Quantum algorithms for eigenvalue problems

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Joint work with

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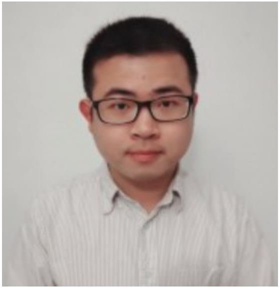


Yulong Dong
(Berkeley)

Outline

Quantum numerical linear algebra

- Solving numerical linear algebra problems on a quantum computer.
- Many interesting, exciting progresses in the past few years.
- Lecture notes on "Quantum Algorithms for Scientific Computation"[1]
- Reasonable way towards "quantum advantage".
- Ground state energy: an eigenvalue problem

$$H|\psi_0\rangle = \lambda_0 |\psi_0\rangle$$

  $H \in \mathbb{C}^{N\times N}$ Hermitian matrix (Hamiltonian).
  Find the algebraically smallest λ_0 and/or prepare $|\psi_0\rangle$
- Under which conditions the cost can be $\mathcal{O}(\mathrm{polylog}(N))$?

[1] https://math.berkeley.edu/~linlin/qasc/

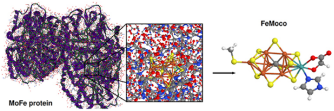
Ground state preparation and energy estimation

$$H|\psi_0\rangle = \lambda_0 |\psi_0\rangle$$

- An efficient input model (local, sparse, etc.) for H:
- QMA-hard (i.e., difficult for quantum computers) of the local Hamiltonian problem without additional assumptions.
- Some physically relevant assumptions:
  1. Good initial guess : $|\langle\phi|\psi_0\rangle| \geq \gamma$.
  2. Spectral gap: $\Delta = \lambda_1 - \lambda_0$. (only necessary for preparing the ground state but not for estimating ground state energy)

Quantum advantage for quantum chemistry?

- Ground state energy: useful in predicting material structures, simulating chemical reactions, etc. FeMoco: primary cofactor of nitrogenase for nitrogen fixation.



- Quantum many body Hamiltonian (second quantization, $\dim(H) = 2^n$)

$$H = \sum_{ij=1}^{n} h_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl=1}^{n} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

- Even for strongly correlated quantum chemistry, exponential quantum advantage (EQA) is under debate[1].

[1] S. Lee et al, Is there evidence for exponential quantum advantage in quantum chemistry?

Input models

- Dimension of Hilbert space is $N = 2^n$.
  Access to initial state: U_I to prepare $|\phi\rangle = U_I |0^n\rangle$.

- Access to Hamiltonian H
  1. Block encoding (BE): $\dim U_H = MN = 2^{m+n}$

  $$U_H = \begin{pmatrix} H/\alpha & * \\ * & * \end{pmatrix} \qquad \text{for some } \alpha$$

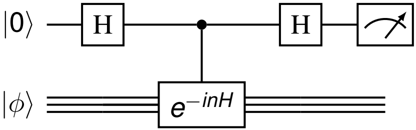
  2. Hamiltonian evolution (HE): $\dim U_H = N = 2^n$

  $$U_H = e^{-\mathrm{i}\tau H} \qquad \text{for some } \tau$$

- Cost of implementing U_H, U_I is $\mathcal{O}(\mathrm{polylog}(N))$.

- Query complexity: the number of accesses to U_H, U_I.

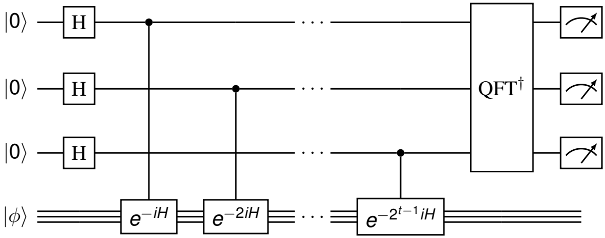
Textbook algorithm with Hamiltonian evolution access: Kitaev's algorithm



- Useful when $|\phi\rangle$ is the exact eigenstate with eigenvalue λ.
- $n = 1$: Hadamard test. Estimate $p(0) \to \mathrm{Re}\,\langle\phi|e^{-iH}|\phi\rangle = \cos(\lambda)$. Cost is $\widetilde{\mathcal{O}}(\epsilon^{-2})$ due to repetition.
- $n = 1, 2, \ldots, 2^{t-1} = \epsilon^{-1}$: Kitaev's algorithm. Cost is $\widetilde{\mathcal{O}}(\epsilon^{-1})$ (Heisenberg limit)
- Can be modified for inexact eigenstate, called the semi-classical QPE (or single ancilla QPE)[1]

[1] (Higgins et al, Nature 2007; Berry et al, PRA 2009)

Textbook algorithm with Hamiltonian evolution access: standard quantum phase estimation (QPE)



- Use multiple control qubits to store eigenvalues in a quantum register.
- Run multiple times and take the lowest value as estimate to λ_0. Useful when $|\phi\rangle$ is not an exact eigenstate.
- Why not stop here? Need to study the query complexity with respect to γ, ϵ, Δ. Suitability for early fault-tolerant devices?

What is special about early fault tolerant quantum computers?

- Limited number of logical qubits.
- It can be difficult to execute certain multiqubit controlled (MQC) gate operations.
  - ✗ High-level : $\mathrm{poly}(n)$ two-qubit gates and ancilla qubits, e.g., quantum median.
  - ✓ Low-level: $\mathcal{O}(n)$ two-qubit gates and $\mathcal{O}(1)$ ancilla qubit, e.g., n-qubit reflection operator.
- It can be important to reduce the circuit depth, sometimes even at the expense of a larger total runtime (via a larger number of repetitions).

Pros and cons of different input models

- Block encoding access:
  - ✓ Natural expression of non-unitary matrices, e.g. sparse matrices, using quantum circuits
  - ✓ Matrix functions $f(H)$ via quantum signal processing (QSP) / quantum singular value transformation (QSVT)
  - ✗ Many ancilla qubits; High-level multi-qubit control. Suitable for fully fault-tolerant quantum devices.
- Hamiltonian evolution access:
  - ✓ Implementation can be ancilla-free, e.g., Trotter method. Perhaps the most important reason for stating that it can be suitable for early fault-tolerant quantum devices.
  - ✗ Trotter method introduces discretization error (though asymptotically amendable using high order methods)
- HE is the “traditional” way of thinking about quantum algorithms (e.g., QPE). Historically, complexity can be sub-optimal

Progresses for ground state energy estimation

	Query depth	Query complexity	# ancilla qubits	Need MQC?	Input model
QPE (high conf.)	$\widetilde{\mathcal{O}}(\epsilon^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-2})$	$\mathcal{O}(\mathrm{polylog}(\gamma^{-1}\epsilon^{-1}))$	High	HE
QPE (1 ancilla)	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-2})$	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-4})$	$\mathcal{O}(1)$	No	HE
Som19	$\widetilde{\mathcal{O}}(\epsilon^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-4}\gamma^{-4})$	$\mathcal{O}(1)$	No	HE
GTC19	$\widetilde{\mathcal{O}}(\epsilon^{-3/2}\gamma^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-3/2}\gamma^{-1})$	$\mathcal{O}(\log(\epsilon^{-1}))$	High	HE
LT20*	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-1})$	$m+\mathcal{O}(\log(\epsilon^{-1}))$	High	BE
LT22 (short depth)	$\widetilde{\mathcal{O}}(\epsilon^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-4})$	$\mathcal{O}(1)$	No	HE
DLT22 (short depth)	$\widetilde{\mathcal{O}}(\epsilon^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-2})$	$\mathcal{O}(1)$	No	HE
DLT22 *	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-1})$	$\mathcal{O}(1)$	Low	HE

* Achieves near optimal complexity w.r.t. γ, ϵ. Knowledge on gap Δ is not necessary.
Initial guess $|\langle\phi|\psi_0\rangle| \geq \gamma$

Som19: (Somma New J. Phys., 2019; slightly improved by LT22); GTC19: (Ge-Tura-Cirac, J. Math. Phys. 2019)
(**Lin**-Tong, Quantum 2020); (**Lin**-Tong, PRX Quantum 2022); (Dong-**Lin**-Tong, 2204.05955)

Progresses for ground state preparation

	Query depth	Query complexity	# ancilla qubits	Need MQC?	Input model
QPE (high conf.)	$\widetilde{\mathcal{O}}(\Delta^{-1})$	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-2})$	$\mathcal{O}(\mathrm{polylog}(\Delta^{-1}\gamma^{-1}\epsilon^{-1}))$	High	HE
QPE (1 ancilla)	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-2})$	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-4})$	$\mathcal{O}(1)$	No	HE
GTC19	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-1})$	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-1})$	$\mathcal{O}(\log(\Delta^{-1}) + \log\log(\epsilon^{-1}))$	High	HE
LT20*	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-1})$	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-1})$	m	High	BE
DLT22 (short depth)	$\widetilde{\mathcal{O}}(\Delta^{-1})$	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-2})$	$\mathcal{O}(1)$	No	HE
DLT22*	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-1})$	$\widetilde{\mathcal{O}}(\Delta^{-1}\gamma^{-1})$	$\mathcal{O}(1)$	Low	HE

* Achieves near optimal complexity w.r.t. γ, Δ.
Initial guess $|\langle\phi|\psi_0\rangle| \geq \gamma$; $\Delta = \lambda_1 - \lambda_0$: spectral gap

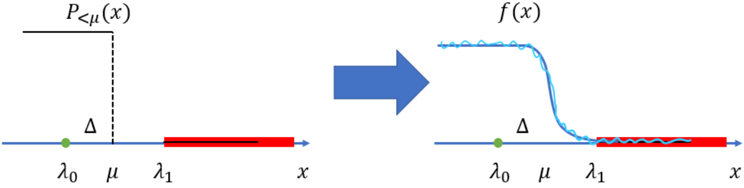
Omitting up to $\log \epsilon^{-1}$ dependence on precision.

GTC19: (Ge-Tura-Cirac, J. Math. Phys. 2019)

(**Lin**-Tong, Quantum 2020); (Dong-**Lin**-Tong, 2204.05955)

Outline

Ground state preparation: eigenstate filtering

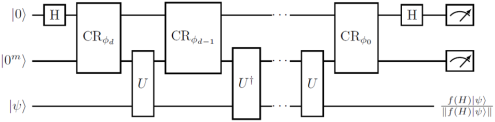


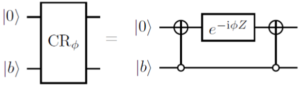
- First assume μ is given.
- Polynomial / trigonometric approximation to step functions.
- Implement a matrix function via an efficient quantum circuit

$$f(H/\alpha)\left|\phi\right\rangle = \sum_{k=0}^{N-1} f(\lambda_k/\alpha)\left|\psi_k\right\rangle\left\langle\psi_k|\phi\right\rangle .$$

Implementation of eigenstate filtering function

- Quantum signal processing (QSP) / quantum singular value transformation (QSVT). Block encoding access.





$$f(H/\alpha)\,|\phi\rangle = \sum_{k=0}^{N-1} f(\lambda_k/\alpha)\,|\psi_k\rangle\,\langle\psi_k|\phi\rangle\,.$$

$$U = \begin{pmatrix} H/\alpha & * \\ * & * \end{pmatrix}, \quad \mathcal{U} = \begin{pmatrix} f(H/\alpha) & * \\ * & * \end{pmatrix}$$

Low and Chuang, “Optimal Hamiltonian simulation by quantum signal processing”, PRL 2017

Gilyén, Su, Low, Wiebe, “Quantum singular value transformation and beyond”, STOC 2019

Martyn et al, “A Grand Unification of Quantum Algorithms”, PRX Quantum 2021

Lin, “Lecture notes on Quantum Algorithms for Scientific Computation”, Ch7,Ch8

Finding the phase factors: Quantum Signal Processing PACKage (QSPPACK)

QSPPACK

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QSPPACK

Quantum Signal Processing PACKage

a package for quantum numerical linear algebra

Developed and maintained by the department of Mathematics, University of California, Berkeley

qsp (dot) package (at) gmail (dot) com

[About]

Latest news

- [June 2022] The official site of QSPPACK has been released.

Download

You can install qsppack to your current directory by pasting the code below to your MATLAB command window:

```
unzip('https://github.com/qsppack/qsppack/archive/master.zip')
movefile('QSPPACK-master', 'qsppack')
addpath(fullfile(cd,'qsppack','Solvers','Optimization')), savepath
```

(Dong-Meng-Whaley-**Lin**, PRA 2021) https://github.com/qsppack/QSPPACK (website still under construction)

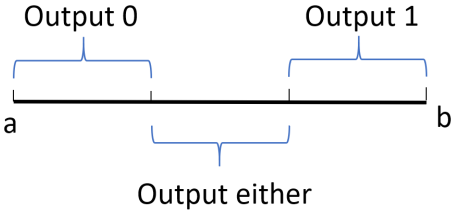
Binary search based ground state energy estimation

- Idea: use binary search. Need to solve the following problem: if we know $a \leq \lambda_0 \leq b$, decide $\lambda_0 > (a+b)/2$ or $\lambda_0 < (a+b)/2$.
- This does not work because we are essentially asking the quantum circuit to compute a discontinuous function while the output probability distribution is a continuous function of λ_0.
- Need to account for the fuzziness and statistical uncertainty.

A decision problem

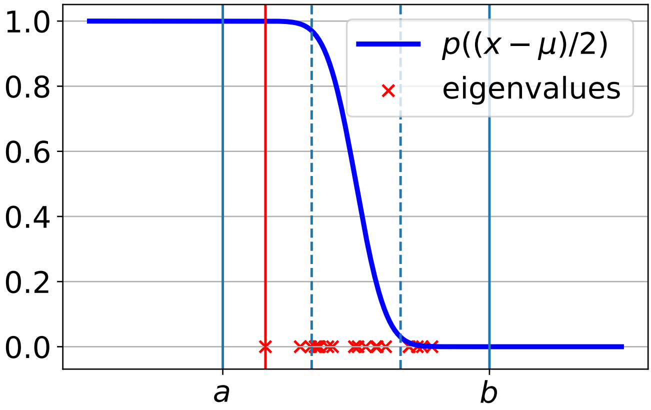
Assuming we know $a \leq \lambda_0 \leq b$.

(i) When $a \leq \lambda_0 \leq \frac{2}{3}a + \frac{1}{3}b$, output 0;
(ii) When $\frac{2}{3}a + \frac{1}{3}b \leq \lambda_0 \leq \frac{1}{3}a + \frac{2}{3}b$, output 0 or 1;
(iii) When $\frac{1}{3}a + \frac{2}{3}b \leq \lambda_0 \leq b$, output 1.



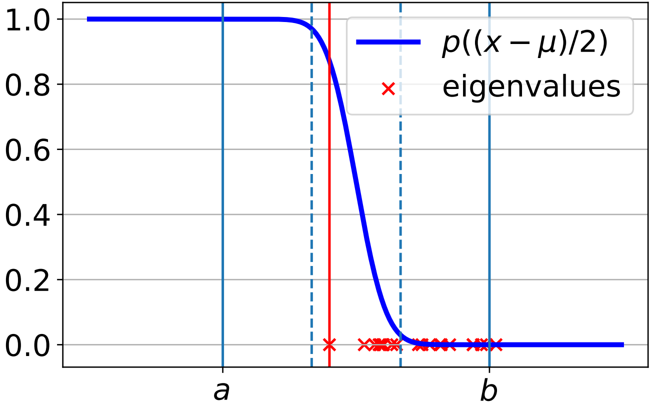
- Success probability of measuring ancilla $p = \| f(H) |\phi\rangle \|^2$.
- Distinguish between $\| f(H) |\phi\rangle \| \geq \gamma(1 - \epsilon')$ and $\| f(H) |\phi\rangle \| \leq \epsilon'$.

Solving the decision problem (i)



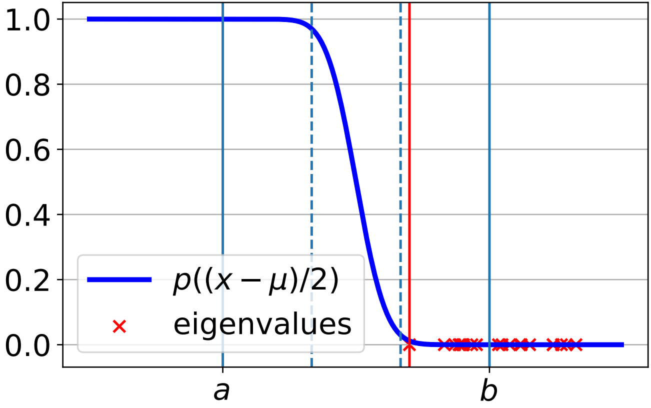
$$\lambda_0 \leq \frac{2}{3}a + \frac{1}{3}b \implies \| f(H) |\phi\rangle \| \geq \gamma(1-\epsilon')$$

Solving the decision problem (ii)



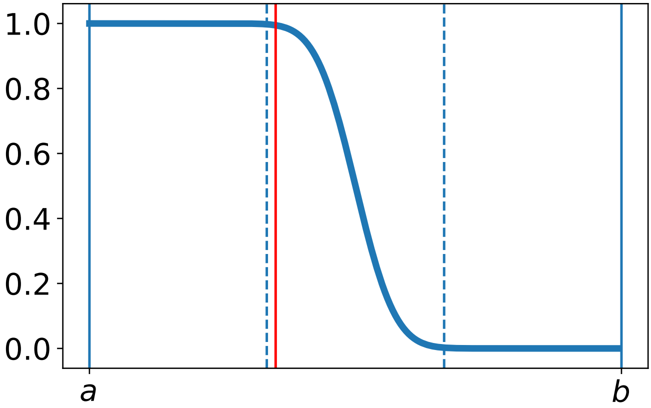
$$\frac{2}{3}a + \frac{1}{3}b \leq \lambda_0 \leq \frac{1}{3}a + \frac{2}{3}b$$

Solving the decision problem (iii)

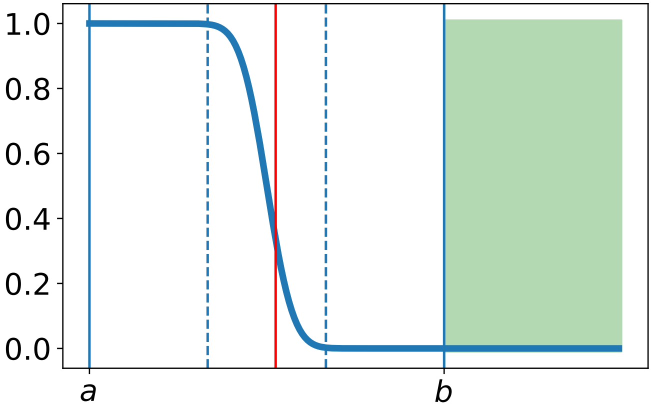


$$\lambda_0 \geq \frac{1}{3}a + \frac{2}{3}b \implies \| f(H) \, |\phi\rangle \, \| \leq \epsilon'$$

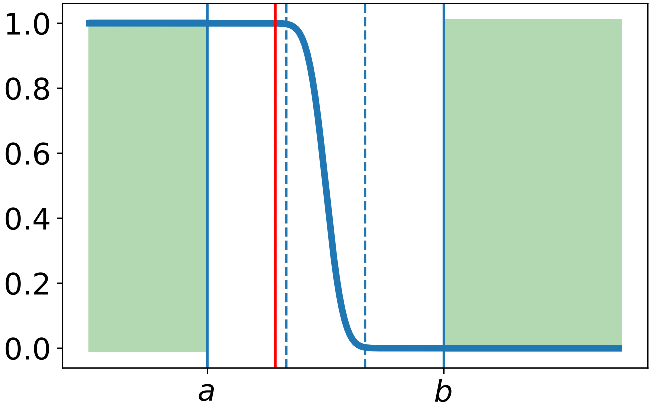
The search process



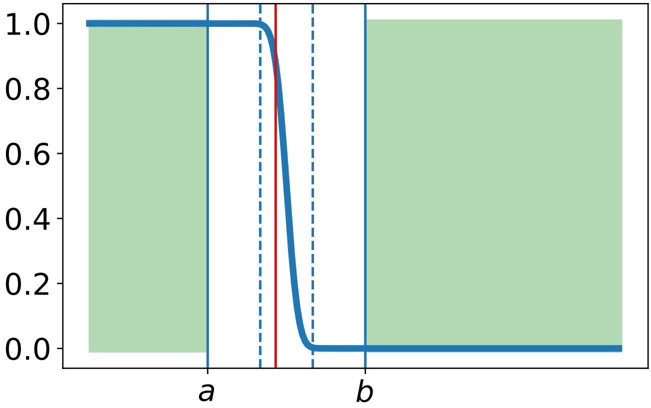
The search process



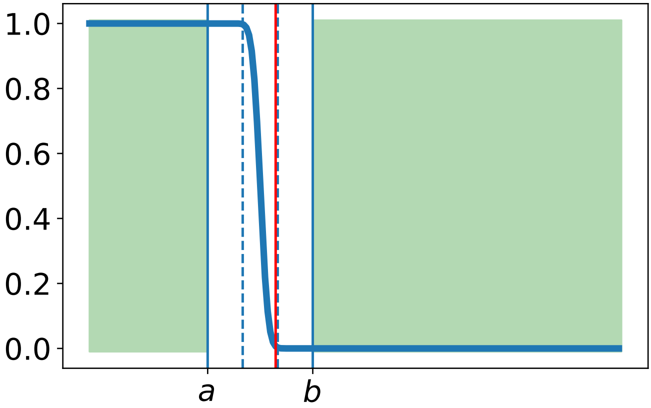
The search process



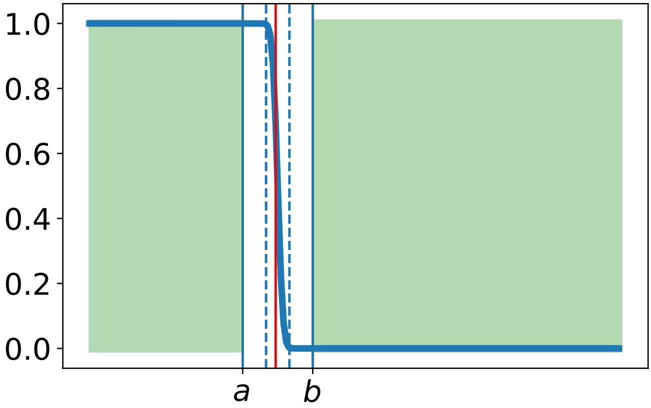
The search process



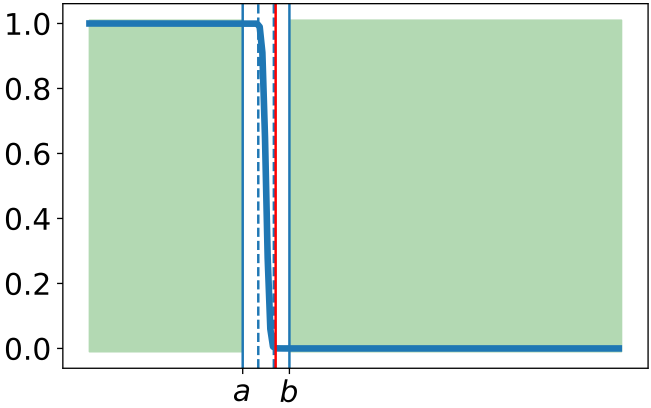
The search process



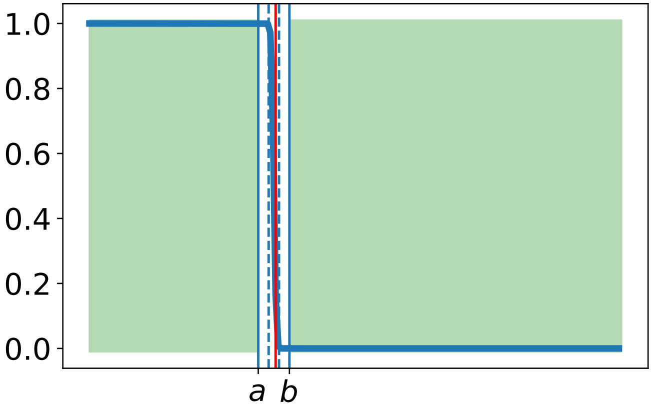
The search process



The search process



The search process



Solving the decision problem

- Success probability of measuring ancilla $p = \|f(H)|\phi\rangle\|^2$.
- Distinguish between $\|f(H)|\phi\rangle\| \geq \gamma(1-\epsilon')$ and $\|f(H)|\phi\rangle\| \leq \epsilon'$.
- Measure the success probability of the ancilla qubit: query complexity $\mathcal{O}(p^{-1}) = \mathcal{O}(\gamma^{-2})$
- Can use binary amplitude estimation[1] reduces query complexity to $\mathcal{O}(\gamma^{-1})$.
- Error probability can be exponentially suppressed using majority voting (Chernoff bound).

[1] (**Lin**-Tong, Quantum 2020). Similar to gapped phase estimation (Ambainis, STACS 12)

Summary of the main steps

- Efficient implementation of a filtering matrix function $f(H-\mu)$. Cost: $\widetilde{\mathcal{O}}(\epsilon^{-1})$ in the worst case.
- Binary amplitude estimation for deciding $\| f(H) \|\phi\rangle \| \geq \gamma(1-\epsilon')$ and $\| f(H) \|\phi\rangle \| \leq \epsilon'$. Cost: $\widetilde{\mathcal{O}}(\gamma^{-1})$.
- Binary search to refine μ: Cost: $\mathcal{O}(\log \epsilon^{-1})$.

Total cost: $\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-1})$

Outline

Introduction

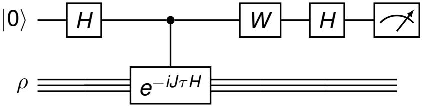
Algorithms for fully fault-tolerant quantum devices

Algorithms for early fault-tolerant quantum devices

(Recall) limitations of early fault tolerant quantum computers

- Limited number of logical qubits.
- It can be difficult to execute certain controlled operations.
- It can be important to reduce the circuit depth, sometimes even at the expense of a larger total runtime (via a larger number of repetitions).

A simple statistical algorithm for ground state energy estimation



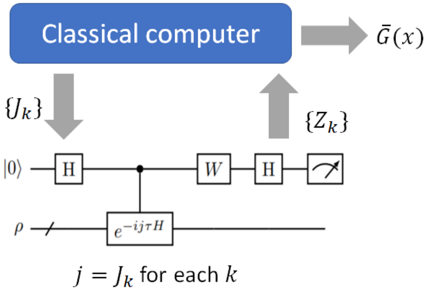
- Similar to circuit in Kitaev's algorithm
- Denote the measurement outcome (± 1) by X (for $W = I$) and Y (for $W = S^\dagger$)

$$\mathbb{E}[X|J] = \mathrm{Re}\,\mathrm{Tr}[\rho e^{-iJ\tau H}]$$
$$\mathbb{E}[Y|J] = \mathrm{Im}\,\mathrm{Tr}[\rho e^{-iJ\tau H}]$$

- Random evolution time J

(**Lin**-Tong, 2102.11340, PRX Quantum 2022)

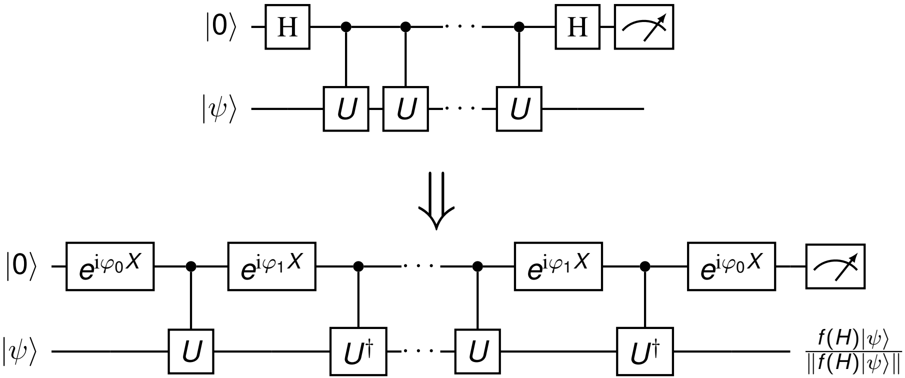
Summary of the algorithm



Combine with bisection algorithm.
Query complexity for $U = e^{-\mathrm{i}\tau H}$ is $\mathcal{O}(\epsilon^{-1}\gamma^{-4})$.

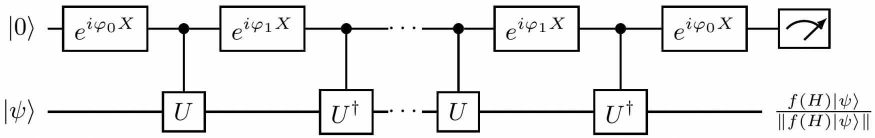
- ✓ Heisenberg limit. One ancilla qubit.
- ✓ Short depth $\mathcal{O}(\epsilon^{-1})$: Heisenberg scaling.
- ✗ Suboptimal scaling with respect to γ.
- ✗ Cannot prepare ground state

From Kitaev's algorithm to quantum eigenvalue transformation of unitary matrices (QET-U)



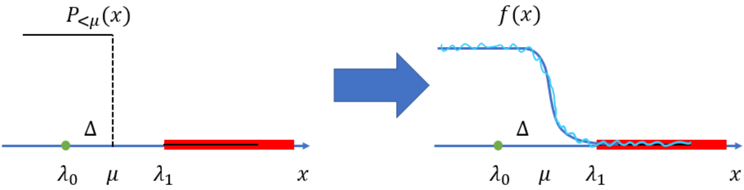
(Dong-**Lin**-Tong, 2204.05955)

Quantum eigenvalue transformation of unitary matrices (QET-U)



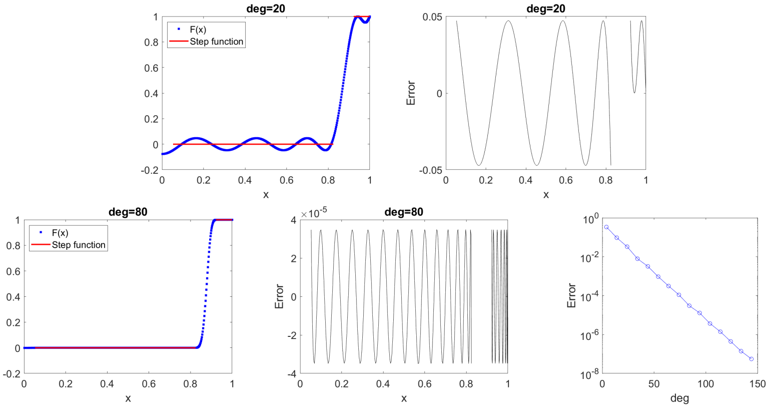
- One ancilla qubit. Hamiltonian evolution access $U = e^{-iH}$, (assuming $0 < \lambda(H) < \pi$).
- $F(x)$ is any real, even polynomial s.t. $\deg(F) = d$, and $|F(x)| \leq 1$ for any $x \in [-1, 1]$.
- Upon measuring ancilla with 0, output quantum state $\propto F\left(\cos \frac{H}{2}\right) |\psi\rangle =: f(H) |\psi\rangle$.
- Probability of success $\left\|F\left(\cos \frac{H}{2}\right) |\psi\rangle\right\|_2^2$.

Ground state preparation via QET-U



- Assume the knowledge of quantity μ s.t. $\lambda_0 \le \mu - \Delta/2 < \mu + \Delta/2 \le \lambda_1$
- $f(H) = F(\cos(H/2))$ or $F(H) = f(2 \arccos(H))$.
- $f(H)$ is a trigonometric polynomial of H.

Approximate polynomial



- $\cos(x/2)$ is monotonically decreasing on $[0, \pi]$.
- Convex optimization based method to find near-optimal polynomial (implemented in QSPPACK).

Binary search: solving the decision problem

- Distinguish

$$\left\| F\left(\cos\frac{H}{2}\right)|\phi\rangle\right\| \geq \gamma(1-\epsilon') \quad \text{and} \quad \left\| F\left(\cos\frac{H}{2}\right)|\phi\rangle\right\| \leq \epsilon'.$$

  by measuring the success probability of ancilla.

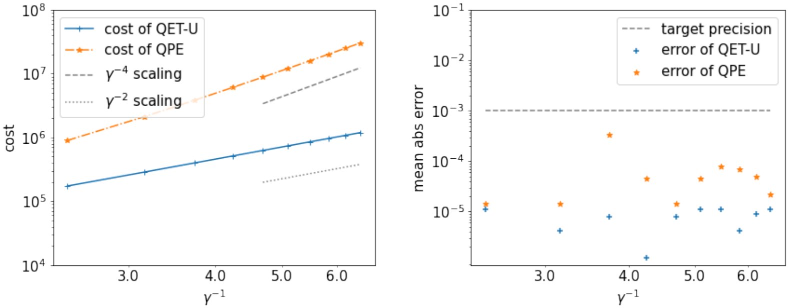
- Short depth algorithm. Circuit depth: $\widetilde{\mathcal{O}}\left(\epsilon^{-1}\right)$. Queries to $U = \widetilde{\mathcal{O}}\left(\epsilon^{-1}\gamma^{-2}\right)$

- Gate count can be small enough to consider on near-term devices.

- Binary amplitude estimation using QET-U[1]: quadratic speedup to near-optimal complexity. Circuit depth: $\widetilde{\mathcal{O}}\left(\epsilon^{-1}\gamma^{-1}\right)$. Queries to $U = \widetilde{\mathcal{O}}\left(\epsilon^{-1}\gamma^{-1}\right)$. Use 2 ancilla qubits.

[1] (Dong-**Lin**-Tong, 2204.05955)

Performance comparison for ground state energy estimation (a simple Kitaev-like circuit)



(Dong-**Lin**-Tong, 2204.05955)

Control-free implementation of certain Hamiltonians

- Based on certain anticommutation relation in Hamiltonian.
- Example: Transverse Field Ising Model (TFIM)

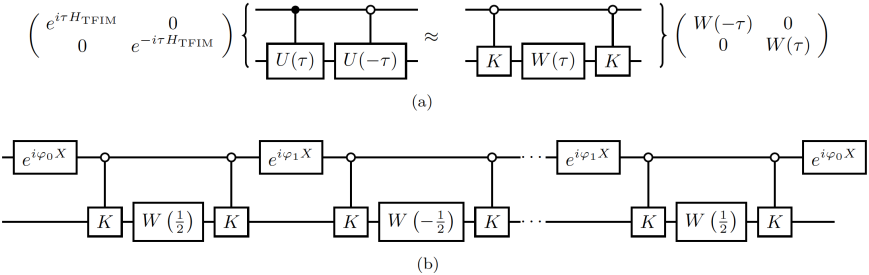
$$H_{\text{TFIM}} = \underbrace{-\sum_{j=1}^{n-1} Z_j Z_{j+1}}_{H^{(1)}_{\text{TFIM}}} \underbrace{-g \sum_{j=1}^{n} X_j}_{H^{(2)}_{\text{TFIM}}} .$$

- Pauli string $K := Y_1 \otimes Z_2 \otimes Y_3 \otimes Z_4 \otimes \cdots$ anticommutes with two sub Hamiltonians

$$\{K, H^{(j)}_{\text{TFIM}}\} = 0 \Rightarrow K e^{itH^{(j)}_{\text{TFIM}}} K = e^{-itH^{(j)}_{\text{TFIM}}}$$

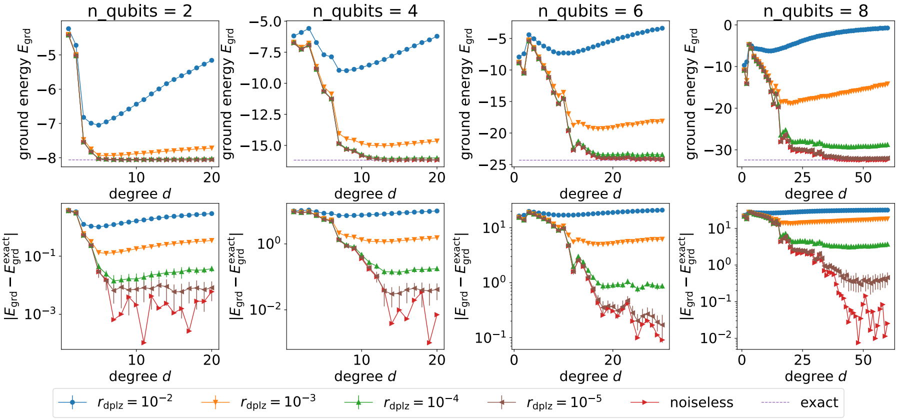
- Conjugating with $K \Rightarrow$ negating evolution time.

Control-free implementation



- $W(\tau)$ is the approximation to the time evolution $U(\tau)$ by Trotter splitting.
- No need to control the time evolution directly.
- Ease of the practical implementation by reducing gates and depth.

Performance of short depth algorithm on TFIM



Implementation in Qiskit. No error mitigation.

Conclusions

Algorithmic ingredients to achieve near-optimal complexity:

- Efficient implementation of eigenstate filtering.
- Binary search based ground state energy estimation.
- Binary amplitude estimation to reduce number of repetitions.

QET-U:

- Hamiltonian evolution access can be as efficient as block encoding access.
- Suitable for early fault-tolerant devices.
- Achieve near-optimal complexity using ≤ 3 ancilla qubits.

Acknowledgment

Thank you for your attention!

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