Quantum Algorithms
Through the Lens of Applied Mathematics

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Solve nature with nature

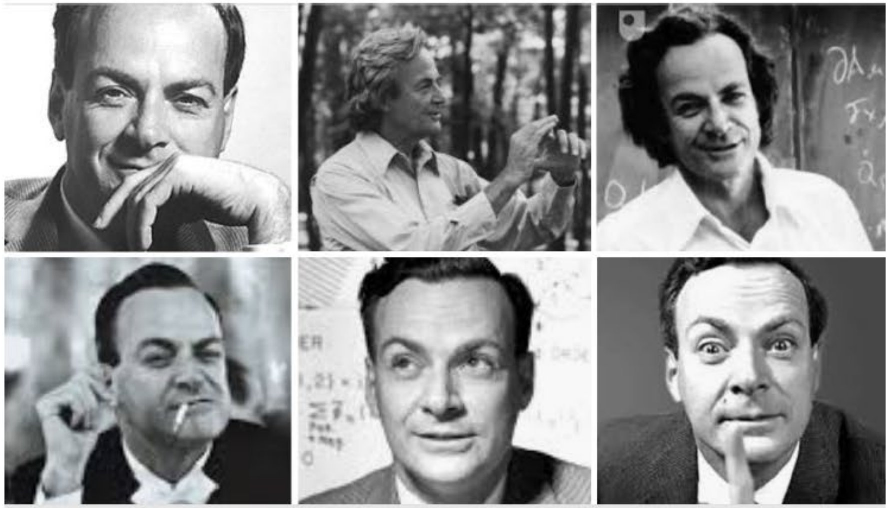


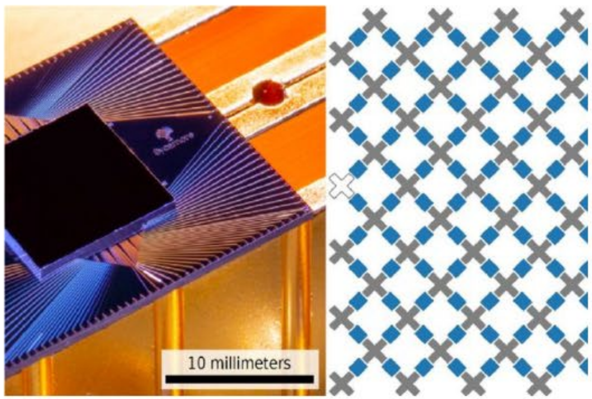
Figure. A superposition of Feynmans

... if you want to make a simulation of nature (quantum many-body problem), you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

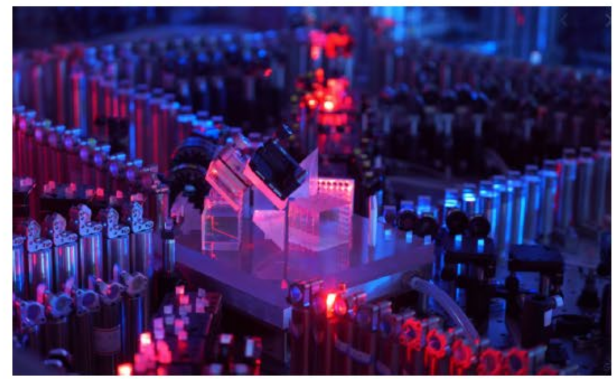
– Richard P. Feynman (1981) 1st Conference on Physics and Computation, MIT

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]



- After about four decades, quantum supremacy has been reached: the point *where quantum computers can do things that classical computers cannot, regardless of whether those tasks are useful.*

- *Is controlling large-scale quantum systems merely really, really hard, or is it ridiculously hard?* – John Preskill (2012)

- Quantum computer does anything useful? called quantum advantage.

What is a quantum computer (mathematically)

- $|\psi\rangle \in \mathbb{C}^N \cong (\mathbb{C}^2)^{\otimes n}$, $\quad N = 2^n$. 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 $\mathcal{O}(\mathrm{polylog}(N))$.
- 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): $MK\mathrm{polylog}(N)$.
- Exponential quantum advantage (EQA): if $MK = \mathcal{O}(\mathrm{polylog}(N))$, and classical algorithm scales as $\mathcal{O}(\mathrm{poly}(N))$.

Quantum advantage in

scientific computing problems?

Quantum speedup

$$\text{Quantum speedup} = \frac{\min \log \text{Cost(classical)}}{\log \text{Cost(quantum)}}.$$

- Task with a system size n, classical cost is $\mathcal{O}(n^{\alpha_c})$ and quantum cost is $\mathcal{O}(n^{\alpha_q})$. $n \to \infty$, quantum speedup is α_c/α_q.
- Quadratic quantum speedup: $\alpha_c/\alpha_q = 2$
  Cubic quantum speedup: $\alpha_c/\alpha_q = 3$.
- $\alpha_c \to \infty$ but α_q remains bounded, quantum speedup is superpolynomial.

Shor's algorithm for prime factorization

- $n = p \cdot q$ (p, q are prime numbers)
- Classical algorithm with best asymptotic complexity:
  General Number Field Sieve
  $\mathcal{O}\left(\exp\left[c(\log n)^{\frac{1}{3}}(\log\log n)^{\frac{2}{3}}\right]\right)$
- (Shor, SIAM J. Comput. 1997)
  Quantum algorithm achieves polynomial complexity $\mathcal{O}\left((\log n)^2(\log\log n)(\log\log\log n)\right)$
- Superpolynomial (but strictly, not exponential) quantum speedup.

Peter Shor

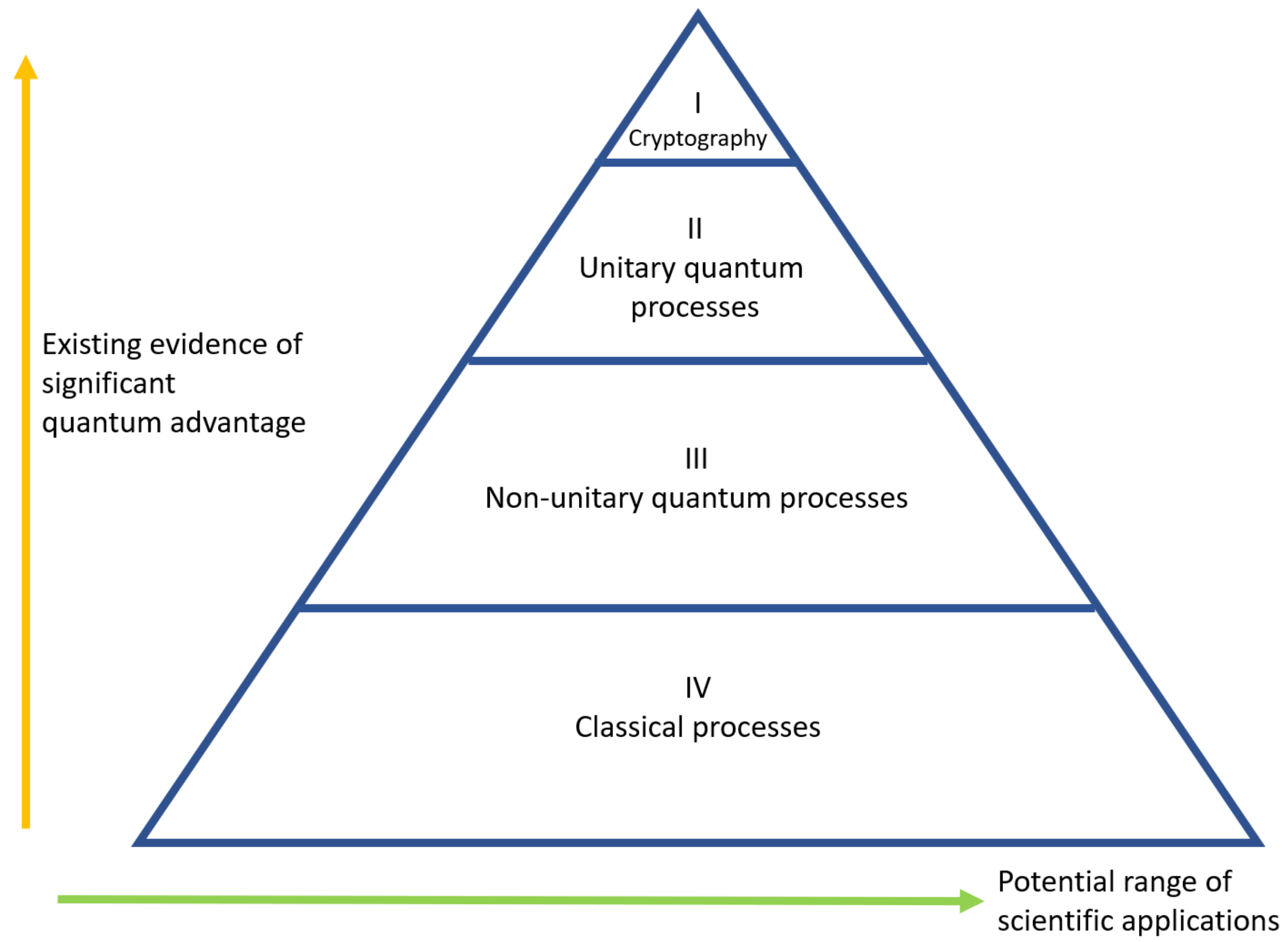
Classical cost

- In principle, the classical cost should be minimized with respect to all classical algorithms, including algorithms that exist today, and those that will ever be developed in the future.
- Extremely challenging for the majority of scientific computing problems.
- Content with an estimate of $\min \mathrm{Cost(classical)}$ using theoretical as well as empirical evidences based on existing classical algorithms.

Quantum cost

- Input cost, or the cost for preparing the input quantum state.
- Output cost, or the cost of quantum measurement.
- Running cost, or the cost of coherent quantum propagation.

Quantum advantage hierarchy (as of now)



Quantum advantage hierarchy (as of now)

Level	Input Cost	Output Cost	Running Cost	Classical Cost	Examples
I	✓	✓	✓	Provably expensive	Shor's algorithm for 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

My personal favorite towards quantum advantage Level III: Non-unitary quantum process

- Ground and excited state energy estimation

$$H\psi = E\psi$$

- Green's function

$$Ax = b$$

- Non-Hermitian quantum dynamics

$$\partial_t u(t) = -Au(t) = -(iH + L)u(t)$$

- Lindblad dynamics

$$\partial_t \rho(t) = \mathcal{L}[\rho(t)]$$

Quantum advantage from open quantum system simulation?

- Empirically challenging
- Rich potential for algorithms
- Interplay between open and closed quantum systems (open boundary condition, thermal states, ground states)

Linear combination of Hamiltonian simulation (LCHS)

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

Theorem

Suppose $A(t) = L(t) + iH(t)$, *then*

$$\mathcal{T} e^{-\int_0^t A(s)ds} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} U_k(t) dk.$$

Here $U_k(t)$ *are unitaries that solve the Schrödinger equation*

$$i\frac{dU_k(t)}{dt} = (kL(t) + H(t))U_k(t), \quad U(0) = I.$$

[An, Liu, **Lin**, arXiv:2303.01029, Phys. Rev. Lett. in press]

Ground-state energy estimation problem

$$H|\psi_0\rangle = \lambda_0 |\psi_0\rangle, \qquad \text{estimate } \lambda_0 \text{ with } \epsilon\text{-accuracy}$$

- Hamiltonian evolution input model: $U_H = e^{-i\tau H}$ for some τ.
- A good initial state $|\phi\rangle = U_I |0^n\rangle$: $p_0 = \gamma^2 = |\langle\phi|\psi_0\rangle|^2 = \Omega(1)$.
- Good initial state is a very strong assumption. But without it, the problem is theoretically intractable in the worst case (QMA-hard).

Progresses for ground-state energy estimation

	Maximal runtime	Total runtime	# ancilla qubits	Need MQC?	Input model
QPE (high confidence)	$\widetilde{\mathcal{O}}(\epsilon^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-1}\gamma^{-2})$	$\mathcal{O}(\mathrm{polylog}(\gamma^{-1}\epsilon^{-1}))$	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 (short depth)	$\widetilde{\mathcal{O}}(\epsilon^{-1})$	$\widetilde{\mathcal{O}}(\epsilon^{-4}\gamma^{-4})$	$\mathcal{O}(1)$	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
DL22 (even shorter depth)⋄	$\widetilde{\mathcal{O}}(D^{-1}) + \frac{\delta}{\epsilon}$	$\widetilde{\mathcal{O}}((D^{-1} + \delta/\epsilon)\,\gamma^{-4})$	$\mathcal{O}(1)$	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. γ, ϵ.
⋄ 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)

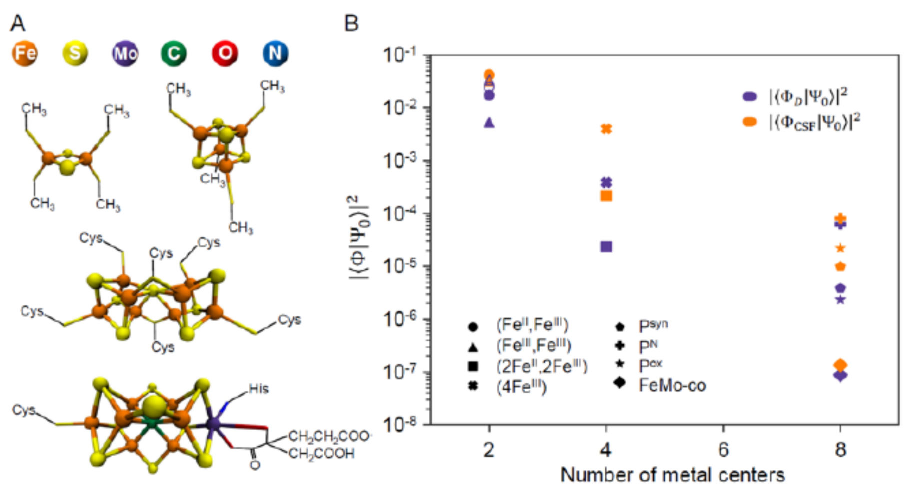
Can we obtain good initial overlap?

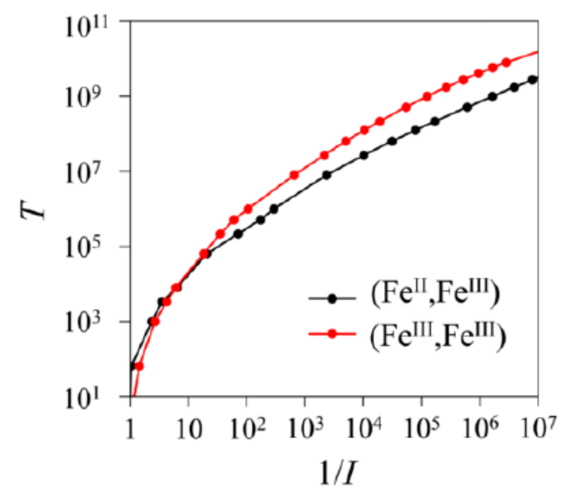
nature communications

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





Eliminate the p_0 dependence?

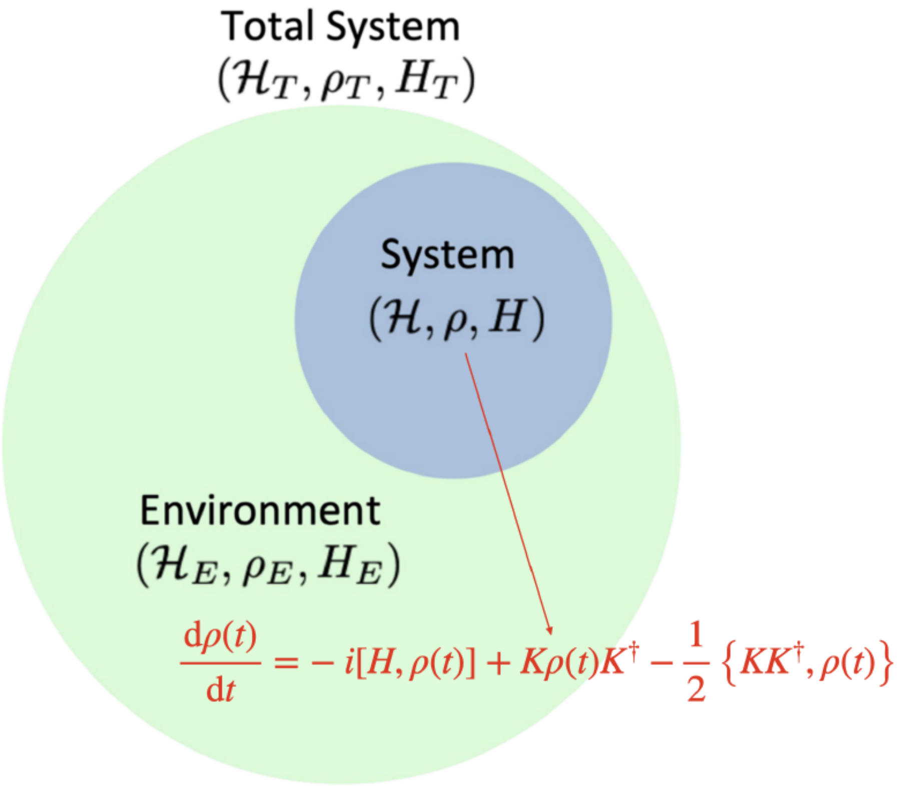
- QMA-hardness: cannot prepare ground state just by knowing H.
- Open quantum system for preparing ground state:
  - System bath coupling, Lindblad dynamics
- Potential advantage:
  - $p_0 = \Omega(1/\mathrm{poly}(n))$ is sufficient but not necessary for efficient preparation.
  - Replace assumption on p_0 by mixing time.

(Chen-Brandao, 2112.07646), (Shtanko, Movassagh, 2112.14688), (Cubitt, 2303.11962), (Rall et al, 2210.01670), (Chen et al, 2303.18224)

Lindblad dynamics

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i[H, \rho(t)] + \sum K_\alpha \rho(t) K_\alpha^\dagger - \frac{1}{2}\left\{K_\alpha K_\alpha^\dagger, \rho(t)\right\} .$$

Lindblad dynamics for open quantum system[1]:



New method (Lindblad for ground state)[1]

Lindblad dynamics with one jump operator

$$\partial_t \rho(t) = -i[H, \rho(t)] + K\rho(t)K^\dagger - \frac{1}{2}\left\{KK^\dagger, \rho(t)\right\}$$

- Jump operator $K = \int_{-\infty}^{\infty} f(s) e^{iHs} A e^{-iHs} \, \mathrm{d}s$

  Simple “Detailed balance" $\Rightarrow$ only requires one jump operator

- Choose proper f such that:
  - $\mathcal{L}_K(|\psi_0\rangle\langle\psi_0|) = 0$

    fix ground state
  - $\langle\psi_i| \mathcal{L}_K(|\psi_j\rangle\langle\psi_j|) |\psi_i\rangle > 0$ for some $i < j$

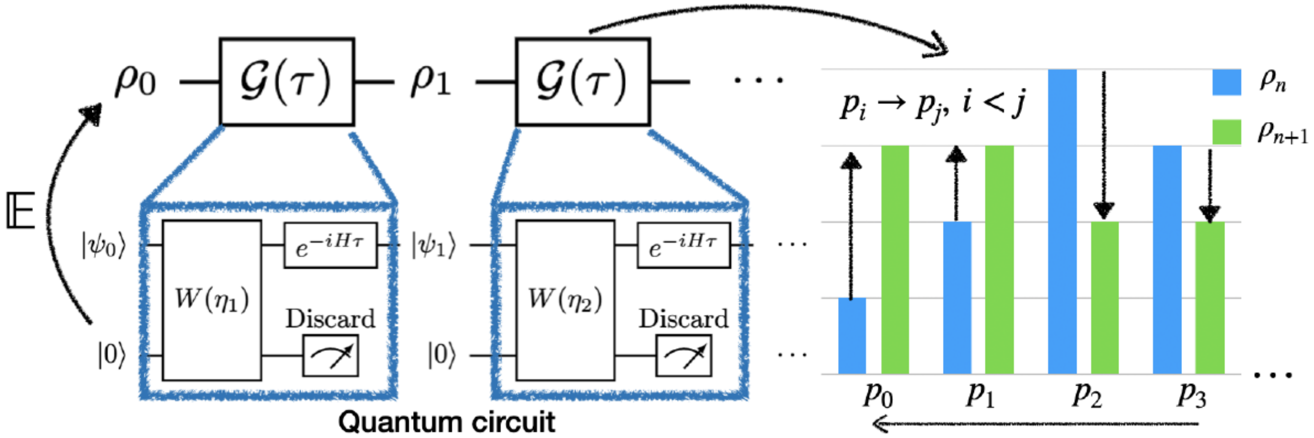
    push high energy state to low energy state

[1] (Ding, Chen, **Lin**, arXiv/2308.15676)

Simulate Lindblad dynamics on quantum computer

$$\partial_t \rho(t) = -i[H, \rho(t)] + K\rho(t)K^\dagger - \frac{1}{2}\left\{KK^\dagger, \rho(t)\right\}$$

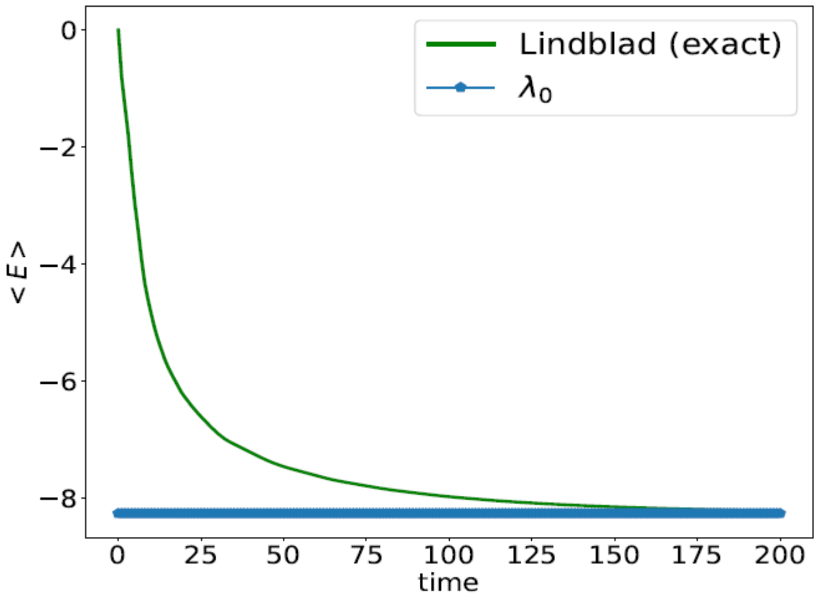
- Simple simulation: One jump operator. One ancilla qubit.



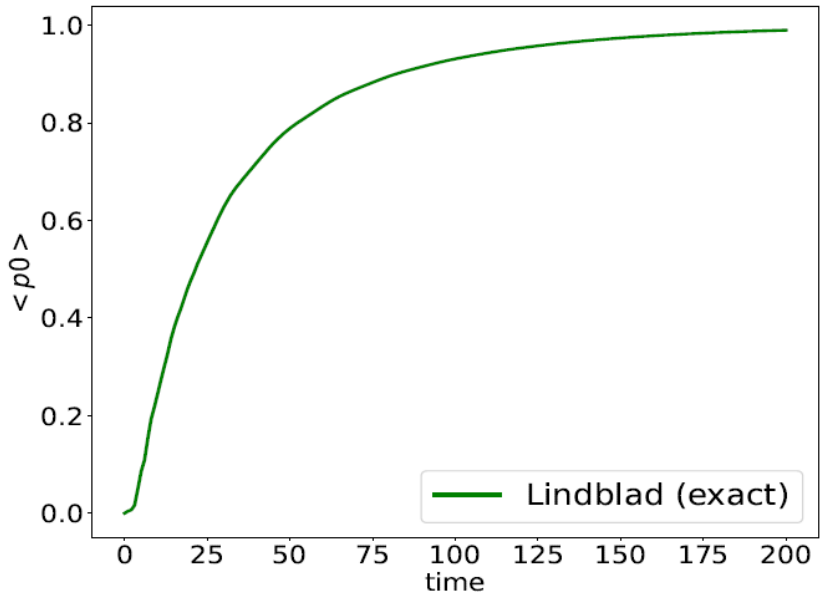
- Accelerated Lindblad dynamics: large time step with cost $\sim \widetilde{\Theta}(t_{\text{mix}}^{1+o(1)}\epsilon^{-o(1)})$

[1] (Ding, Chen, **Lin**, arXiv/2308.15676)

TFIM-6 model:



(a) Simulation time vs energy



(b) Simulation time vs overlap

Start from $p_0 = 0$!

Conclusion

- Quantum advantage:

  Quantum input, quantum output, quantum running, Classical

- I think quantum advantage in Level I and II (unitary quantum) will be achieved.

- Level III (non-unitary quantum)? Many interesting questions! Open quantum systems are ever more interesting. Polynomial mixing time?

- Level IV (Classical)?

Early fault tolerant quantum computation

“Ten digit numerical algorithms”

Ten digits,
Five seconds,
And just one page.

Lloyd N. Trefethen

A ten digit algorithm is a little gem of a program to compute something numerical. The jingle summarizes the three defining conditions. The program can be at most one page long, and it has to solve your problem to at least ten digits of accuracy on your machine in less than five seconds.

[Trefethen, A. R. Mitchell Lecture, 2005]

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

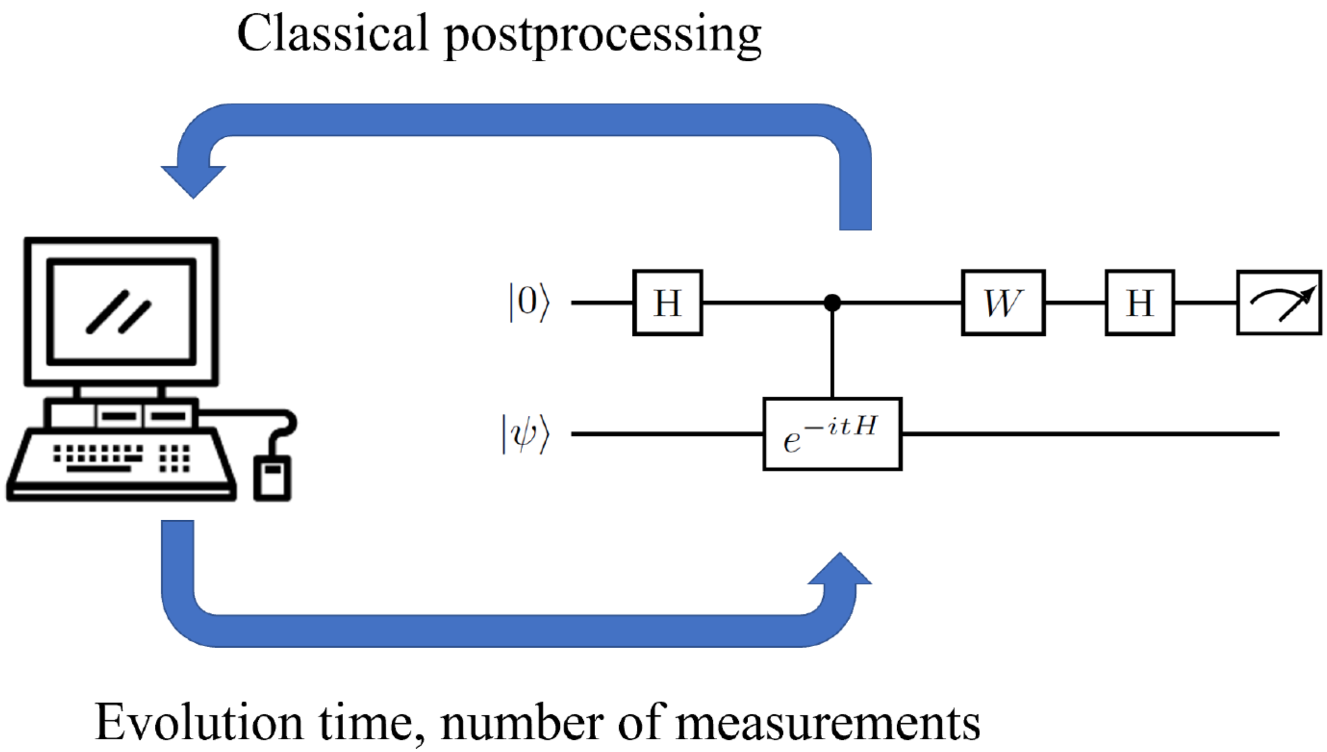
- O(1) ancilla qubits
- Short circuit depth
- Simple gates
- Larger number of repetitions and total cost

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

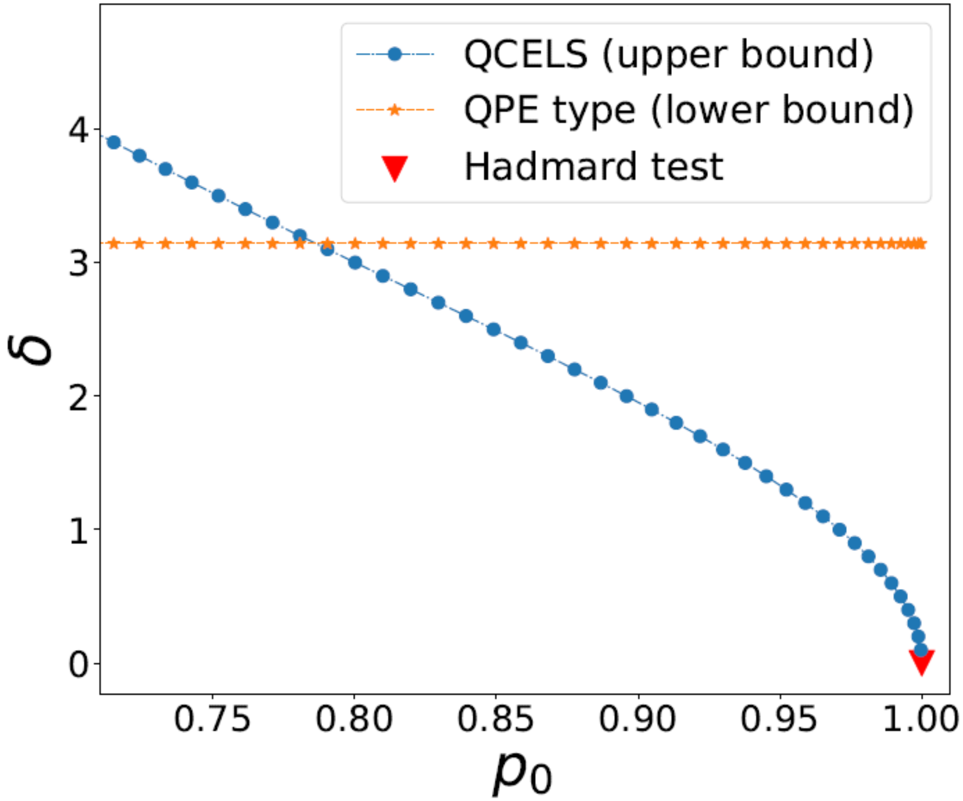
“333 quantum algorithms”

- Can demonstrate 3 digits of (meaningful) accuracy
- Use at most 3 ancilla qubits
- Can be expressed within 3 lines of circuit diagrams.

Classical post-processing of Hadamard test circuit



Simple and surprisingly powerful.

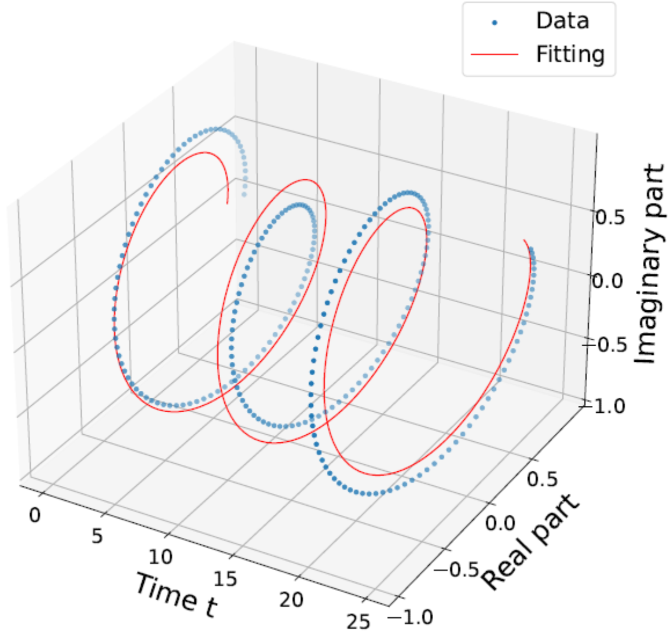


$$T_{\max} = \frac{\delta}{\epsilon}$$

QCELS: quantum complex exponential least squares

[Ding, **Lin**, PRX Quantum, 2023]

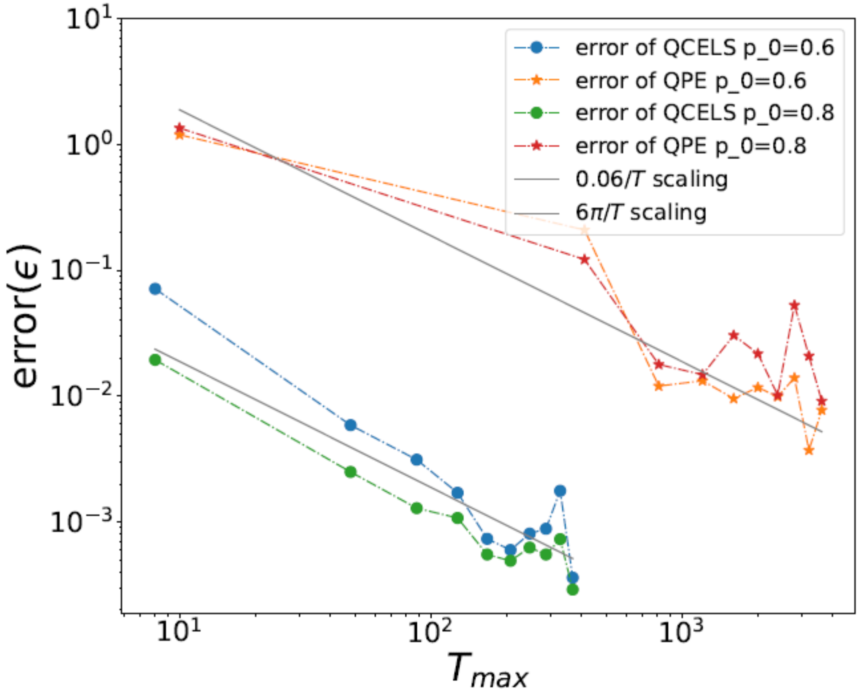
Quantum complex exponential least squares

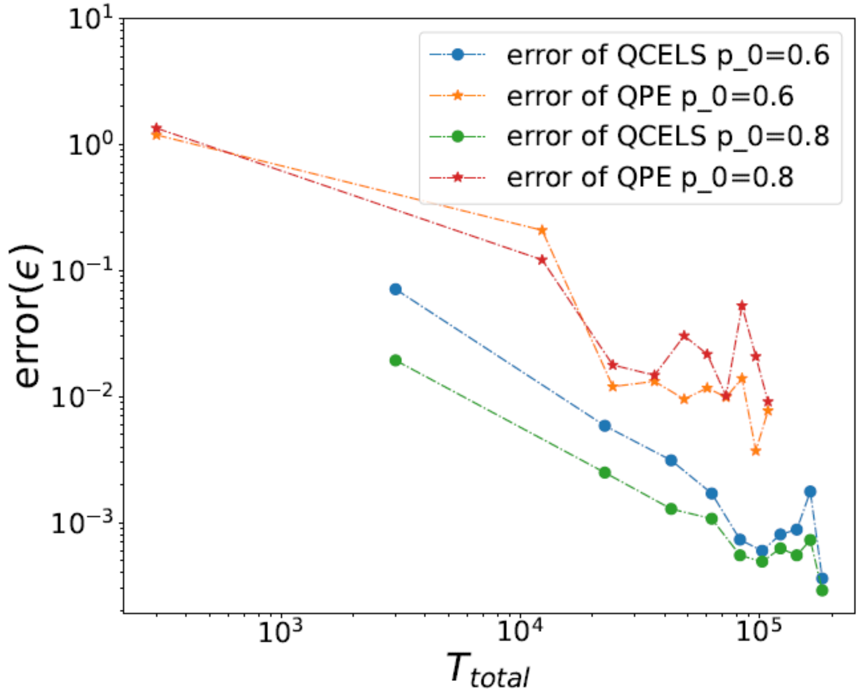


- Minimize mean square error (MSE)

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

- Fitting can be inexact when $p_0 < 1$, but can still estimate λ_0 to any precision ϵ.





Two order of magnitude reduction of maximal runtime!

Thank you for your attention!

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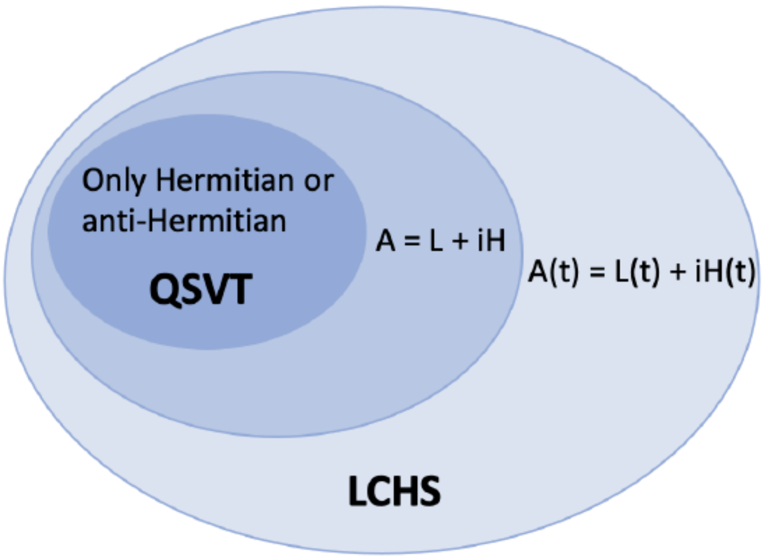
Comparison

LCHS vs Quantum singular value transformation (QSVT)



LCHS vs other quantum ODE algorithms