

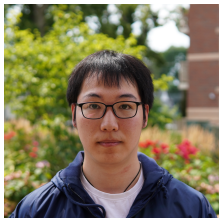
# Quantum algorithms for eigenvalue problems

Lin Lin

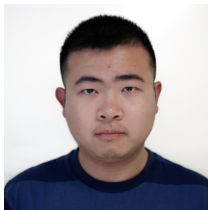
Department of Mathematics, UC Berkeley  
Lawrence Berkeley National Laboratory  
Challenge Institute for Quantum Computation

Ordway lecture, University of Minnesota  
April, 2023

## Joint work with



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Prof.)



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(Berkeley)



**Yu Tong**  
(Caltech, IQIM Fellow)

# Outline

Introduction

Main results

Algorithms

Current directions

Proof ideas

# What is a quantum computer (mathematically)

- $|\psi\rangle \in \mathbb{C}^N \cong (\mathbb{C}^2)^{\otimes n}$ ,  $N = 2^n$ .  $n$ : number of **qubits**.
- Normalization condition  $\langle\psi|\psi\rangle = \sum_{j=0}^{N-1} |\psi_j|^2 = 1$ .
- Quantum gate: unitary matrix  $U \in \mathbb{C}^{N \times N}$ . For some  $U$ , application  $U|\psi\rangle$  is **efficient**: cost is  $\mathcal{O}(\text{polylog}(N))$ .
- Quantum algorithm: a series of large matrix-vector multiplications:  $U_K \cdots U_1 |\psi\rangle$ . Then measure some qubits and repeat  $M$  times for classical output.
- Quantum cost (roughly):  $MK \text{polylog}(N)$ .
- Exponential quantum advantage (EQA): if  $MK = \mathcal{O}(\text{polylog}(N))$ , **and** classical algorithm scales as  $\mathcal{O}(\text{poly}(N))$ .

# A fast growing industry



I don't know. Maybe this is going to be like nuclear fusion (always 10 years away)..

Will a fault-tolerant quantum computer ever be built?

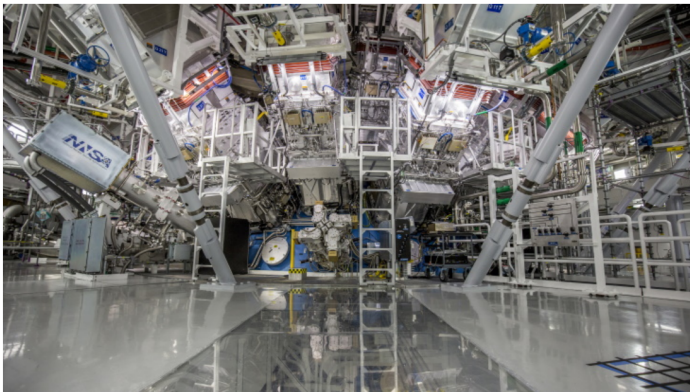


## US researchers achieve historic fusion ignition

13 December 2022



**The first ever controlled fusion experiment to produce more energy from fusion than the laser energy used to drive it was conducted at the National Ignition Facility (NIF) at the Lawrence Livermore National Laboratory (LLNL) on 5 December - a breakthrough that has been decades in the making.**



*The target chamber at NIF (Image: LLNL)*

# Quantum numerical linear algebra

- Solving numerical linear algebra problems on a quantum computer. Exciting progress in the past few years.
- Note “Quantum algorithms for scientific computation”<sup>1</sup>
- This talk is about **eigenvalue problems**:

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

$H \in \mathbb{C}^{N \times N}$  Hermitian matrix (Hamiltonian).

Find the **smallest**  $\lambda_0$  and/or prepare  $|\psi_0\rangle$

- **One of the most important** problems in quantum physics, quantum chemistry and materials science.

<sup>1</sup>arXiv:2201.08309. More frequently updated: <https://math.berkeley.edu/~linlin/qasc/>



## Hamiltonian evolution input model

- Unitary matrix:  $U_H = e^{-i\tau H}$  for some  $\tau$ .
- e.g.,  $H = \sum_{i=1}^n Z_i$ ,  $U_H = \prod_{i=1}^n e^{-i\tau Z_i}$  can be implemented with  $n$  single qubit gate rotations. **Gate complexity** is  $n = \log_2 N$ .
- Approximate implementation  $\|U_H - e^{-i\tau H}\| \leq \epsilon$  via e.g., Trotter expansion is acceptable.
- Long time evolution  $e^{-iTH} = U_H^d$ .  
**Runtime**  $T = d\tau$ . Query depth  $d$ .  
Both measure **query complexities**

# Assumptions in this talk

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

- Hamiltonian evolution input model:  $U_H = e^{-i\tau H}$  for some  $\tau$ .
- A **good**<sup>1</sup> initial state  $|\phi\rangle = U_I|0^n\rangle$ ,  $p_0 = |\langle\phi|\psi_0\rangle|^2 = \Omega(1)$ .  
 $|0^n\rangle = |0\rangle^{\otimes n} = (1, 0, \dots, 0)^\top$ .
- **Ground-state energy estimation**: estimate  $\lambda_0$  to precision  $\epsilon$ .
- Good initial state is a very strong assumption. But without it, the problem is theoretically intractable in the worst case<sup>2</sup>.
- Focus on methods with **performance guarantee**. Can be **combined** with e.g., VQE (prepare good initial state)

<sup>1</sup>Can be theoretically relaxed to  $\gamma = \Omega(1/\text{poly}(n))$ .

<sup>2</sup>The worst case is QMA-hard, which is a quantum analogue of NP hardness. In other words, the task can be difficult even with a perfect quantum computer.

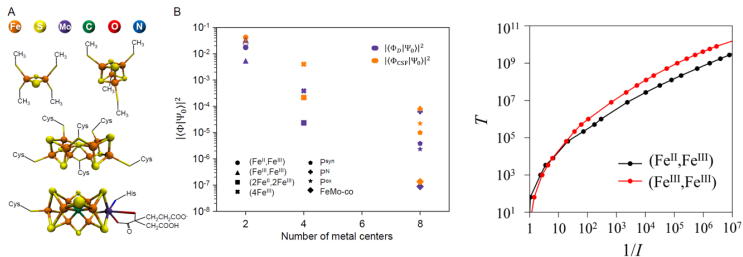
# Exponential quantum advantage under debate

## nature communications

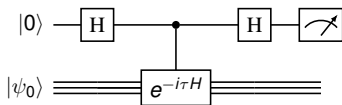
### Evaluating the evidence for exponential quantum advantage in ground-state quantum chemistry

[Seunghoon Lee](#), [Joonho Lee](#), [Huanchen Zhai](#), [Yu Tong](#), [Alexander M. Dalzell](#), [Ashutosh Kumar](#), [Phillip Helms](#), [Johnnie Gray](#), [Zhi-Hao Cui](#), [Wenyuan Liu](#), [Michael Kastoryano](#), [Ryan Babbush](#), [John Preskill](#), [David R. Reichman](#), [Earl T. Campbell](#), [Edward F. Valeev](#), [Lin Lin](#) & [Garnet Kin-Lic Chan](#) 

*Nature Communications* **14**, Article number: 1952 (2023) | [Cite this article](#)



## Textbook algorithm 1: Hadamard test



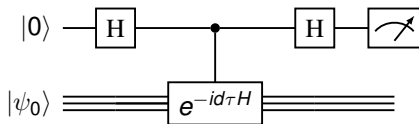
$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

- Readout the success probability

$$p(0) = \frac{1}{2} (1 + \text{Re} \langle \psi_0 | e^{-i\tau H} | \psi_0 \rangle) = \frac{1}{2} (1 + \cos(\lambda_0 \tau)).$$

- **Maximal runtime**  $T_{\max} = \tau$  can be **arbitrarily small**: very short circuit depth. At the expense of larger number of repetitions.
- Monte Carlo algorithm: To reach precision  $\epsilon$ , the number of repetitions is  $\mathcal{O}((\epsilon\tau)^{-2})$ . **Total runtime**:  $T_{\text{total}} = \mathcal{O}(\epsilon^{-2}\tau^{-1})$
- Need to prepare **exact eigenstate**, i.e.  $p_0 = |\langle \phi | \psi_0 \rangle|^2 = 1$ .

## Textbook algorithm 2: Kitaev's algorithm

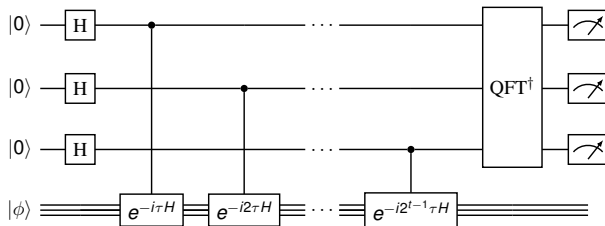


- $d = 1, 2, 4, \dots, 2^{t-1} = \pi(\epsilon\tau)^{-1}$ .
- Maximal runtime  $T_{\max} = 2^{t-1}\tau = \pi/\epsilon$ .
- Total runtime is  $T_{\text{total}} = \tilde{O}(\epsilon^{-1})$ . Heisenberg-limited scaling<sup>1</sup>
- Need to prepare **exact eigenstate**, i.e.  $p_0 = |\langle\phi|\psi_0\rangle|^2 = 1$ .
- Can be modified to accommodate inexact eigenstate<sup>2</sup>  
In this case,  $T_{\max} = \mathcal{O}(\epsilon^{-1}p_0^{-1})$ ,  $T_{\text{total}} = \tilde{O}(\epsilon^{-1}p_0^{-2})$ .

<sup>1</sup>Best scaling allowed by quantum mechanics

<sup>2</sup>The first work is semi-classical QPE, or single ancilla QPE: (Griffiths, Niu, PRL 1996; Higgins et al, Nature 2007)

## Textbook algorithm 3: Quantum phase estimation



- Use many ancilla qubits.
- Exact eigenstate:  $T_{\max} = 2^t \tau = 2\pi/\epsilon$ ,  $T_{\text{total}} = \tilde{\mathcal{O}}(\epsilon^{-1})$ .
- **Naturally** accommodate inexact eigenstate  $p_0 < 1$ .  
In this case,  $T_{\max} = \mathcal{O}(\epsilon^{-1} p_0^{-1})$ ,  $T_{\text{total}} = \tilde{\mathcal{O}}(\epsilon^{-1} p_0^{-2})$ .

# Outline

Introduction

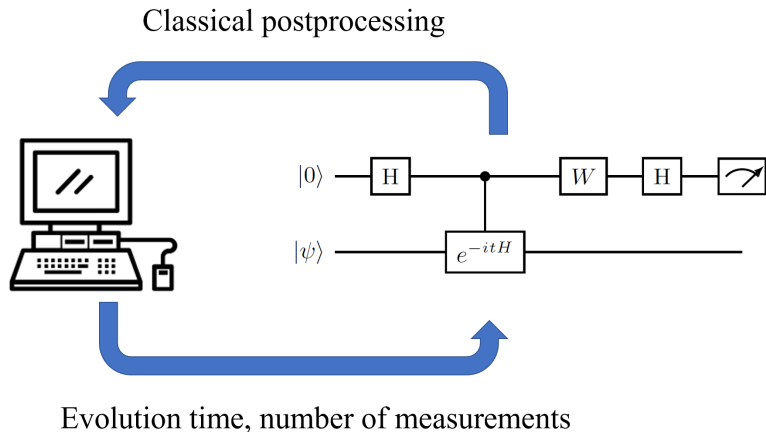
**Main results**

Algorithms

Current directions

Proof ideas

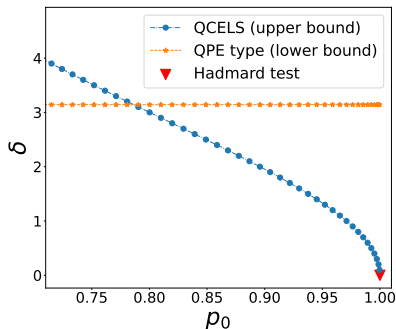
# Classical post-processing of Hadamard test circuit



Simple and surprisingly powerful.



# Theoretical comparison of preconstants with large $\rho_0$

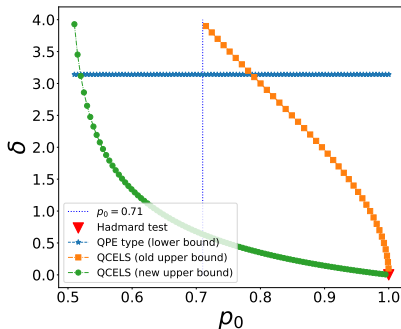


$$T_{\max} = \frac{\delta}{\epsilon}$$

QCELS: quantum complex exponential least squares

## Further improvement of preconstant

$$\delta = \Theta(\sqrt{1 - \rho_0}) \rightarrow \delta = \Theta(1 - \rho_0), \quad T_{\max} = \frac{\delta}{\epsilon}.$$



Earlier bound (Ding-Lin, , PRX Quantum 2023); New bound: (Ding-Lin, 2303.05714)

See also (Ni-Li-Ying, 2302.0245) for proving robust phase estimation (RPE) satisfies  $\delta = \Theta(1 - \rho_0)$ .

## Large $p_0$

### Theorem (Ding-Lin, 2211.11973)

If  $p_0 > 0.71$ , choose

$$\delta = \Theta(\sqrt{1 - p_0}).$$

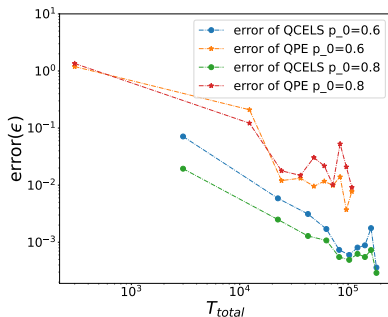
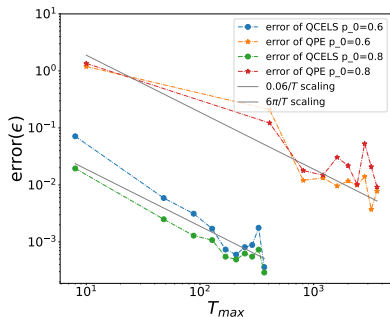
*There exists an algorithm that uses 1 ancilla qubit to estimate  $\lambda_0$  to precision  $\epsilon$  with*

$$T_{\max} = \frac{\delta}{\epsilon}, \quad T_{\text{total}} = \tilde{\Theta} \left( \delta^{-(1+o(1))} \epsilon^{-1} \right).$$

- Distinct feature: the preconstant  $\delta$  can be **arbitrarily small** as  $p_0 \rightarrow 1$ .

# Numerical results for large $\rho_0$

## Transverse field Ising model (TFIM)<sup>1</sup>

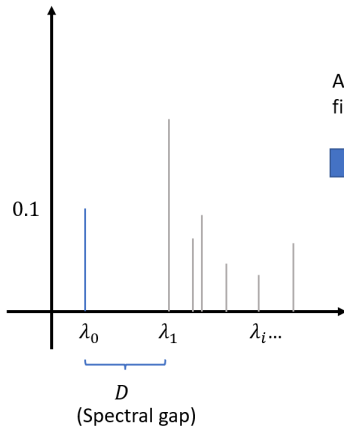


- Numerical performance is much better than theoretical prediction, and the bound 0.71 can be pushed downward.
- **Two order of magnitude reduction** of maximal runtime!

<sup>1</sup>QCELS refers to the multi-level version of quantum complex exponential least squares

# Small $p_0$ : convert to large $p_0$ with a spectral gap

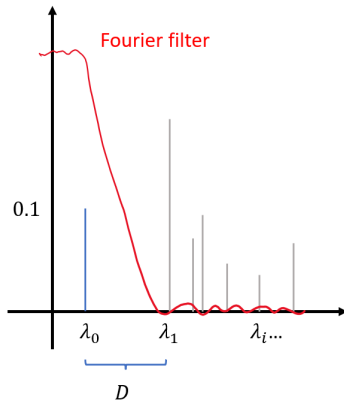
$$p_i = |\langle \phi | \psi_i \rangle|^2$$



Approximate  
filtering

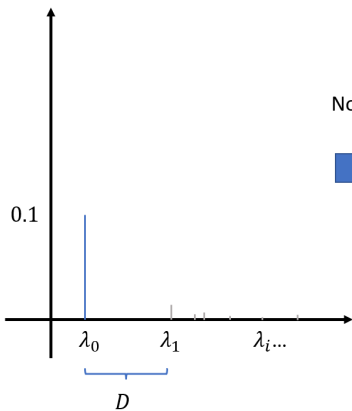


$$p_i = |\langle \phi | \psi_i \rangle|^2$$



## Small $p_0$ : convert to large $p_0$ with a spectral gap

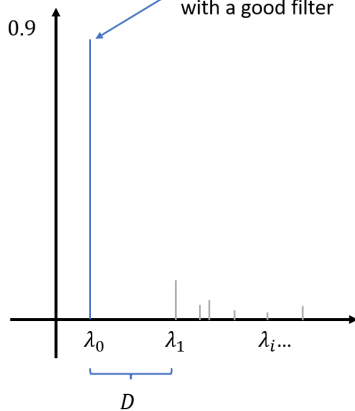
$$p_i = |\langle \phi | \psi_i \rangle|^2$$



Normalization



$$p_i = |\langle \phi | \psi_i \rangle|^2$$

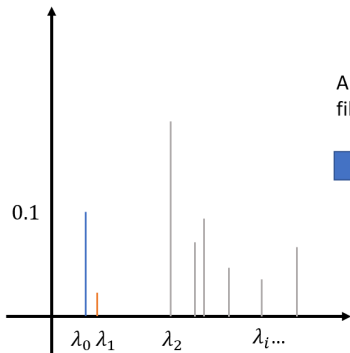


Can approach 1  
with a good filter

Apply the algorithm for the case of large  $p_0$ !

# Small $p_0$ : what if the spectral gap is small?

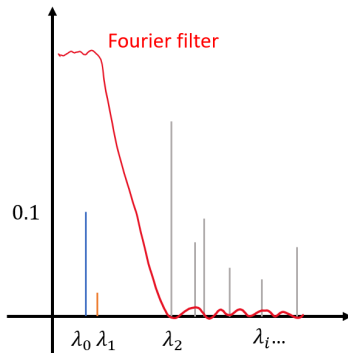
$$p_i = |\langle \phi | \psi_i \rangle|^2$$



Approximate  
filtering

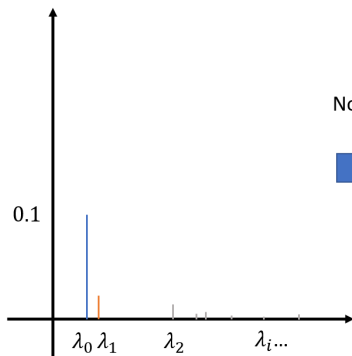


$$p_i = |\langle \phi | \psi_i \rangle|^2$$



## Small $p_0$ : what if the spectral gap is small?

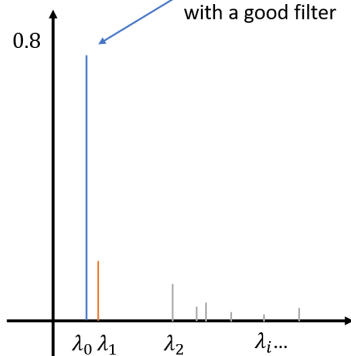
$$p_i = |\langle \phi | \psi_i \rangle|^2$$



Normalization



$$p_i = |\langle \phi | \psi_i \rangle|^2$$

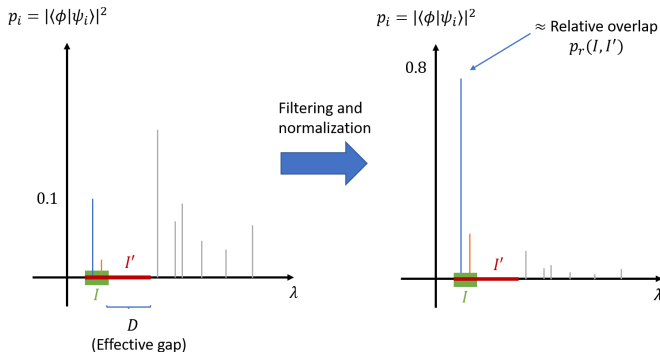


Apply the algorithm for the case of large  $p_0$ !



# Relative overlap

$$p_r(I, I') = \frac{|\langle \psi | \psi_0 \rangle|^2 \mathbb{1}_{\lambda_0 \in I}}{\sum_{\lambda_k \in I'} |\langle \psi | \psi_k \rangle|^2}$$



The concept of relative overlap is applicable to certain **small gapped quantum systems**, and is aware of the information of the **initial state**.

## Small $p_0$

### Theorem (Ding-Lin, 2211.11973)

Given relative overlap  $p_r(I, I') \geq 0.71$ ,  $D = \min_{x_1 \notin I', x_2 \in I} |x_1 - x_2|$ , choose

$$\delta = \Theta(\sqrt{1 - p_r(I, I')}).$$

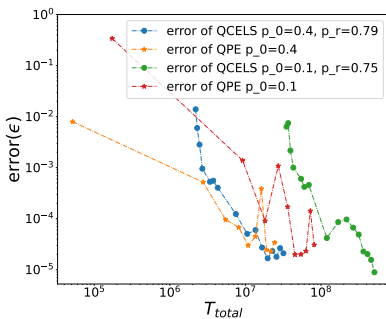
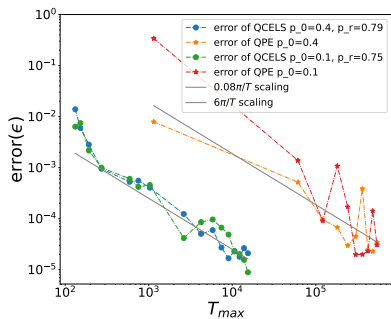
There exists an algorithm that uses 1 ancilla qubit to estimate  $\lambda_0$  to precision  $\epsilon$  with

$$T_{\max} = \tilde{\Theta}(D^{-1}) + \delta/\epsilon, \quad T_{\text{total}} = \tilde{\Theta}\left(p_0^{-2}\delta^{-(2+o(1))}\left(D^{-1} + \delta/\epsilon\right)\right).$$

- Distinct feature: can use the information of relative overlap (all previous algorithms are agnostic to it)
- Reduce circuit depth when  $D \gg \epsilon$  and  $p_r(I, I')$  is large.

# Numerical results for small $\rho_0$

## Hubbard model



Two order of magnitude reduction of maximal runtime!

## Criterion for comparing quantum algorithms

Number of  
ancilla qubits

Circuit depth

Gate set

Total cost

# Full fault-tolerant quantum computer

Large number  
of ancilla qubits

Long circuit  
depth

Multi-qubit  
control gates

Asymptotic  
total cost

## Early fault-tolerant quantum computer

$O(1)$  ancilla qubits

Short circuit depth

Simple gates

Larger number of repetitions and total cost

Eventually, lead to a small **non-Clifford (Toffoli/T)** gate count.

# Progresses for ground-state energy estimation

	Maximal runtime	Total runtime	# ancilla qubits	Need MQC?	Input model
QPE (high confidence)	$\tilde{O}(\epsilon^{-1})$	$\tilde{O}(\epsilon^{-1}\gamma^{-2})$	$\mathcal{O}(\text{polylog}(\gamma^{-1}\epsilon^{-1}))$	High	HE
QPE (1 ancilla)	$\tilde{O}(\epsilon^{-1}\gamma^{-2})$	$\tilde{O}(\epsilon^{-1}\gamma^{-4})$	$\mathcal{O}(1)$	No	HE
Som19 (short depth)	$\tilde{O}(\epsilon^{-1})$	$\tilde{O}(\epsilon^{-4}\gamma^{-4})$	$\mathcal{O}(1)$	No	HE
GTC19	$\tilde{O}(\epsilon^{-3/2}\gamma^{-1})$	$\tilde{O}(\epsilon^{-3/2}\gamma^{-1})$	$\mathcal{O}(\log(\epsilon^{-1}))$	High	HE
LT20*	$\tilde{O}(\epsilon^{-1}\gamma^{-1})$	$\tilde{O}(\epsilon^{-1}\gamma^{-1})$	$m + \mathcal{O}(\log(\epsilon^{-1}))$	High	BE
LT22 (short depth)	$\tilde{O}(\epsilon^{-1})$	$\tilde{O}(\epsilon^{-1}\gamma^{-4})$	$\mathcal{O}(1)$	No	HE
DLT22 (short depth)	$\tilde{O}(\epsilon^{-1})$	$\tilde{O}(\epsilon^{-1}\gamma^{-2})$	$\mathcal{O}(1)$	No	HE
DLT22*	$\tilde{O}(\epsilon^{-1}\gamma^{-1})$	$\tilde{O}(\epsilon^{-1}\gamma^{-1})$	$\mathcal{O}(1)$	Low	HE
<b>DL22</b> (even shorter depth) <sup>◊</sup>	$\tilde{O}(D^{-1}) + \frac{\delta}{\epsilon}$	$\tilde{O}((D^{-1} + \delta/\epsilon)\gamma^{-4})$	$\mathcal{O}(1)$	No	HE

Initial guess  $p_0 = |\langle \phi | \psi_0 \rangle|^2 = \gamma^2$ .

MQC: Multi-qubit control. HE: Hamiltonian evolution. BE: Block encoding

\* Achieves near optimal complexity w.r.t.  $\gamma, \epsilon$ .

◊ Significantly reduced preconstant in depth with large overlap / relative overlap.

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, PRX Quantum 2022);

(Ding-Lin, PRX Quantum 2023)

# Exponential improvement of dependence on precision for gapped system

## Corollary (Ding-Lin, 2211.11973)

*If  $\epsilon \ll D$ , there exists an algorithm that uses 1 ancilla qubit to estimate  $\lambda_0$  to precision  $\epsilon$  with high probability using*

$$T_{\max} = \tilde{\Theta}(D^{-1}), \quad T_{\text{total}} = \tilde{\Theta}\left(D/(p_0^2 \epsilon^2)\right).$$

- $T_{\max}$  is independent of  $\epsilon$ , though this does not satisfy Heisenberg-limited scaling.



# Outline

Introduction

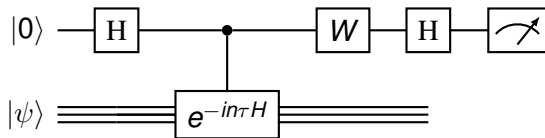
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## Classical post-processing of Hadamard test circuit



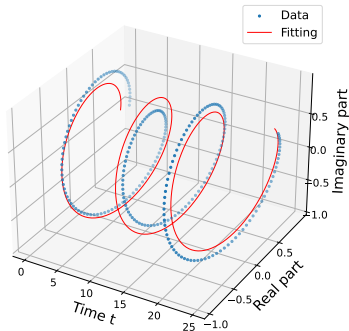
- $W = I$ ,  $\mathbb{E}(X_n) = \text{Re}(\langle\psi|\exp(-in\tau H)|\psi\rangle)$ .
- $W = S^\dagger$ ,  $\mathbb{E}(Y_n) = \text{Im}(\langle\psi|\exp(-in\tau H)|\psi\rangle)$ .
- Sample  $N_s$  times

$$Z_n = \frac{1}{N_s} \sum_{k=1}^{N_s} (X_{k,n} + iY_{k,n}) \approx \langle\psi|\exp(-in\tau H)|\psi\rangle.$$

- **Post-processing** of time series

$$\mathcal{D}_H = \{(n\tau, Z_n)\}_{n=0}^{N-1}.$$

# Quantum complex exponential least squares



- Minimize mean square error (MSE)

$$(r^*, \theta^*) = \arg \min_{r \in \mathbb{C}, \theta \in \mathbb{R}} L(r, \theta), \quad L(r, \theta) = \frac{1}{N} \sum_{n=0}^{N-1} |Z_n - r \exp(-i\theta n\tau)|^2.$$

- Fitting can be inexact when  $p_0 < 1$ , but can still accurately estimate  $\lambda_0$  (*not* an obvious fact).

## Solve the optimization problem

- Fix  $\theta$ , optimize  $r$

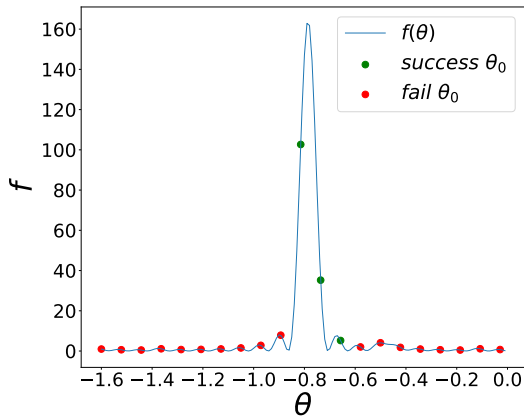
$$\min_{r \in \mathbb{C}} L(r, \theta) = \frac{1}{N} \sum_{n=0}^{N-1} |z_n|^2 - \frac{1}{N} \left| \sum_{n=0}^{N-1} z_n e^{i\theta n\tau} \right|^2.$$

- Only optimize w.r.t.  $\theta$ :

$$\theta^* = \arg \max_{\theta \in \mathbb{R}} f(\theta), \quad f(\theta) = \frac{1}{N} \left| \sum_{n=0}^{N-1} z_n e^{i\theta n\tau} \right|^2.$$

- Energy landscape is rugged but can be handled **classically** (there is only one scalar variable  $\theta$ ).

# Optimization landscape



## Convergence

### Theorem (Basic version QCELS)

Given  $p_0 > 0.71$ , we can choose

$$\delta = \Theta(\sqrt{1 - p_0}), \quad T_{\max} = \frac{\delta}{\epsilon}, \quad NN_S = \tilde{\Omega}(\delta^{-(2+o(1))}).$$

Let  $\theta^*$  be the optimizer. Then with high probability

$$|(\theta^* - \lambda_0) \bmod [-\pi/\tau, \pi/\tau]| < \epsilon.$$

- **Short maximal runtime** (circuit depth).
- **Does not** achieve Heisenberg-limited scaling.

$$T_{\max} = N\tau \quad \Rightarrow \quad N = \mathcal{O}(\epsilon^{-1}) \text{ if } \tau \text{ is small}$$

$$T_{\text{total}} = \tau N_S N(N - 1)/2 = \tilde{\mathcal{O}}(\epsilon^{-2})$$

## Multi-level QCELS

- The result  $T_{\max} = \frac{\delta}{\epsilon}$ ,  $NN_s = \tilde{\Omega}(\delta^{-(2+o(1))})$  is independent of  $\tau$ 

$$|(\theta^* - \lambda_0) \bmod [-\pi/\tau, \pi/\tau]| < \epsilon.$$
- Choose  $\tau_{j+1} = 2\tau_j$  to refine the search interval

### Algorithm

For  $j = 1, \dots, J$

Generate data set  $\mathcal{D}_{H,j} = \{(n\tau_j, Z_{n,j})\}_{n=0}^{N-1}$ .

Solve

$$(r_j^*, \theta_j^*) \leftarrow \arg \min_{r \in \mathbb{C}, \theta \in [-\lambda_{\min}, \lambda_{\max}]} L(r, \theta),$$

Shrink search interval

$$\lambda_{\min} \leftarrow \theta_j^* - \frac{\pi}{2\tau_j}, \quad \lambda_{\max} \leftarrow \theta_j^* + \frac{\pi}{2\tau_j}$$

# Convergence

## Theorem (Multi-level QCELS)

If  $p_0 > 0.71$ , choose

$$\delta = \Theta(\sqrt{1 - p_0}),$$

and

$$T_{\max} = \frac{\delta}{\epsilon}, \quad T_{\text{total}} = \tilde{\Theta}\left(\delta^{-(1+o(1))} \epsilon^{-1}\right).$$

Let  $\theta^*$  be the output of multi-level QCELS. Then with high probability

$$|(\theta^* - \lambda_0) \bmod [-\pi, \pi]| < \epsilon.$$

- Short maximal runtime (circuit depth).
- Achieve Heisenberg-limited scaling.



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## Estimating multiple eigenvalues

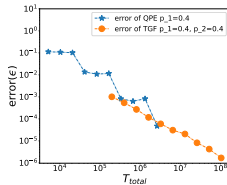
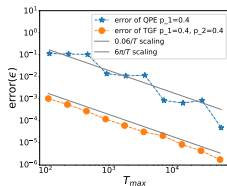
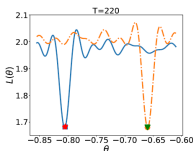
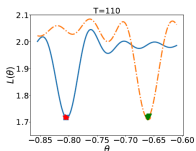
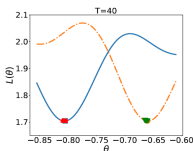
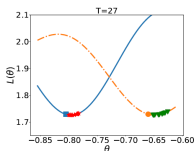
$$H|\psi_i\rangle = \lambda_i|\psi_i\rangle, \quad i = 1, 2, \dots, M$$

- **Dominant modes**  $\lambda_m, m \in \mathcal{D} \subset \{1, 2, \dots, M\}, |\mathcal{D}| = K$ .
- Overlap  $p_m = |\langle \psi_m | \psi \rangle|^2$ . Residual overlap  $R^K = \sum_{m' \in \mathcal{D}^c} p_{m'}$ .
- Assume  $p_{\min}^K = \min_{m \in \mathcal{D}} p_m = \Omega(R^K)$ .
- Heisenberg-limited scaling: Total cost  $\tilde{O}(\epsilon^{-1})$ .
- **Short-depth**:  $T_{\max} = \delta/\epsilon, \delta = \tilde{\Theta}(R^K/p_{\min}^K)$ .

# Estimating multiple eigenvalues with short-depth quantum circuit

$$\left(\{r_k^*\}_{k=1}^K, \{\theta_k^*\}_{k=1}^K\right) = \arg \min_{r_k \in \mathbb{C}, \theta_k \in \mathbb{R}} L_K \left(\{r_k\}_{k=1}^K, \{\theta_k\}_{k=1}^K\right).$$

$$L_K \left(\{r_k\}_{k=1}^K, \{\theta_k\}_{k=1}^K\right) = \frac{1}{N} \sum_{n=1}^N \left| Z_n - \sum_{k=1}^K r_k \exp(-i\theta_k t_n) \right|^2$$



Transverse field Ising model (TFIM)

## Complexity

Theorem (Ding-Lin, 2303.05714)

If  $p_{\min}^K > 3R^K$ , choose

$$\delta = \tilde{\Theta}(R^K / p_{\min}^K).$$

There exists an algorithm that uses 1 ancilla qubit to estimate dominant  $\{\lambda_m\}_{m \in \mathcal{D}}$  to precision  $\epsilon$  with high probability using

$$T_{\max} = \frac{\delta}{\epsilon}, \quad T_{\text{total}} = \tilde{\Theta} \left( \frac{1}{(p_{\min}^K)^4 \delta^{1+o(1)} \epsilon} \right).$$

- Direct generalization of QCELS
- Current drawback: classical optimization cost can be  $\exp(cK)$  in the worst case (this has not effect on the quantum cost)

## Ground-state energy estimation with global depolarized noise

- Global depolarized noise channel

$$\rho \mapsto e^{-\alpha\tau} \rho + \frac{1 - e^{-\alpha\tau}}{M} I,$$

- Not possible to run to  $T_{\max} \gg \alpha^{-1} \Rightarrow$  No Heisenberg-limited scaling.
- New result:** For gapped system  $\Delta_\lambda > 0$ , choose

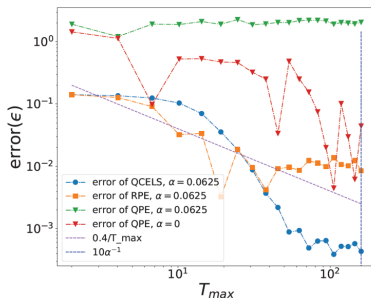
$$T_{\max} = \Theta\left(\frac{1}{\Delta_\lambda} \log\left(\frac{1}{\epsilon}\right)\right), \quad N = \Theta(\text{poly}(\epsilon^{-1})),$$

can still approximate ground-state energy to **arbitrary precision**  $\epsilon$ .

# QCELS with global depolarized noise channel

$$L_\beta(r, \theta) = \frac{1}{N_t} \sum_{n=1}^{N_t} |\exp(\beta|t_n|)Z_n - r \exp(-i\theta t_n)|^2$$

$$(r^*, \theta^*) = \operatorname{argmin}_{r \in \mathbb{R}, \theta \in [-\pi, \pi]} L_\beta(r, \theta)$$



## Conclusion

- Early fault-tolerant quantum algorithm:  
Small number of ancilla qubits, simple gates, short circuit depth
- Recommend **QCELS** for short-depth simulation, and in general **signal processing** based methods.
- Compare with quantum subspace methods / matrix pencil methods; More general noise channel Applications and initialize with VQE / DMRG; Excited state properties and Green's functions.
- Not discussed:
  - Randomized implementation of Fourier filtering and binary search based ground-state energy estimation<sup>1</sup>;
  - Quantum eigenvalue transformation of unitary matrices and preparation of ground state<sup>2</sup>

<sup>1</sup>(Lin-Tong, PRX Quantum 3, 010318, 2022)

<sup>2</sup>(Dong-Lin-Tong, PRX Quantum 3, 040305, 2022)

# Acknowledgment

Thank you for your attention!

Lin Lin

<https://math.berkeley.edu/~linlin/>



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# Outline

Introduction

Main results

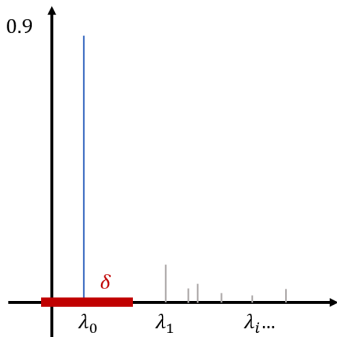
Algorithms

Current directions

Proof ideas

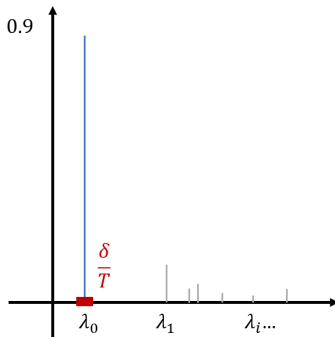
# Phase cancellation in long time simulation

$$p_i = |\langle \phi | \psi_i \rangle|^2$$



Uncertainty in short time simulation

$$p_i = |\langle \phi | \psi_i \rangle|^2$$



Uncertainty in long time simulation

## Intuitive analysis of basic version of QCELS

- Recall

$$\theta^* = \arg \max_{\theta \in \mathbb{R}} f(\theta), \quad f(\theta) = \frac{1}{N} \left| \sum_{n=0}^{N-1} z_n e^{i\theta n \tau} \right|^2.$$

- Need to bound

$$R_0 = |(\lambda_0 - \theta^*)\tau \bmod [-\pi, \pi]|.$$

- Lower bound  $f(\lambda_0)$

$$(2p_0 - 1)N \leq \sqrt{f(\lambda_0)}$$

- Upper bound  $f(\theta^*)$

$$\sqrt{f(\theta^*)} \leq \left| \frac{\sin(NR_0/2)}{\sin(R_0/2)} \right| + (1 - p_0)N.$$

## Intuitive analysis of basic version of QCELS

- Optimality  $\sqrt{f(\theta^*)} \geq \sqrt{f(\lambda_0)}$  gives

$$\left| \frac{\sin(NR_0/2)}{\sin(R_0/2)} \right| \geq (3p_0 - 2)N \equiv \frac{\sin(N(\delta/2N))}{\sin(\delta/2N)} \approx N \left( 1 - \frac{\delta^2}{24} \right)$$

- $\delta^2 \approx 72(1 - p_0) \Rightarrow \delta \rightarrow 0$  as  $p_0 \rightarrow 1$ .
- $\frac{\sin(Nx)}{\sin(x)}$  is decreasing on  $[0, \pi/(2N)] \Rightarrow R_0 \leq \frac{\delta}{N}$  or

$$|(\lambda_0 - \theta^*) \bmod [-\pi/\tau, \pi/\tau]| < \frac{\delta}{T_{max}} = \epsilon$$

- This gives  $T_{max} = \delta/\epsilon$ : **short runtime!**

## A more careful analysis

- Everything is **noisy**. Take into account failure probability.
- Need to bound **Monte Carlo error**

$$E_n = Z_n - \langle \psi | \exp(-in\tau H) | \psi \rangle, \quad \bar{E}_\theta = \frac{1}{N} \sum_{n=0}^{N-1} E_n \exp(i\theta n\tau)$$

- Lipschitz continuity and Hoeffding's inequality

$$\mathbb{P} \left( \sup_{\theta \in [\lambda_0 - \frac{\rho}{\tau}, \lambda_0 + \frac{\rho}{\tau}]} |\bar{E}_\theta - \bar{E}_{\lambda_0}| \geq \left( 4\sqrt{2} \log^{1/2} \left( \frac{8\sqrt{N_s N}}{\eta} \right) + 1 \right) \frac{\rho}{\sqrt{N_s N}} \right) \leq \eta$$

- A somewhat elaborate **iterative refinement** procedure to improve the  $\delta$  dependence of  $NN_s$ .
- Finally, multi-level QCELS just applies the analysis to each level.