`qpe-toolbox`: Tensor Network Simulation of Quantum Phase Estimation

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Entanglement and topology in interacting quantum matter
Benasque

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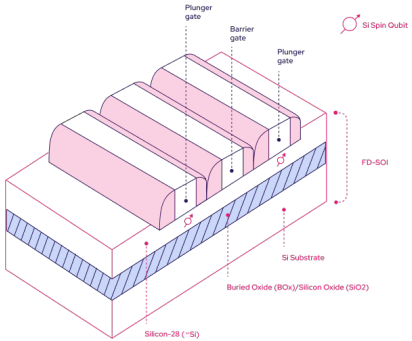
quobly

Mandatory corporate slide

- Quobly is a quantum startup based in Grenoble, France
- building quantum computer
- semiconductor spin qubits technology
- Quantum information team:
  - simulation of (noisy) quantum hardware
  - simulation of quantum circuits
  - classical and quantum resources estimation



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NISQ and FACT

NISQ: Noisy Intermediate-Scale Quantum

- quantum hardware exists
- small number of qubits
- gate fidelity is limited
- noise is a major issue

FASQ: Fault-tolerant Application-Scale Quantum

- large number of qubits
- quantum error correction suppresses noise
- deep circuits can be run

Mind the gaps: The fraught road to quantum advantage

Jens Eisert[1,2,3] and John Preskill[4,5]

The Quest for a Quantum Advantage

Race between NISQ and classical simulations (non exhaustive)

Experiment	qubits	gates	Type	Simulated?	Useful?
Google 2019	53	430	Random circuit sampling	Yes (TN)	No
USTC 2023	50	?	Gaussian boson sampling	Yes (TN)	No
IBM 2023	127	2880	Ising model	Yes (TN, Pauli path)	Yes
Google 2025	65	1000	OTOC measurement	No	No

Why Quantum Phase Estimation?

- There is a variety of quantum algorithms. We chose to focus on one
- The “zoo” of quantum algorithms breaks down into many variations of fewer algorithmic primitives
- We believe the first useful application of a QPU will require fault tolerant quantum computing (FTQC)
- QPE is:
  - a key subroutine in Shor’s algorithm
  - FTQC: requires deep circuits (hard to simulate classically)
  - expected to solve problems in chemistry, condensed matter

Quantum Fourier Transform

$$|j\rangle \to \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{2\pi jk/2^n} |k\rangle$$

- Classical Fast Fourier Transform (FFT): cost $\mathcal{O}(n2^n)$
- Quantum Fourier Transform: $\mathcal{O}(n^2)$
- actually no quantum speed-up: MPS-based QFT simulated with cost $\mathcal{O}(n)$

PRX QUANTUM **4,** 040318 (2023)

Quantum Fourier Transform Has Small Entanglement

Jielun Chen (陈捷伦),[1,2,*] E.M. Stoudenmire,[3] and Steven R. White[1]

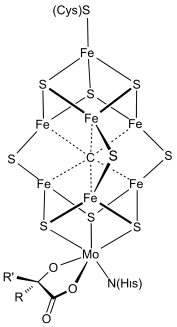
Contents

Quantum chemistry and molecules

- N electrons, M molecular orbitals
- Molecular electronic Hamiltonian:

$$\hat{\mathcal{H}} = \hat{T}_{el} + \hat{V}_{nuc-el} + \hat{V}_{el-el} + \hat{V}_{nuc-nuc}$$

- Exact Diagonalization (FCI): exponential in M
- Approximate methods: DFT for weakly correlated molecules
- strongly correlated molecules: tensor networks, quantum computers (?)



FeMocCO cluster of nitrogenase

Effective Hamiltonian for quantum chemistry

- Born-Oppenheimer approximation: fixed ion positions
- chemistry basis set: `sto-3g`, `6-31g`, `ccpvdz`...
- project on finite dimensional space
- Hartree-Fock to get molecular orbitals
- compute kinetic and Coulomb matrix elements

$$\hat{V}_{el-el} = \frac{1}{2} \sum_{p,q,r,s=1}^{M} V_{pqrs} \hat{c}_p^\dagger \hat{c}_p^\dagger \hat{c}_r \hat{c}_s$$

- TL;DR: Quantum chemistry is Fermi-Hubbard with long-range t and U

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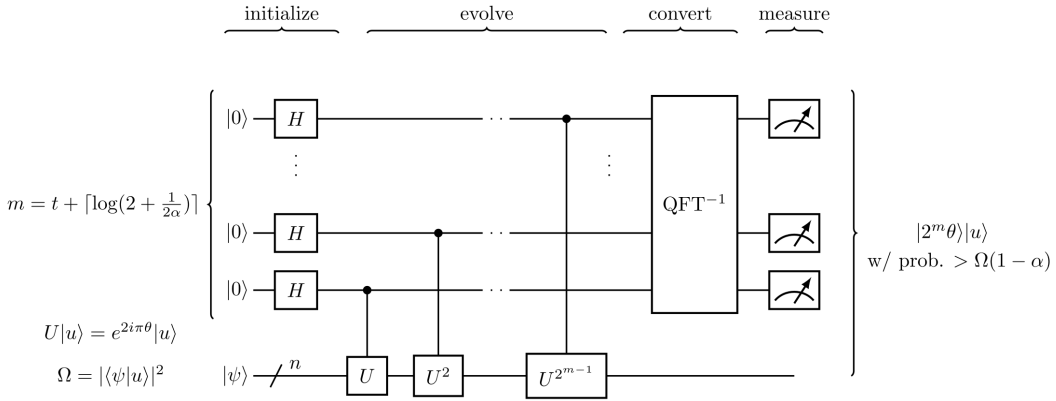
Textbook Quantum Phase Estimation

- $U(t) = \exp(-iHt)$
- QPE finds eigenvalue with t bits precision
- initial state projected on eigenvector with probability $\Omega = |\langle\psi|u\rangle|^2$



Trotterized Quantum Phase Estimation

- cannot directly encode $U(t) = \exp(iHt)$
- decompose $H = \sum_k h_k$
- Trotter-Suzuki decomposition

$$U(\delta t) = \prod_k \exp(-ih_k \delta t) + O(\delta t^2)$$

- formulate each h_k as quantum gate
- control error with number of Trotter steps and time step length
- naïve implementation: cost $\mathcal{O}(2^m(E_{\max} - E_{\min})M^4)$
  m number of precision bits, M number of orbitals

Progress in QPE resource use

Year	Innovation	FeMoco-54 [37]			FeMoco-76 [38]		
		Qubits	Toffolis	Reference	Qubits	Toffolis	Reference
2017	First resource estimate by Trotterization [37]	111	5.0×10^{13}	[37]	-	-	-
2019	Qubitization of Single-Factorization [17]	3320	9.5×10^{10}	[7]	3628	1.2×10^{11}	[7]
2020	Qubitization of Double-Factorization (DF) [9]	3600	2.3×10^{10}	[9]	6404	5.3×10^{10}	[7]
2020	Tensor-Hyper-Contraction (THC) [7]	2142	5.3×10^{9}	[7]	2196	3.2×10^{10}	[7]
2024	Symmetry compression of DF [39]	1994	2.6×10^{9}	[39]	-	-	-
2025	Symmetry compression of THC [8]	-	-	-	1512	4.3×10^{9}	[8]
This work	Spectrum amplification & DFTHC	1137	3.41×10^{8}		1459	9.99×10^{8}	
Improvement of this work over [39] and [8][a]		1.8×	7.0×		1.0 ×	4.3 ×	

Resources for FeMoCo - from Low et al. (Google team), PRX 15 2025

Advanced QPE: Linear Combination of Unitaries

- Rewrite Hamiltonian as sum of unitaries

$$H = \sum_{\ell=0}^{L-1} w_\ell H_\ell \qquad \text{s.t.} \qquad w_\ell \geq 0, \qquad H_\ell^2 = 1$$

- Define "one norm" $\lambda \equiv \sum_{\ell=0}^{L-1} w_\ell$
- walk operator $\mathcal{W} = \exp\big(-i \arccos(H/\lambda)\big)$
- apply QPE on $\mathcal{W}$
- cost $\mathcal{O}(2^m C_{\mathcal{W}} \frac{\lambda}{\Omega})$

Advanced QPE: Robust Phase Estimation

- single ancilla qubit / many repetitions of the circuit
- Inspired from J. Günther et al. arXiv:2503.05647
- Hadamard test: measure $\langle U|\psi|U\rangle$ with $U = \exp(-iHt)$ for $t = 2^k, k = 1...R$
- Find an estimate of $2^k E \bmod 2\pi$ within measurement and Trotter error
- For each k, select the estimate closest to the previous one: improve precision on E by one bit
- Measure E up to $\mathcal{O}(2^{-R})$ error with R circuits

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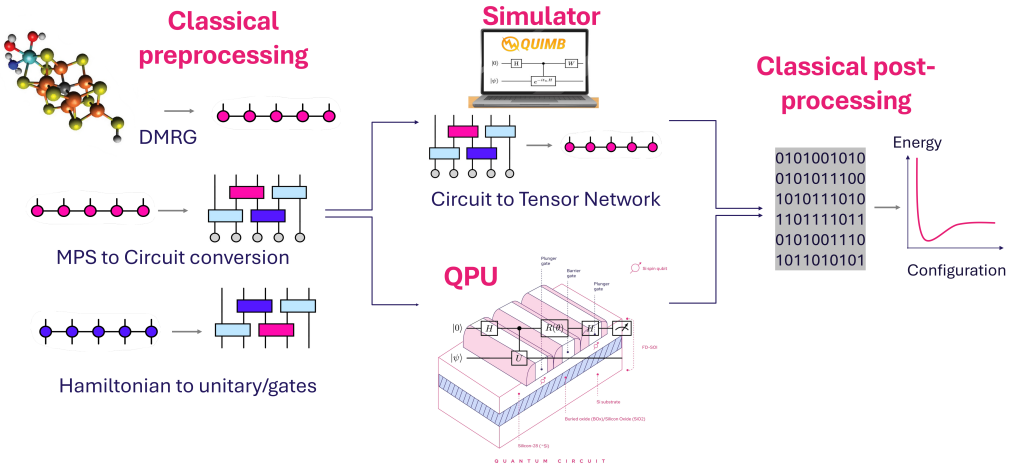
Introducing `qpe-toolbox`

Objective: Simulate the full QPE pipeline. Get ready for QPE in the long term

Requirements	Features
Include the best classical algorithms	Component 1: Classical solution via DMRG
A classical-to-quantum converter	Component 2: Tensor-network state preparation
Advanced QPE schemes to reduce quantum resources	Component 3: qubitization, single-ancilla
Circuit simulations to quantify the boundary of a quantum advantage, prepare experiments	Component 4: Large-scale tensor network simulations and optimization

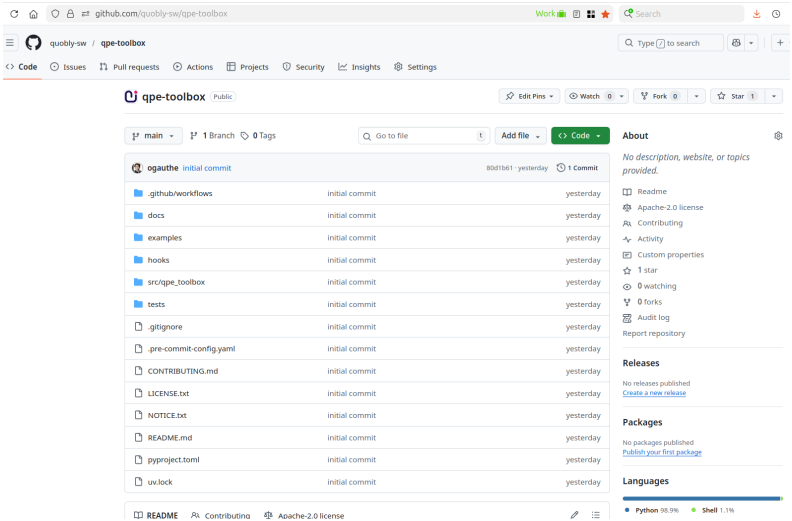
qpe-toolbox in One Slide



`qpe-toolbox` beyond QPE

- overview of tensor network possibilities for quantum circuit simulation
- benchmark: `quimb` vs `qiskit` for circuit simulation
- variational circuit optimization
- complete pipeline from quantum chemistry problem to QPE
- more to come in the future!

Code is Available!



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Thibaud Louvet

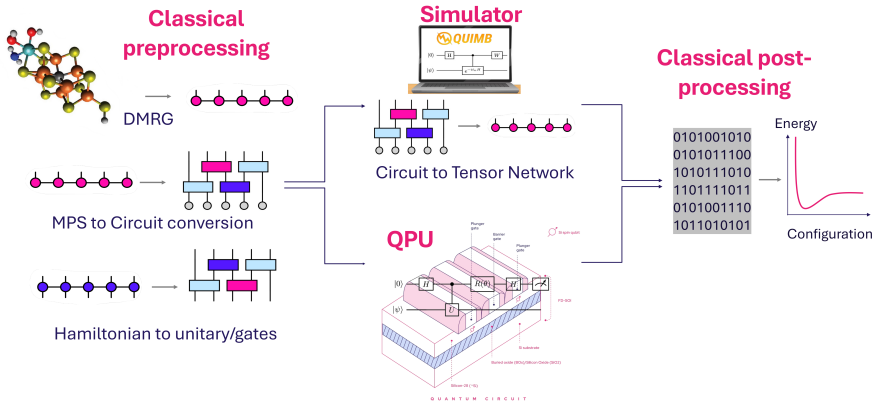
Summary

- We develop an open-source numerical toolbox
  - Based on advanced tensor-network techniques
  - explore and evaluate performances of QPE variants

- First stage release “My pedagogical toolbox” (coming soon)
  - complete pipeline from quantum chemistry problem to QPE
  - Initialization: DMRG or circuit optimization
  - Hamiltonian encoding: Trotterization or naïve qubitization
  - Phase estimation: textbook QPE or Robust Phase Estimation

`https://github.com/quobly-sw/qpe-toolbox`

Thank you for your attention



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