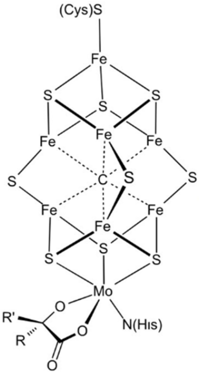
Eigenvalue problems

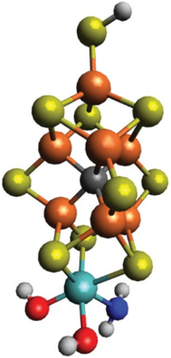
Lin Lin

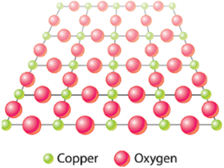
Department of Mathematics, UC Berkeley

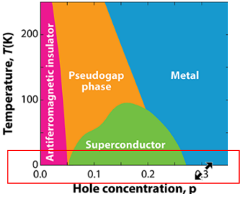
April, 2026

Quantum ground state preparation and ground-state energy estimation









Ground state preparation and ground state energy estimation

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

- Estimate the smallest eigenvalue λ_0 to precision ϵ.

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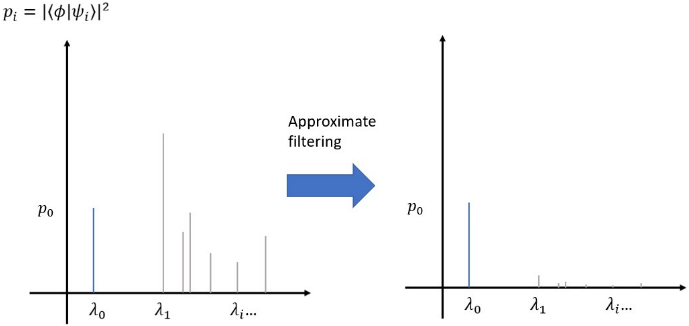
- Standard assumption: good initial state $|\phi\rangle$:
  $p_0 = \gamma^2 = |\langle\phi|\psi_0\rangle|^2 = \Omega(1)$.
- Methods with performance guarantee. Can be combined with e.g., VQE (prepare good initial state)

Quantum phase estimation (and post-QPE methods)



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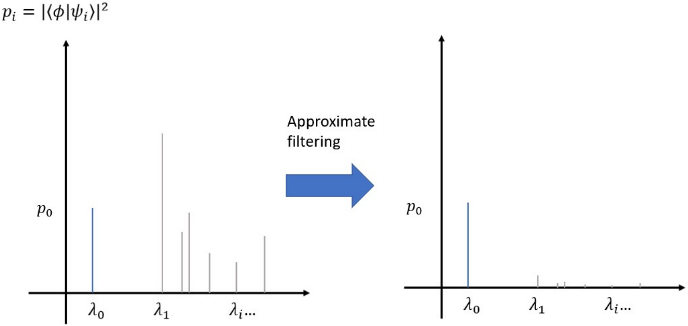

- Filtering or post-selection.
- # repetition p_0^{-1}; optimal scaling[1] is $p_0^{-\frac{1}{2}}$
- Do not work if $p_0 = |\langle\phi|\psi_0\rangle|^2$ is small

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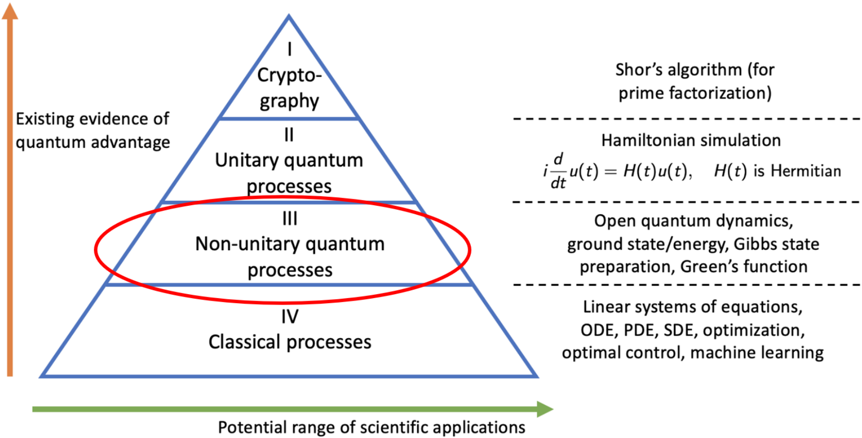
[1] (**L.**-Tong, *Near-optimal ground state preparation*, Quantum 2020)



Existing evidence of quantum advantage

I
Crypto-graphy

II
Unitary quantum processes

III
Non-unitary quantum processes

IV
Classical processes

Potential range of scientific applications

Shor's algorithm (for prime factorization)

Hamiltonian simulation

$i\frac{d}{dt}u(t) = H(t)u(t), \quad H(t)$ is Hermitian

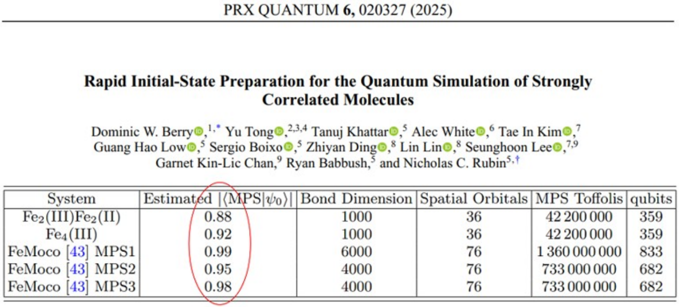
Open quantum dynamics, ground state/energy, Gibbs state preparation, Green's function

Linear systems of equations, ODE, PDE, SDE, optimization, optimal control, machine learning

Can we prepare a good initial state? Given that classical computer can prepare a good initial state, is the problem still classically hard?

(Lee et al, Nature Communications 14, 1952, 2023)

Maybe we can prepare a good initial state



PRX QUANTUM **6,** 020327 (2025)

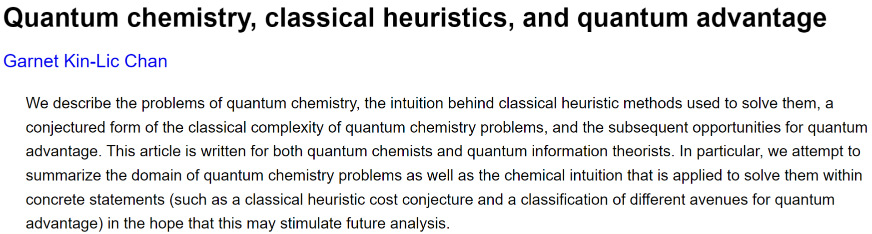
Rapid Initial-State Preparation for the Quantum Simulation of Strongly Correlated Molecules

Dominic W. Berry[1,*] Yu Tong[2,3,4] Tanuj Khattar[5] Alec White[6] Tae In Kim[7]
Guang Hao Low[5] Sergio Boixo[5] Zhiyan Ding[8] Lin Lin[8] Seunghoon Lee[7,9]
Garnet Kin-Lic Chan[9] Ryan Babbush[5] and Nicholas C. Rubin[5,†]

System	Estimated $\|\langle \mathrm{MPS}\|\psi_0\rangle\|$	Bond Dimension	Spatial Orbitals	MPS Toffolis	qubits
$\mathrm{Fe_2(III)Fe_2(II)}$	0.88	1000	36	42 200 000	359
$\mathrm{Fe_4(III)}$	0.92	1000	36	42 200 000	359
FeMoco [43] MPS1	0.99	6000	76	1 360 000 000	833
FeMoco [43] MPS2	0.95	4000	76	733 000 000	682
FeMoco [43] MPS3	0.98	4000	76	733 000 000	682

Given that classical computer can prepare a good initial state, is the problem still classically hard?

Maybe still worth it to refine to error ϵ with $\mathcal{O}(\epsilon^{-1})$ quantum queries.



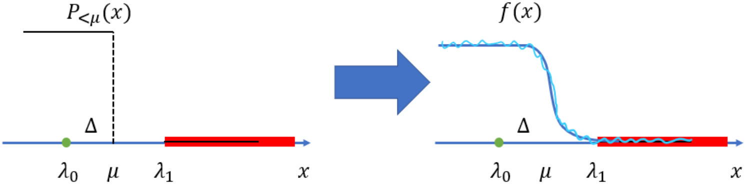
Quantum chemistry, classical heuristics, and quantum advantage

Garnet Kin-Lic Chan

We describe the problems of quantum chemistry, the intuition behind classical heuristic methods used to solve them, a conjectured form of the classical complexity of quantum chemistry problems, and the subsequent opportunities for quantum advantage. This article is written for both quantum chemists and quantum information theorists. In particular, we attempt to summarize the domain of quantum chemistry problems as well as the chemical intuition that is applied to solve them within concrete statements (such as a classical heuristic cost conjecture and a classification of different avenues for quantum advantage) in the hope that this may stimulate future analysis.

(Chan, Spiers Memorial Lecture, arXiv:2407.11235)

Ground state preparation: eigenstate filtering



- First assume μ is given.

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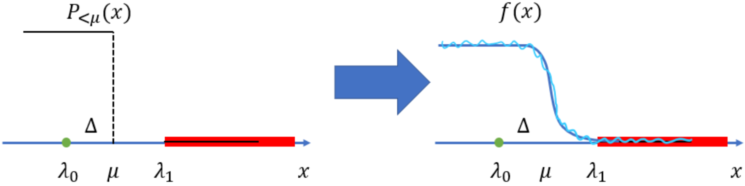

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- Polynomial / trigonometric approximation to step functions.

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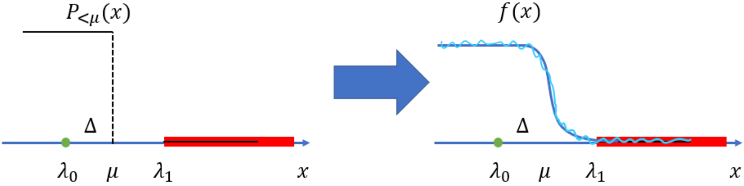

- First assume μ is given.
- Polynomial / trigonometric approximation to step functions.
- Implement a matrix function via an efficient quantum circuit

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

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 $\lambda_0 < (a+b)/2$.

Binary search based ground state energy estimation

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- 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.

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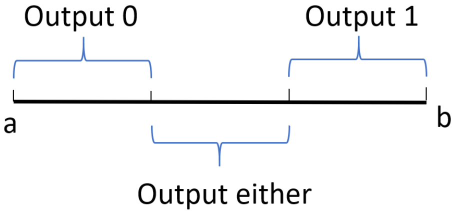
- This does not work because we are essentially asking the quantum circuit to compute a discontinuous function while the output probability distribution is a continuous function of λ_0.
- Need to account for the fuzziness and statistical uncertainty.

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.



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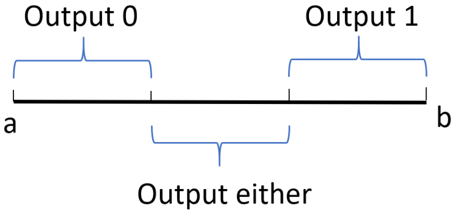
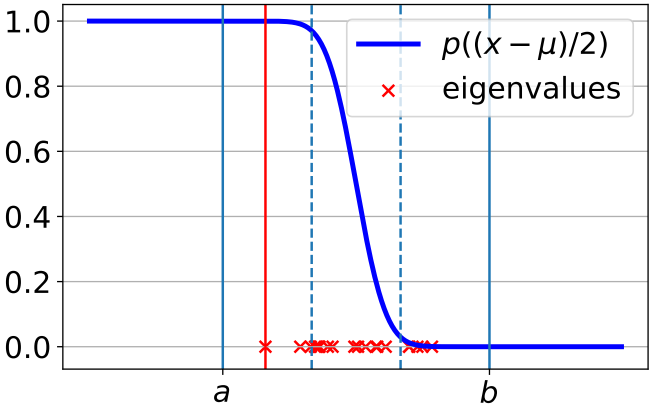


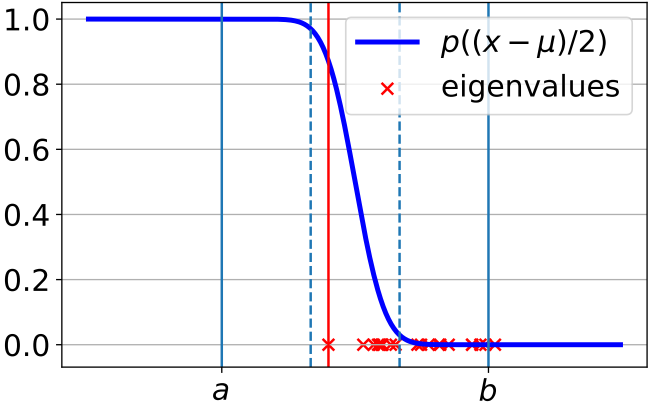
- Success probability of measuring ancilla $p = \| f(H) \left|\phi\right\rangle \|^2$.
- Distinguish between $\| f(H) \left|\phi\right\rangle \| \ge \gamma(1-\epsilon')$ and $\| f(H) \left|\phi\right\rangle \| \le \epsilon'$.

Solving the decision problem (i)



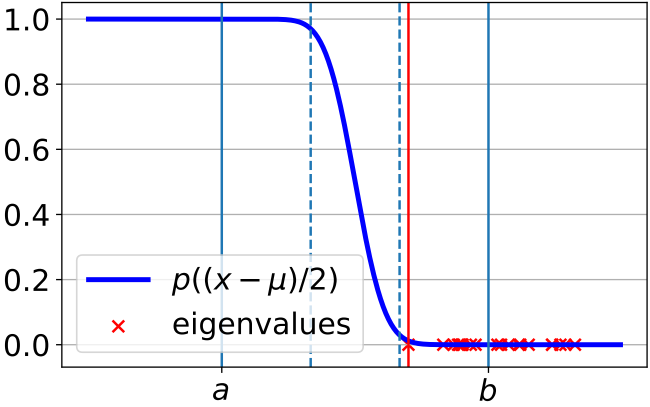
$$\lambda_0 \leq \frac{2}{3}a + \frac{1}{3}b \implies \| f(H) \, |\phi\rangle \, \| \geq \gamma(1-\epsilon')$$

Solving the decision problem (ii)



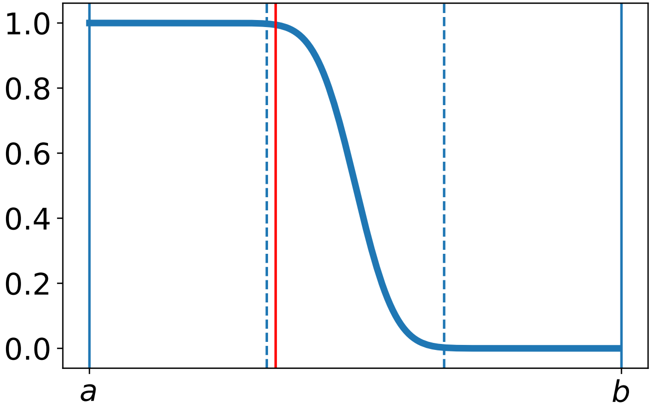
$$\tfrac{2}{3}a + \tfrac{1}{3}b \leq \lambda_0 \leq \tfrac{1}{3}a + \tfrac{2}{3}b$$

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



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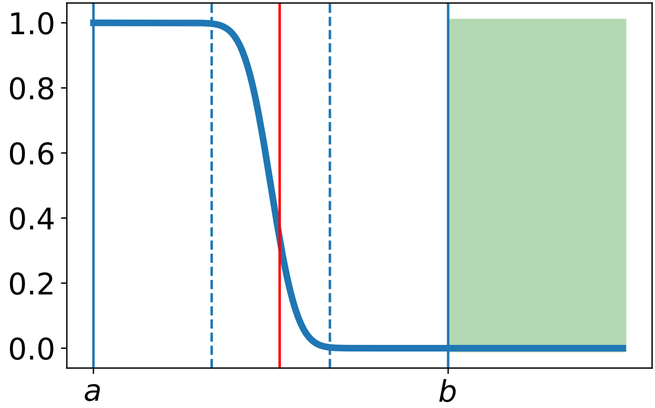

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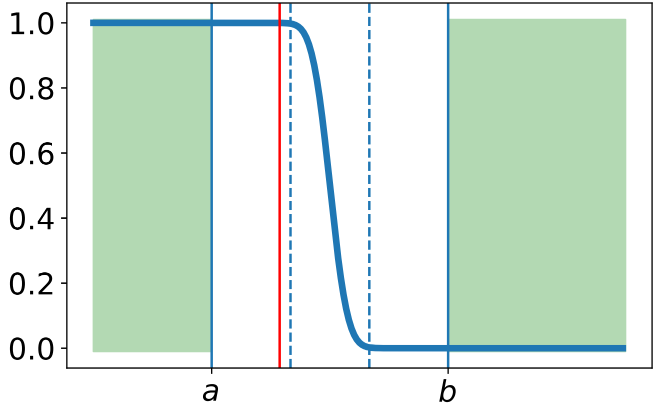

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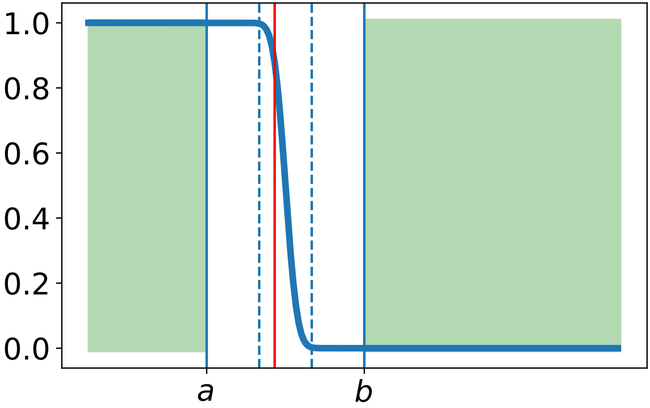

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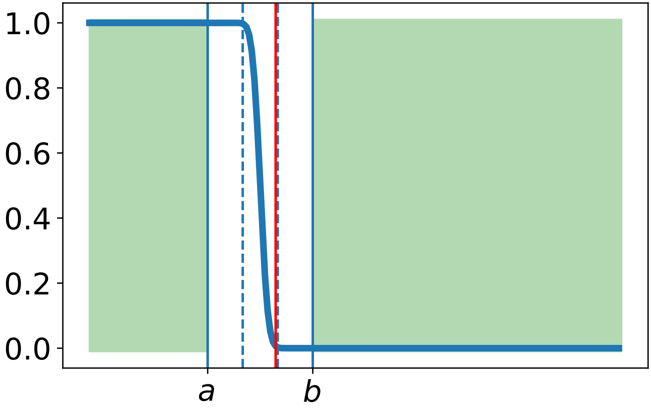

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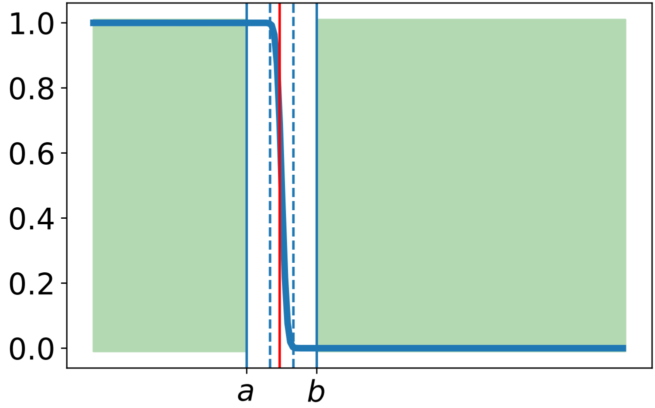

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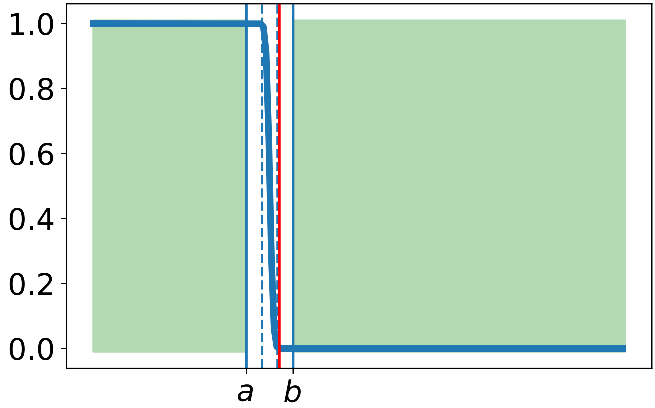

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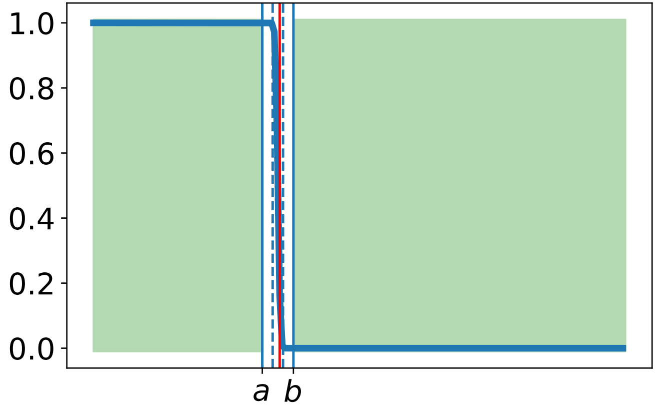

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- Error probability can be exponentially suppressed using majority voting (Chernoff bound).

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Summary of the main steps

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

Towards early fault-tolerant quantum eigensolver

[LT20] uses the block encoding framework:

- Many ancillary qubits.
- Long circuit depth (preconstant).
- Complex control logics.

Efficient quantum eigensolvers for early fault tolerant quantum computer?

Early fault-tolerant (EFT) quantum algorithm

Limited useful quantum resources:

- Selective application of quantum error correction to components most susceptible to noise

No universally accepted definition of an early fault-tolerant quantum computer. See recent discussions: (Katabarwa et al, *Early fault-tolerant quantum computing*, PRX Quantum 2024)

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Need significantly simplified algorithm for practical deployment.

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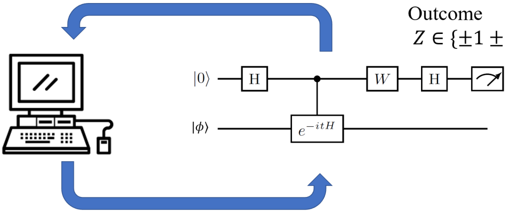
Single ancilla quantum phase estimation

Classical postprocessing



Outcome
$Z \in \{\pm 1 \pm i\}$

Evolution time t

Alexei Kitaev

Kitaev algorithm: $p_0 = \gamma^2 \approx 1$. (Kitaev, Shen, Vyalyi, 2002)

Post-Kitaev type: (**L.**, Tong, PRX Quantum 2022); (Dong-**L.**-Tong, PRX Quantum 2022); (Wan, Berta, Campbell, PRL 2022); (Ding-**L.**, PRX Quantum 2023); (Ding-**L.**, Quantum, 2023); (Wang et al, Quantum 2023); (Ni, Li, Ying, Quantum 2023); (Ding et al, Quantum 2024)...

Quantum Krylov subspace type: (Parrish, McMahon, 2019); (Stair, Huang, Evangelista, JCTC 2020); (Epperly, **L.**, Nakatsukasa, SIMAX 2022); (Klymko et al, PRX Quantum 2022); (Shen et al, QCE 2023); (Li, Ni, Ying, PRA 2023); (Ding, Epperly, **L.**, Zhang, arXiv: 2404.03885, FOCS 2024)(Yoshioka et al, Nature Comm. 2025)(Barison et al, QST 2025)...

Experimental relevance: (Blunt et al, PRX Quantum 2023); (Kiss et al, arXiv:2405.03754)..

Workflow

Evolution
time $t_n = \color{red}{n\tau}$

$Z_n \in \{\pm 1 \pm i\}$

$T_{\max} = \max t_n$: Maximal evolution time (circuit depth)
$T_{\text{total}} = \sum_n t_n$: Total evolution time (total cost)

Dataset

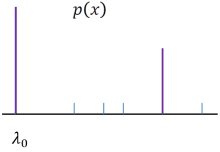
$$\mathcal{D}_H = \{(t_n, Z_n)\}_{n=0}^{N-1}, \quad t_n \in \mathbb{R}, \quad Z_n \in \{\pm 1 \pm i\}$$

so that

$$\mathbb{E} Z_n = \langle \phi | \exp(-i t_n H) | \phi \rangle = \sum_j p_j e^{-i t_n \lambda_j} =: \int e^{-i t_n x} p(x) \, \mathrm{d}x.$$

- Choice of $\{t_n\}$ is important. Allow repetition. $T_{\text{total}} = \sum_n t_n$.
- Classical signal processing of noisy data to estimate spectral density

$$p(x) = \sum_j p_j \delta(x - \lambda_j).$$



Ground state energy: first peak of $p(x)$.

Choice of $\{t_n\}$

Consider $|\phi\rangle = |\psi_0\rangle$ (or $p_0 = 1$)

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- Uniform grid: $t_n = n\tau$. $N\tau = \epsilon^{-1}$
  $T_{\mathrm{total}} = \widetilde{\mathcal{O}}(\epsilon^{-2})$. Standard quantum limit

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  $T_{\text{total}} = \widetilde{\mathcal{O}}(\epsilon^{-2})$. Standard quantum limit

- Kitaev's algorithm: logarithmic grid: $t_n = 2^n \tau$, $2^N \tau = \epsilon^{-1}$.
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Choice of $\{t_n\}$

Consider $|\phi\rangle = |\psi_0\rangle$ (or $p_0 = 1$)

$$\mathcal{D}_H = \{(t_n, Z_n)\}_{n=0}^{N-1}, \quad t_n \in \mathbb{R}, \quad Z_n \in \{\pm 1 \pm i\}$$

so that

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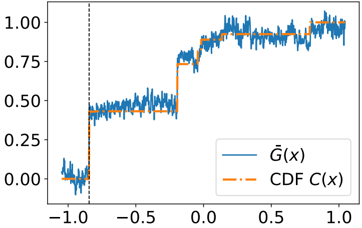
Early fault tolerant eigensolver with Heisenberg limited scaling?

First EFT eigensolver with Heisenberg scaling

- Randomized evolution time:
  $\mathbb{P}(t_n = j\tau) \propto j$-th Fourier coefficient of Heaviside function

- Noisy approximation to the cumulative density function (CDF)
  $C(\mu) = \int_{-\infty}^{\mu} p(x)\,\mathrm{d}x$.



- Works for any $p_0 > 0$. $T_{\text{total}} = \widetilde{\mathcal{O}}(\epsilon^{-1} p_0^{-2})$

(**L.**-Tong, *Heisenberg-limited ground state energy estimation for early fault-tolerant quantum computers*, PRX Quantum 2022)

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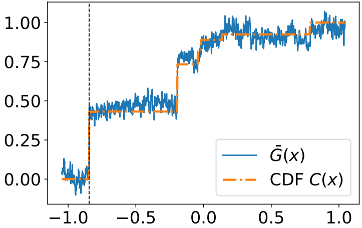

- Can improve to near optimal complexity $T_{\text{total}} = \widetilde{\mathcal{O}}(\epsilon^{-1} p_0^{-\frac{1}{2}})$ with 3 ancilla qubits

(Dong-**L.**-Tong, *Ground state preparation and energy estimation on early fault-tolerant quantum computers via quantum eigenvalue transformation of unitary matrices*, PRX Quantum 2022)

Short-depth quantum eigensolver?

- Assume $\|H\| \leq 1$, so far, all algorithms require circuit depth

$$T_{\max} := \max_n t_n \geq \frac{\pi}{\epsilon}.$$

$\epsilon = 10^{-3}$ gives $T_{\max} \approx 3000$.

Short-depth quantum eigensolver?

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$$T_{\max} := \max_n t_n \geq \frac{\pi}{\epsilon}.$$

$\epsilon = 10^{-3}$ gives $T_{\max} \approx 3000$.

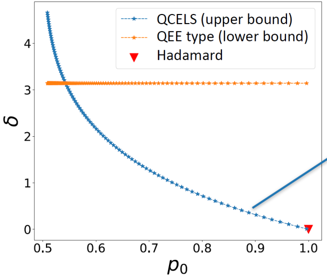
- As $p_0 \to 1$, can we design quantum eigensolvers with short circuit depth while maintaining Heisenberg limited scaling?

$$T_{\max} = \frac{\delta}{\epsilon}, \quad \delta \ll 1.$$

First short-depth quantum eigensolver

- Quantum complex exponential least squares (QCELS)[1]
- Randomized evolution time: Truncated Gaussian distribution

$$\mathbb{P}(t_n = t) \propto e^{-\frac{t^2}{2T_{\max}^2}} \mathbf{1}_{[-\gamma T_{\max}, \gamma T_{\max}]}, \quad T_{\max} = \frac{\delta}{\epsilon}, \quad \delta = \mathcal{O}(1 - p_0).$$



$T_{\max} = \mathcal{O}\left(\frac{1 - p_0}{\epsilon}\right)$

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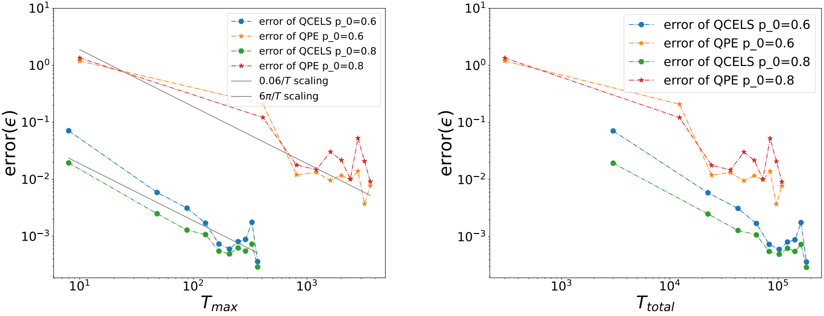
[1] Ding-**L.**, *Even shorter quantum circuit for phase estimation on early fault-tolerant quantum computers with applications to ground-state energy estimation*, PRX Quantum 2023
See also (Ni-Li-Ying, Quantum 2023)(Ding-**L.**, Quantum 2023).

Numerical results for QCELS

Transverse field Ising model (TFIM)



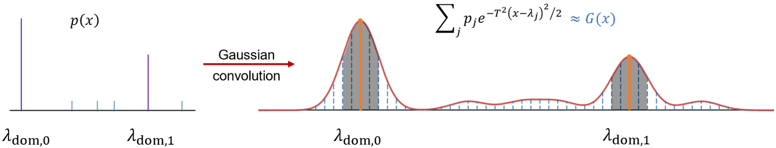
- Two order of magnitude reduction of T_{max}
- Comparable (in fact, a bit smaller) T_{total}.

Quantum Multiple Eigenvalue Gaussian filtered Search (QMEGS)

- Randomized evolution time: Truncated Gaussian distribution

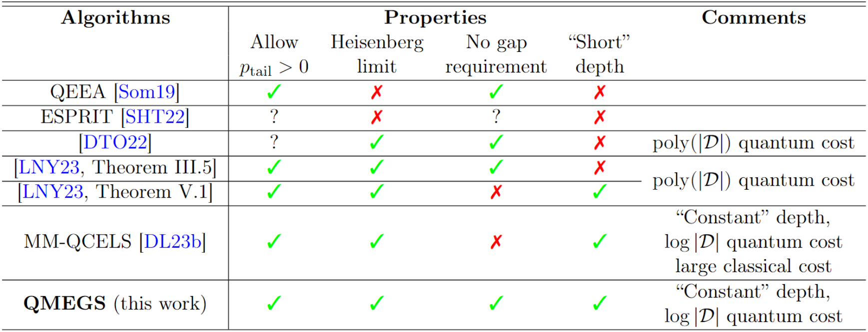
$$\mathbb{P}(t_n = t) \propto e^{-\frac{t^2}{2T_{\max}^2}} \mathbf{1}_{[-\gamma T_{\max}, \gamma T_{\max}]}, \quad T_{\max} = \frac{\delta}{\epsilon}, \quad \delta = \mathcal{O}(1 - p_0).$$

- Compute $G(x) \propto \left|\sum_n Z_n e^{i t_n x}\right|$ at each grid point x. Find the maximum point and block a neighborhood; and repeat



(Ding, Li, **L.**, Ni, Ying, Zhang, Quantum 2024)

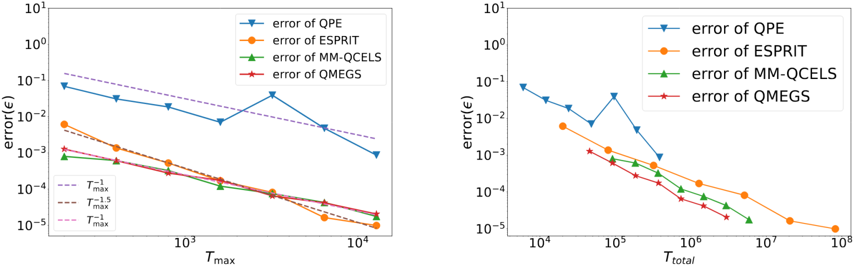
Quantum Multiple Eigenvalue Gaussian filtered Search (QMEGS)



Algorithms	**Properties**				**Comments**
	Allow $p_{\text{tail}} > 0$	Heisenberg limit	No gap requirement	"Short" depth	
QEEA [Som19]	✓	✗	✓	✗	
ESPRIT [SHT22]	?	✗	?	✗	
[DTO22]	?	✓	✓	✗	poly($\lvert\mathcal{D}\rvert$) quantum cost
[LNY23, Theorem III.5]	✓	✓	✓	✗	poly($\lvert\mathcal{D}\rvert$) quantum cost
[LNY23, Theorem V.1]	✓	✓	✗	✓	
MM-QCELS [DL23b]	✓	✓	✗	✓	"Constant" depth, $\log\lvert\mathcal{D}\rvert$ quantum cost large classical cost
QMEGS (this work)	✓	✓	✓	✓	"Constant" depth, $\log\lvert\mathcal{D}\rvert$ quantum cost

- Dominant modes $\lambda_{\text{dom},m}$, $m \in \mathcal{D}$. $p_{\text{tail}} = \sum_{i \in \mathcal{D}^c} p_i$.
- $p_{\min} = \min_{i \in \mathcal{D}} p_{\text{dom},i} \gtrsim p_{\text{tail}}$. Gap $\Delta := \min_{i \in \mathcal{D}, j \neq i} \left|\lambda_{\text{dom},i} - \lambda_j\right|$
- "Short" depth: $T_{\max} = \widetilde{\mathcal{O}}(p_{\text{tail}}/\epsilon)$
- "Constant" depth: $T_{\max} = \widetilde{\mathcal{O}}(\Delta \log \epsilon^{-1})$

Numerical results for QMEGS



ESPRIT: Estimation of signal parameters via rotational invariance techniques.
See (Roy, Kailath, 1989). Used recently for quantum eigensolver (Shen et al, QCE 2023)
Noisy super-resolution of ESPRIT: (Ding, Epperly, **L.**, Zhang, FOCS 2024)