Quantum algorithms for eigenvalue problems

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Herbert Keller Colloquium,
Caltech, October, 2024

Outline

Criteria for achieving quantum advantage in scientific computation

Early fault tolerant quantum eigensolver

Noisy super-resolution in classical signal processing

Conclusion

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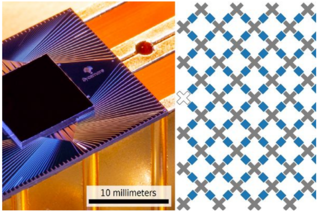
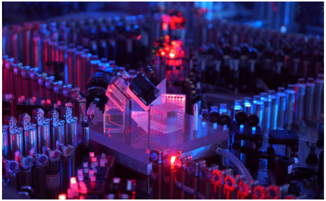
Quantum computation meets public attention

Google, Nature 2019
Random circuit sampling
Theory: [Boixo et al, 2018]



USTC, Science 2020
Boson sampling.
Theory: [Aaronson–Arkhipov, 2011]



Quantum supremacy

Quantum supremacy and quantum advantage

- Is controlling large-scale quantum systems merely really, really hard, or is it ridiculously hard?[1]
- Quantum supremacy: quantum computer is faster than classical computer on some (contrived) task.
- Quantum advantage: quantum computer is faster than classical computer on a useful task.

John Preskill

[1] (Preskill, 25th Solvay Conference on Physics, arXiv:1203.5813)

Crash course on quantum computing

- $|\psi\rangle \in \mathbb{C}^{2^n} \cong (\mathbb{C}^2)^{\otimes n}$, n : number of qubits.
- Quantum superpower: For certain unitary matrices $U \in \mathbb{C}^{2^n \times 2^n}$, cost of quantum implementation of matrix-vector multiplication $U|\psi\rangle$ can be $\mathrm{poly}(n)$. (Potential) exponential speedup.

Read the fine print:

- Input vector $|\psi_{\mathrm{in}}\rangle$ prepared using classical information.
- Run quantum algorithm: $|\psi_{\mathrm{out}}\rangle = U_T \cdots U_1 |\psi_{\mathrm{in}}\rangle$.
  Circuit depth: $\mathcal{O}(T)$
- Output via measurement of e.g., a qubit: $p = \langle\psi_{\mathrm{out}}|P|\psi_{\mathrm{out}}\rangle$.
  Outcome is a Bernoulli random variable $\sim \mathrm{Bern}(p)$.
  Can also estimate p via repetition.

Criteria for Quantum Advantage?

Useful; Quantumly easy; Classically hard

- Low quantum input cost
- Low quantum running cost
- Low quantum output cost

Shor's algorithm for prime number factorization

- Useful: RSA cryptosystem
- Input: $N \in \mathbb{N}$ with promise $N = p \cdot q$. number of bits $n = \log N$
- Output: Prime numbers p, q.
- Quantum running cost[1]: $\widetilde{\mathcal{O}}\left(n^2\right)$.
- Best available classically cost[2]: $\widetilde{\mathcal{O}}\left(\exp\left[cn^{\frac{1}{3}}\right]\right)$

Peter Shor

[1] (Shor, FOCS 1994; SIAM J. Comput. 1997)
[2] General number field sieve, see e.g., (Lenstra and Lenstra, 1993)

Unitary dynamics / Hamiltonian simulation

Richard Feynman

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle, \quad |\psi(0)\rangle \in \mathbb{C}^{2^n}.$$

- Useful: Dynamics of quantum many-body systems. Feynman's original vision.
- Input state: Often simple initial state (such as product state)
- Quantum running cost[1]: $\mathrm{poly}(n)$
- Output: Measure $\langle\psi(t)|O|\psi(t)\rangle$
- Empirically challenging for classical simulation beyond 1D[2]

[1] (Lloyd, Science, 1996) and numerous works
[2] This question is constantly being re-examined see e.g., (Angrisani et al, arXiv:2409.01706)

Scientific Computation: Numerical tasks

- Linear systems of equations $Ax = b$
- Matrix function $x = A^{-p}b$
- Differential equations $u'(t) = -Au$
- Eigenvalue problems $Au = \lambda u$

...

How to express these non-unitary processes?

Scientific Computation: Applications

High dimensional problems ($\mathbb{R}^d$, $d \gg 3$)

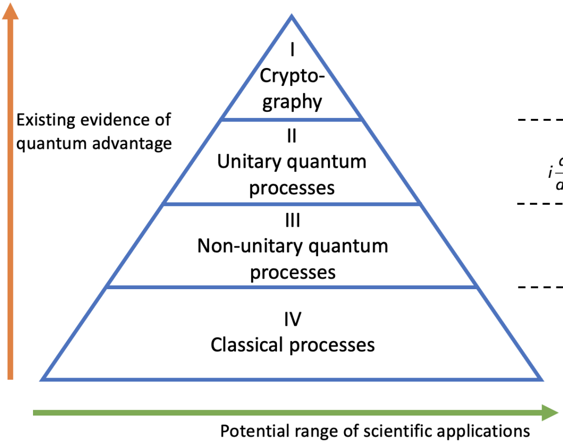
- Quantum many body system: (Schrödinger equation, Dirac equation, Lindblad equation)
- Control theory, game theory (Hamilton-Jacobi equation)
- Probability theory, sampling (Fokker-Planck equation)

Low dimensional problems ($\mathbb{R}^d$, $d \leq 3$)

- Fluid dynamics (Navier-Stokes equation)
- Electromagnetism (Maxwell equation, Helmholtz equation)
- Approximate models for high dimensional problems (Kohn-Sham density functional theory, Mean-field games)

Which one(s) hold promise for quantum advantage?

Quantum advantage hierarchy (as of now)



Shor's algorithm (for prime factorization)

Hamiltonian simulation

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

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

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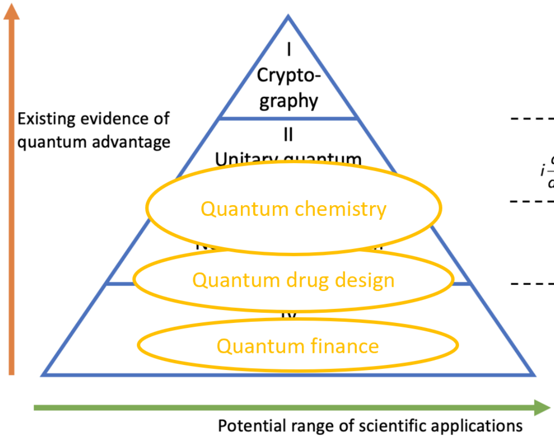
Linear systems of equations, ODE, PDE, SDE, optimization, optimal control, machine learning

Quantum advantage hierarchy (as of now)



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Quantum advantage hierarchy (as of now)

Level	Input Cost	Output Cost	Running Cost	Classical Cost	Examples
I	✓	✓	✓	Provably expensive	Prime number factorization
II	✓	✓	✓	Empirically expensive	Hamiltonian simulation
III	?	?	✓	Empirically expensive	Ground state energy estimation, thermal state preparation, Green's function, open quantum system dynamics
IV	?	?	?	?	Classical partial differential equations, stochastic differential equations, optimization problems, sampling problems

Table: Examples of problems in the quantum advantage hierarchy and existing amount of evidence justifying significant quantum speedups.

End-to-end complexities

arXiv > quant-ph > arXiv:2310.03011

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Quantum Physics

[Submitted on 4 Oct 2023]

Quantum algorithms: A survey of applications and end-to-end complexities

Alexander M. Dalzell, Sam McArdle, Mario Berta, Przemyslaw Bienias, Chi-Fang Chen, András Gilyén, Connor T. Hann, Michael J. Kastoryano, Emil T. Khabiboulline, Aleksander Kubica, Grant Salton, Samson Wang, Fernando G. S. L. Brandão

Cambridge Univ. Press (to be published)

SIAM NEWS **APRIL 2024**

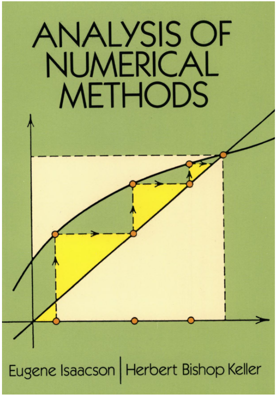
Research | April 01, 2024

Quantum Advantages and End-to-end Complexity

By Lin Lin

https://sinews.siam.org/Details-Page/quantum-advantages-and-end-to-end-complexity

Outline

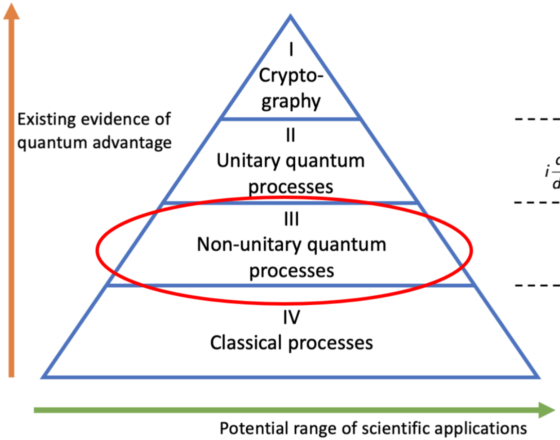


Chapter 4 Computation of Eigenvalues and Eigenvectors

Ground-state energy estimation problem

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

- Estimate the smallest eigenvalue λ_0 to precision ϵ.
- Theoretically intractable in the worst case (QMA-hard).
- Main assumption: good initial state $|\phi\rangle$: $p_0 = \gamma^2 = |\langle\phi|\psi_0\rangle|^2 = \Omega(1)$.
- Focus on methods with performance guarantee. Can be combined with e.g., VQE (prepare good initial state)



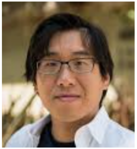
Given that classical computer can prepare a good initial state, is the problem still classically hard?

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

Quantum chemistry, classical heuristics, and quantum advantage

Garnet Kin-Lic Chan

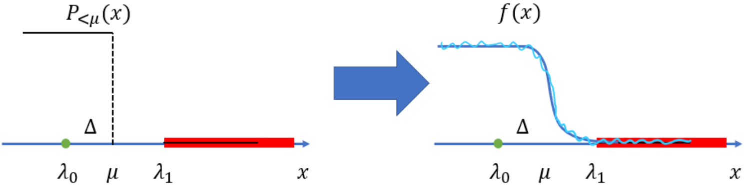
We describe the problems of quantum chemistry, the intuition behind classical heuristic methods used to solve them, a conjectured form of the classical complexity of quantum chemistry problems, and the subsequent opportunities for quantum advantage. This article is written for both quantum chemists and 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.



Garnet Chan

(Chan, Spiers Memorial Lecture, arXiv:2407.11235)

First near-optimal quantum eigensolver



- Efficient implementation of a filtering matrix function $f(H-\mu)$. Cost: $\widetilde{\mathcal{O}}(\epsilon^{-1})$ in the worst case (take $\Delta = \epsilon$).
- Binary amplitude estimation for deciding $\|f(H-\mu)\,|\phi\rangle\,\| \geq \sqrt{p_0}(1-\epsilon')$ or $\|f(H-\mu)\,|\phi\rangle\,\| \leq \epsilon'$. Cost: $\widetilde{\mathcal{O}}(p_0^{-\frac{1}{2}})$. ($p_0 = |\langle\phi|\psi_0\rangle|^2$)
- Binary search to refine μ: Cost: $\mathcal{O}(\log \epsilon^{-1})$.
- Total cost: $\widetilde{\mathcal{O}}(\epsilon^{-1} p_0^{-\frac{1}{2}})$.

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

Towards early fault-tolerant quantum eigensolver

[LT20] uses the block encoding framework:

- Many ancillary qubits.
- Long circuit depth (preconstant).

Efficient quantum eigensolvers for early fault tolerant quantum computer?

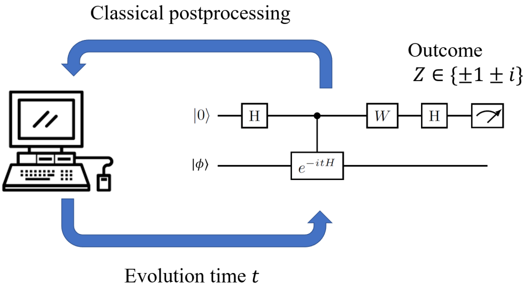
Early fault-tolerant (EFT) quantum computer

Be very frugal with quantum resource usage:

- Few ancillary qubits.
- Short circuit depth.
- Small number of repetitions.
- Proper error mitigation and correction strategies.

There is no universally accepted definition of an early fault-tolerant quantum computer. See recent discussions: (Katabarwa, Gratsea, Caesura, Johnson, *Early fault-tolerant quantum computing*, PRX Quantum 2024)

Single ancilla quantum phase estimation




Alexei Kitaev

Kitaev algorithm: $p_0 = \gamma^2 \approx 1$.

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)...

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

Workflow

Evolution time t_n

$|\phi\rangle$

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

$T_{\max} = \max t_n$: Maximal evolution time (circuit depth)

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

Dataset

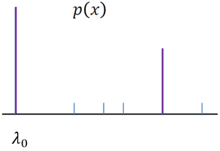
$$\mathcal{D}_H = \{(t_n, Z_n)\}_{n=0}^{N-1}, \quad t_n \in \mathbb{R}, \quad Z_n \in \{\pm 1 \pm i\}$$

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 $p_0 = 1$)

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

so that

$$\mathbb{E} Z_n = \langle\phi| \exp(-i t_n H) |\phi\rangle = e^{-i t_n \lambda_0}.$$

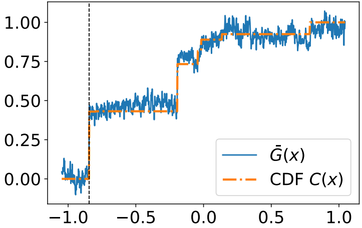
- Uniform grid: $t_n = n\tau$. $N\tau = \epsilon^{-1}$
  $T_{\text{total}} = \widetilde{\mathcal{O}}(\epsilon^{-2})$. Standard quantum limit
- Kitaev's algorithm: logarithmic grid: $t_n = 2^n\tau$, $2^N\tau = \epsilon^{-1}$.
  $T_{\text{total}} = \widetilde{\mathcal{O}}(\epsilon^{-1})$. Heisenberg limit (saturates lower bound)

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

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

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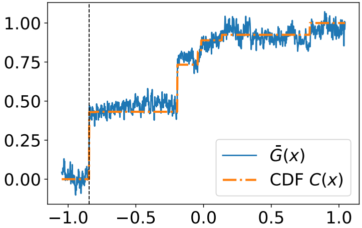


- Can improve to near optimal complexity $T_{\text{total}} = \widetilde{\mathcal{O}}(\epsilon^{-1} p_0^{-\frac{1}{2}})$ with 3 ancilla qubits

(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 $T_{\max} \approx 3000$.

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

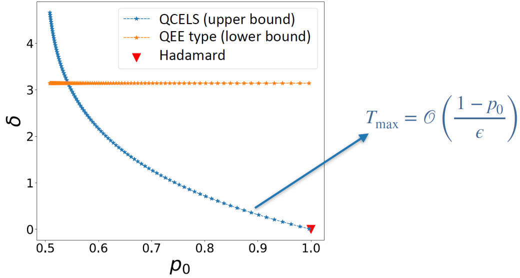
$$T_{\max} = \frac{\delta}{\epsilon}, \quad \delta \ll 1.$$

First short-depth quantum eigensolver

- Quantum complex exponential least squares (QCELS)[1]

- Randomized evolution time: Truncated Gaussian distribution

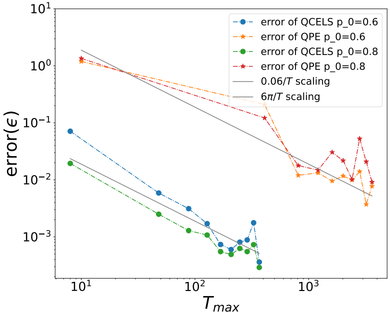
$$\mathbb{P}(t_n = t) \propto e^{-\frac{t^2}{2T_{\max}^2}} \mathbf{1}_{[-\gamma T_{\max}, \gamma T_{\max}]}, \quad T_{\max} = \frac{\delta}{\epsilon}, \quad \delta = \mathcal{O}(1 - p_0).$$

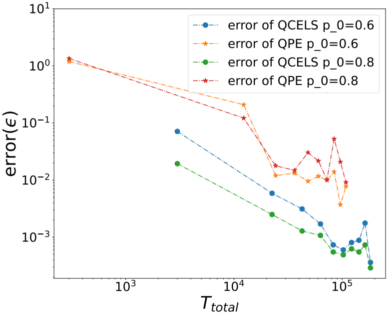


[1] Ding-**L.**, *Even shorter quantum circuit for phase estimation on early fault-tolerant quantum computers with applications to ground-state energy estimation*, PRX Quantum 2023
See also (Ni-Li-Ying, Quantum 2023)(Ding-**L.**, Quantum 2023).

Numerical results for QCELS

Transverse field Ising model (TFIM)





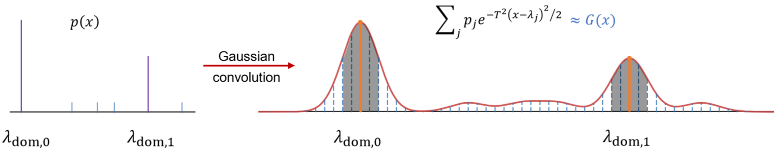
- Two order of magnitude reduction of $T_{\max}$
- Comparable (in fact, a bit smaller) T_{total}.

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



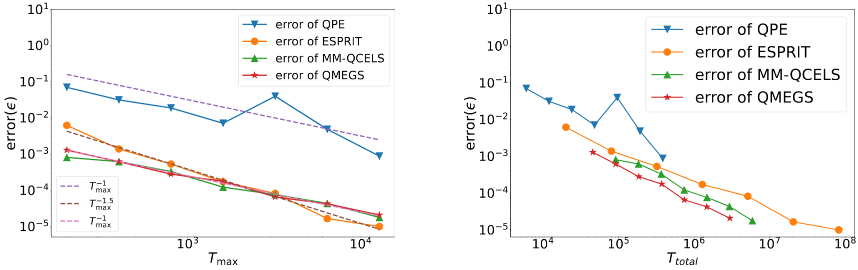
(Ding, Li, **L.**, Ni, Ying, Zhang, Quantum 2024, arXiv:2402.01013)

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]	?	✓	✓	✗	$\text{poly}(\lvert\mathcal{D}\rvert)$ quantum cost
[LNY23, Theorem III.5]	✓	✓	✓	✗	$\text{poly}(\lvert\mathcal{D}\rvert)$ 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)

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ESPRIT

One of the most widely used classical signal processing method[1]

ESPRIT -estimation of signal parameters via rotational invariance techniques

R Roy, T Kailath - IEEE Transactions on acoustics, speech, and …, 1989 - ieeexplore.ieee.org

… In this paper, a new algorithm (**ESPRIT**) that dramatically reduces these computation and… the signals are elements of the **ESPRIT** solution as well. **ESPRIT** is also manifestly more robust…

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- Uniform time grid: $\mathcal{D}_H = \{(t_n = n\tau, Z_n)\}_{n=0}^{N-1}, \quad T_{\max} = \max_n t_n$
- Noisy measurement:

$$Z_n = \mathbb{E} Z_n + \eta_n = \sum_j p_j e^{-i t_n \lambda_j} + \text{Noise}.$$

Goal: Dominant mode estimation $(\lambda_{\mathrm{dom},m}, p_{\mathrm{dom},m}), m \in \mathcal{D}$.

[1] Similar type algorithms: Prony, Matrix pencil, MUSIC..

Workflow

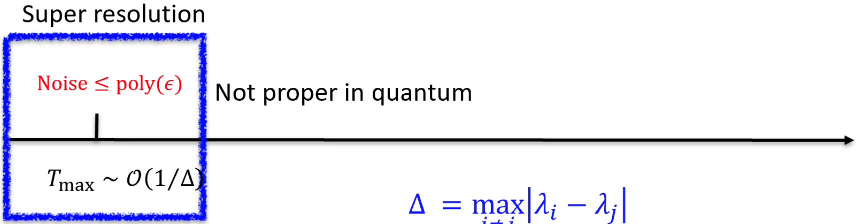
Evolution
time $t_n = n\tau$

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

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

Super-resolution of ESPRIT

Super resolution: Beyond Nyquist limit $\epsilon = \mathcal{O}\left(T_{\max}^{-1}\right)$.



$$\Delta = \max_{i \neq j} |\lambda_i - \lambda_j|$$

gap between eigenvalues

[Ankur Moitra, STOC, 2015]
[Weilin Li, et al, IEEE Transactions on Information Theory, 2020]
[M E Stroeks, New Journal of Physics, 2022]

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[Ankur Moitra, STOC, 2015]
[Weilin Li, et al, IEEE Transactions on Information Theory, 2020]
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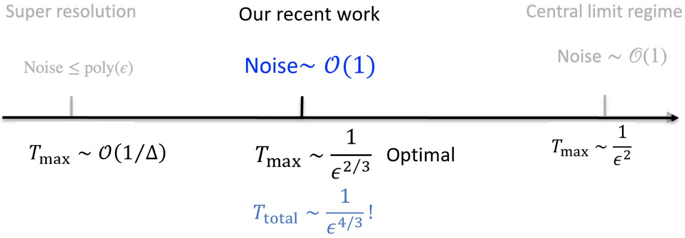
Noisy super-resolution of ESPRIT



- $\epsilon = \mathcal{O}\left(\frac{1}{T_{\max}^{3/2}}\right)$: Beyond Nyquist limit.
  Match Cramér-Rao type lower bound and numerical results
- $T_{\text{total}} = \mathcal{O}\left(T_{\max}^2\right) = \mathcal{O}\left(\frac{1}{\epsilon^{4/3}}\right)$. Not Heisenberg limit scaling due to uniform sampling.

(Ding, Epperly, **L.**, Zhang, FOCS 2024, arXiv:2404.03885)

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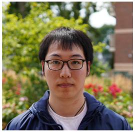
Conclusion

- Recommend QMEGS[1] as early fault-tolerant eigensolver.
- Short $T_{\max}$ with a good initial state.
  T_{total} comparable to most advanced quantum phase estimation[2]
- Overcome dependence on good initial state?
  Ideas from quantum Markov Chain / Lindblad dynamics [3]

[1](Ding, Li, **L.**, Ni, Ying, Zhang, Quantum 2024, arXiv:2402.01013)
[2](Berry at al, arXiv:2409.11748)
[3](Ding, Chen, **L.**, Phys. Rev. Research 2024, arXiv:2308.15676)

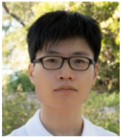
- *Is it fair to say that there has not been much progress in quantum algorithms since Shor's algorithm?* – Sebastian Hassinger
- Reflection that Shor's algorithm is still essentially the only Level I application on the quantum advantage hierarchy!
- Find better ways to communicate with the public on what have been achieved and what are achievable!

Acknowledgment



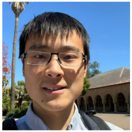
Zhiyan Ding

Ethan Epperly



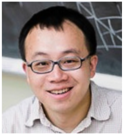
Ruizhe Zhang

Yulong Dong



Hongkang Ni

Yu Tong



Lexing Ying

Acknowledgment

Thank you for your attention!

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Linear combination of Hamiltonian simulation (LCHS)

Express non-unitary dynamics (Level III)
as Hamiltonian simulation problems (Level II)

Theorem (LCHS)

Let $A = L + iH$ with Hermitian H, L and $L \succeq 0$, then there exists a kernel function $f : \mathbb{C} \to \mathbb{C}$ s.t.

$$e^{-At} = \int_{\mathbb{R}} \frac{f(k)}{1 - ik} e^{-it(kL+H)} \, \mathrm{d}k.$$

An asymptotically near-optimal choice of $f(k)$ is

$$f(z) = \frac{1}{2\pi e^{-2^\beta} e^{(1+iz)^\beta}}, \quad \beta \in (0, 1).$$

(An, Liu, **L.**. Phys. Rev. Lett., 2023, arXiv: 2303.01029) (An, Childs, **L.**, arXiv:2312.03916)

Complexity for solving differential equations

First algorithm to achieve optimal state preparation cost and near-optimal matrix query complexity.

$$u'(t) = -A(t)u(t), \quad u(0) = u_0.$$

Method	**Query complexity**	
	$A(t)$	u_0
Truncated Dyson[1]	$\widetilde{\mathcal{O}}\left(q\alpha T\left(\log\left(\frac{1}{\epsilon}\right)\right)^2\right)$	$\mathcal{O}\left(q\alpha T\log\left(\frac{1}{\epsilon}\right)\right)$
Time-marching[2]	$\widetilde{\mathcal{O}}\left(q\alpha^2 T^2\log\left(\frac{1}{\epsilon}\right)\right)$	$\mathcal{O}(q)$
Original LCHS[3]	$\widetilde{\mathcal{O}}\left(q^2\alpha T/\epsilon\right)$	$\mathcal{O}(q)$
Improved LCHS[4]	$\widetilde{\mathcal{O}}\left(q\alpha T\left(\log\left(\frac{1}{\epsilon}\right)\right)^{1+1/\beta}\right)$	$\mathcal{O}(q)$

$$\alpha = \max_{0\le t\le T}\|A(t)\|, q = \|u_0\|/\|u(T)\|$$

[1][Berry, and Costa. arXiv:2212.03544]
[2][Fang, **L.**, and Tong. Quantum 2023, arXiv:2208.06941]
[3][An, Liu, **L.**. PRL 2023, arXiv: 2303.01029]
[4][An, Childs, **L.**, arXiv:2312.03916]