repeating measurement by making copies is not possible due to no-cloning theorem. Repeat experiment on identically prepared qubits and perform multiple measurements in the end to get the result.

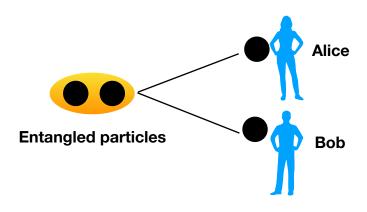
Nature only reveals quantum nature through statistics.



Verification



### **Entanglement**



#### **Correlations between parts**

$$|01\rangle + |10\rangle$$

#### **Measurement Basis**

z : Up/Down

x: Left/Right -

If they measure the same property (basis), they get correlated result. Otherwise, random. Measuring parts, collapses the results.

Spooky action at a distance - EPR paradox, Bell inequalities

Spooky! and faster than light communication? (NOT)

Entanglement is a resource: Dense coding, teleportation, quantum key sharing.

### What can we do with all that quantum?

- Core idea (Feynman): Simulate quantum physics, atomic and molecular interactions.
- Speed-ups for some problems in Computer Science and Mathematics
  - Integer factorisation (Shor). Break RSA.
  - Grover's search (Brute force search in unstructured databases).
  - Random sampling of quantum circuits, Boson sampling ...
- Optimization and Machine Learning.
- Quantum chemistry, drug design and studying complex biological datasets, protein folding.
- Quantum pattern recognition.

Long way to go. But we can still do interesting things with our computers.

### QuTiP Code

### QuTiP speaks quantum

Quantum 
$$|\psi\rangle=\frac{1}{\sqrt(2)}\left(|0\rangle+|1\rangle\right)$$
 state vectors 
$$H=\frac{\sigma_z}{2}$$

$$H = \frac{\sigma_z}{2}$$

Operators and Hamiltonians

$$a, a^{\dagger}$$

**Tensors** 

$$\sigma_z\otimes\sigma_x$$

**Density matrices** 

```
>> from qutip import *
>> psi1 = basis(2, 0)
 >> psi2 = basis(2, 1)
 \gg psi = (psi1 + psi2)/1.414
 \gg H = sigmaz()/2
 >> tensor(rho1, rho2)
 >> tensor(sigmaz(), sigmax())
 >> rho = ket2dm(psi)
 >> op = vector_to_operator(rho)
```

#### The Qobj class

 State and operators are declared as Qobj

- Algebra (bosonic)
- Sparse CSR matrices which interact with specialized Cython enhanced code.

```
>> q = Qobj([1], [0])
Quantum object: dims = [[2], [1]],
shape = (2, 1), type = ket
>> d = destroy(2)
Quantum object: dims = [[2], [2]],
shape = (2, 2), type = oper,
isherm = False
>> q.daq()
Quantum object: dims = [[1], [2]],
shape = (1, 2), type = bra
```

### **Operators**

Operators	Command (# means optional)	Inputs
Charge operator	charge(N, M=-N)	Diagonal operator with entries from M 0 N.
Commutator	commutator(A, B, kind)	kind = 'normal' or 'anti' commutator.
Diagonals operator	qdiags(N)	Quantum object created from arrays of diagonals at given offsets.
Higher spin operator	<pre>jmat(j,#s)</pre>	j = integer or half-integer representing spin, s = 'x', 'y', 'z', '+', or '-'
Identity	qeye (N)	N = number of levels in Hilbert space.
Destruction operator	destroy(N)	same as above
Momentum operator	momentum(N)	same as above
Number operator	num (N)	same as above

### Methods on Qobj

Command	Description
Q.check_herm()	Check if quantum object is Hermitian
Q.conj()	Conjugate of quantum object.
Q.dag()	Returns adjoint (dagger) of object.
Q.diag()	Returns the diagonal elements.
Q.eigenenergies()	Eigenenergies (values) of operator.
Q.eigenstates()	Returns eigenvalues and eigenvectors.
Q.groundstate()	Eigenval & eigket of Qobj groundstate.
Q.matrix_element(bra,ket)	Matrix element bra Q ket>
Q.norm()	Returns L2 norm for states, trace norm for operators.

#### Superoperators, maps, tensors

- $oldsymbol{\cdot}$  spre and spost  $X
  ho X^\dagger$
- Multipartite systems, tensors, two coupled qubits, qubit coupled to an oscillator

```
>> tensor(sigmax(), sigmax())
>> tensor(psi1, psi2)
>> tensor(rho1, rho2)
```

 Composite Hamiltonians, Liouvillians, and super tensors

```
>> H_sys = sigmaz()/2
>> H_cav = destroy(5)
>> H_comp = tensor(H_sys, H_cav)
>> super_tensor(L1, L2)
```

Contractions, exotic maps

```
>> X = sigmax()
>> spre(X) *spost(X.dag())
... type = super, isherm = True
Qobj data =
[[0. 0. 0. 1.]
 [0. 0. 1. 0.]
 [0. 1. 0. 0.]
 [1. 0. 0. 0.]]
>> H = sigmaz()
>> c ops = [sigmax(), sigmay()]
>> liouvillian(H, c ops)
.. type = super, isherm = False
Qobj data =
[[-2.+0.j 0.+0.j 0.+0.j 2.+0.j]
 [0.+0.j -2.+2.j 0.+0.j 0.+0.j]
 [0.+0.j 0.+0.j -2.-2.j 0.+0.j]
 [2.+0.j 0.+0.j 0.+0.j -2.+0.j]
```

#### Gates as Quantum Objects

- All valid Qobj methods work directly.
   Eg: Make a super-operator out of Toffoli
- Quickly move from the picture of circuits and gates to Hamiltonian evolution and use all of the QuTiP machinery
- Noise, quantum control, stochastic evolution

From circuit to physics

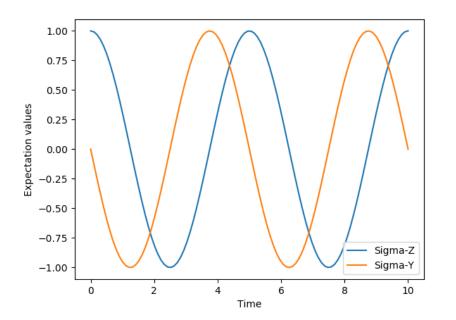
```
# Make a super operator out of a gate
>> spre(toffoli())
Quantum object: dims = [[[2, 2, 2], [2,
2, 2]], [[2, 2, 2], [2, 2, 2]]], shape =
(64, 64), type = super, isherm = True
                               0.0
                   0.0 - 0.0
                   0.0
>> toffoli super = spre(toffoli())
>> toffoli super.iscp
False
```

### QuTiP

Quantum dynamics

#### Lindblad master equation solver

#### Typical workflow



```
\dot{\rho} = -i[H, \rho] + \sum_{i} C_{i} \rho C_{i}^{\dagger} - \frac{1}{2} \left\{ C_{i} C_{i}^{\dagger}, \rho \right\}
\Rightarrow \text{H = sigmaz()}
\Rightarrow \text{c_ops = [sigmam()]}
\Rightarrow \text{psi0 = basis(2, 0)}
\Rightarrow \text{times = np.linspace(0.0, 10.0, 20.0)}
\Rightarrow \text{result = mesolve(H, psi0, times, c ops)}
```

#### Visualization

### Time dependent Hamiltonians

- QuTiP handles time-dependent Hamiltonians with ease
- Time-dependent Hamiltonians arise in control problems or driven systems.
- Smart built in solvers such as Floquet formalism: Evolve the wave function "stroboscopically", i.e., only evaluating at time multiples of the driving period.

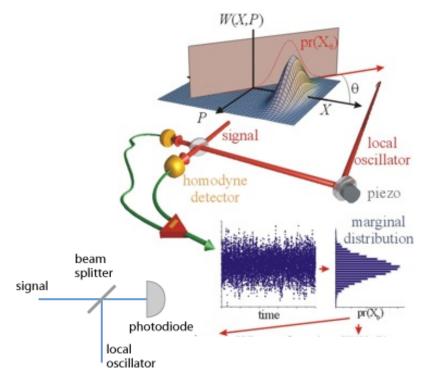
```
>> def f(t, args):
.. return np.exp(-args[0]*t)
>> H0 = sigmax()/2
>> H1 = sigmaz()/2
>> H = [H0,[H1, f]]
```

$$H = H_0 - f(t)H_1$$

>> mesolve(H, ...)
>> floquet markov mesolve

### Stochastic Master Equations

- Quantum stochastic calculus is the non-commutative analogue of Ito's calculus, developed to study noise in open quantum systems. (Barichielli, 1990)
- Useful tool to model continuous weak measurements, and implement feedback-control methods
- For example: Weak continuous
   Heterodyne and Homodyne measurement techniques (used to extract quadrature information with photon counters)



**RP Photonics** 

#### Other master equation solvers

```
\dot{\rho} = -\frac{i}{\hbar}[H,\rho] + \sum_{I=1}^{N^2-1} \gamma_i \left(\mathcal{L}_i \rho \mathcal{L}_i^\dagger - \frac{1}{2} \mathcal{L}_i \mathcal{L}_i^\dagger, \rho\right) >> c_ops = [sigmam()]  
>> psi0 = basis(2, 0)  
>> times = np.linspace(0.0, 10.0, 20.0)  
>> result = mesolve(H, psi0, times, c_ops)
```

Monte Carlo

HsolverDL Hierarchy

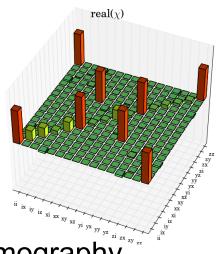
Finnesolve Floquet-Markov

Ssesolve Stochastic

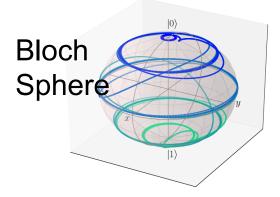
Presolve Reaction coordinate briesolve Bloch redfield

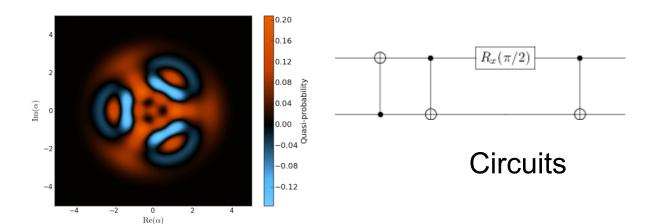
... and more

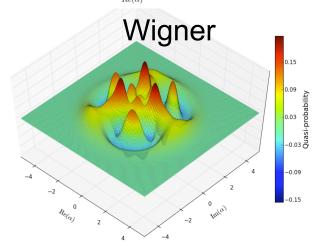
#### **Visualisation**

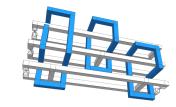


Tomography



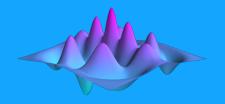






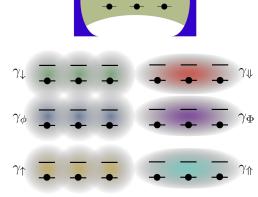
Surface code Topological Circuits

### QuTiP: What's new?



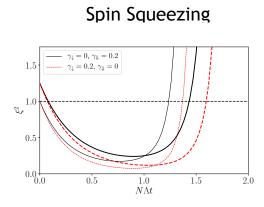
### PIQS: simulating qubit ensembles

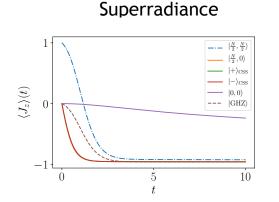
- PIQS (Permutational Invariant Quantum Solver)
   Nathan Shammah, <u>Shahnawaz Ahmed</u>
  - Noisy driven dissipative open quantum systems
  - Collective effects in qubit ensembles (100)



Shammah, N., Ahmed, S., Lambert, N., De Liberato, S., & Nori, F. (2018). Open quantum systems with local and collective incoherent processes: Efficient numerical simulation using permutational invariance. arXiv preprint arXiv: 1805.05129.

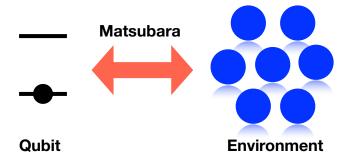
# Ultrastrong Coupling SS (a,b) (a,





### Non-Markovian methods, virtual photons

- A generic Hierarchical Equations of Motion (HEOM) implementation.
   Neill Lambert, Shahnawaz Ahmed
  - Non-Markovian dynamics: Environment has a memory
  - Ultrastrong coupling regime of light and matter
  - Bound states and virtual photons



A. Fruchtman, N. Lambert, and E.M. Gauger, Scientific Reports, **6** 28204 (2016). When do perturbative approaches accurately capture the dynamics of complex quantum systems?

#### **Scattering**

#### qutip.org/tutorials

Photon scattering in Quantum Optical Systems
 Ben Bartlett, P.h.D student, Stanford University



Email: benbartlett@stanford.edu

Github: bencbartlett

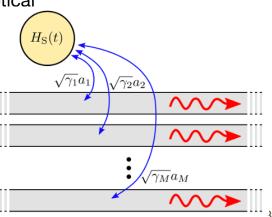
Photon scattering

Multiple waveguides: SPDC, Photon emission

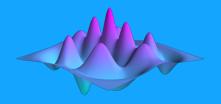
K.A. Fischer, et.al. (2017), "Scattering of Coherent Pulses from Quantum-Optical

Systems" (arXiv: <u>1710.02875</u>)

"How do photons scatter into the waveguide when the system is driven with some excitation field?"



# Open source and open science



### How QuTiP uses open source

Code, Testing



**Publish** 



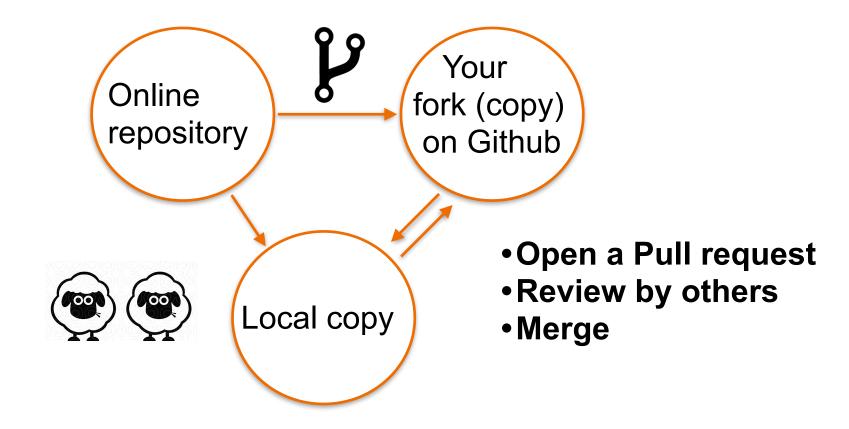








#### **Github**



#### **Testing**

#### "Untested code is broken code"

dist: trusty
language: python









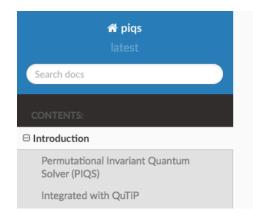
Write a .travis.yml fileavis with GithubAutomated testing online

#### **Documentation**

#### **Auto-generate**

>> sphinx-quickstart





#### **Edit conf**

doc/source/conf.py

# -- Project information
project = 'piqs'

#### Generate doc

C Edit on GitHub

>> make html

#### piqs.readthedocs.com

Docs » Introduction

Introduction

Permutational Invariant Quantum Solver (PIQS)

PIQS is an open-source Python solver to study the exact Lindbladian dynamics of open quantum systems consisting of identical qubits.

### Publishing and distributing code

setup.py

meta.yml

zenodo

Code/Data





DOI 10.5281/zenodo.1212802

Draft a new release



- >> pip install qutip
- >> conda -c conda-forge install qutip
- >> python setup.py install/develop

### QuTiP: summing up

#### The **Quantum Toolbox in Python**





QuTiP

Ouantum Toolbox in Python

>600 citations (Google Scholar)

downloads 43k (conda forge)

More info at <a href="http://gutip.org/">http://gutip.org/</a>

#### Authors

Comp. Phys. Comm. 183, 1760-1772 (2012); ibid. 184, 1234 (2013).

# Code

Robert J. Johansson

Rakuten Inc.



IBM O



#### Users

Distribution of 25k website visitors (2016)



#### Timeline:

Inspired by the Quantum Toolbox in MatLAB.

2011-2012: QuTiP 1.0

Aug 2015: 100 citations

Aug 2016: 200 citations

Jan 2017: QuTiP 4.0

July 2018: QuTiP 4.3

#### **Lead Developers**







Universite de Sherbrooke



Chris Grenade University of Sydney

#### **Contributing Developers**

- Neill Lambert (RIKEN)
- · Denis Vasilyev (Leibniz)
- Kevin Fischer (Stanford)
- Jonathan Zoller (Ulm University)
- · Ben Criger (RWTH Aachen)
- Eric Giguere
- Shahnawaz Ahmed (Chalmers)
- Nathan Shammah (RIKEN)

• GitHub: 44 contributors, 4k commits

License: BSD

Style: PEP8 compliant

#### Libraries used:

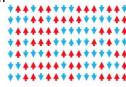
- Scipy
- Matplotlib
- NumPy
   Cython
- SymPy
- Cython
  - Jupyter notebooks
  - Online documentation
  - Independent testing

#### Google summer of Code 2019

#### We are applying to Google Summer of Code 2019 with NumFocus!

https://github.com/qutip/qutip/wiki//Google-Summer-of-Code-2019

- Lattice models in QuTiP. Ising, Hubbard, XY, Heisenberg model
  - Clemens Gneiting (Riken, Japan)
  - Eric Giguere (Université de Sherbrooke)





- GPU backend for dynamics with the Hierarchical Eq of Motion
  - Neill Lambert (Riken, Japan)
  - Alex Pitchford (Université de Sherbrooke)
- An overhaul and abstraction of the quantum object class
  - Alex Pitchford (Université de Sherbrooke)
  - Eric Giguère (Université de Sherbrooke, UK)



medium.com/quantum-tech

Go to menti.com and use code 54 73 02

Thank you

sahmed.in

Twitter @quantshah