Road to Quantum Advantage: Theory

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IBM Quantum One, RPI, April 2024

- Quantum supremacy: *quantum computers can perform certain (can be arbitrarily contrived) tasks much more efficiently than classical computers.* Google, USTC, Xanadu

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

- Quantum computer does anything useful? Quantum advantage.

Quantum advantage: Shor's algorithm

- $n = p \cdot q$ (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.

Quantum advantage: Quantum dynamics

- Feynman's original vision
- $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ (Hamiltonian simulation)
- Often simple initial state (such as product state) $|\psi(0)\rangle$
- Observe $\langle\psi(t)|O|\psi(t)\rangle$
- Challenging for classical simulation beyond 1D

Scientific computing: mathematics

- Linear systems of equations $Ax = b$
- Linear differential equations (Ordinary / Partial / Stochastic)
  $\partial_t u = Au$
- Linear eigenvalue problem $Au = \lambda u$
- (Nonlinear equations)

…

Most of these are non-unitary processes

Ingenious ideas to “shoehorn” into unitary processes

Scientific computing: applications

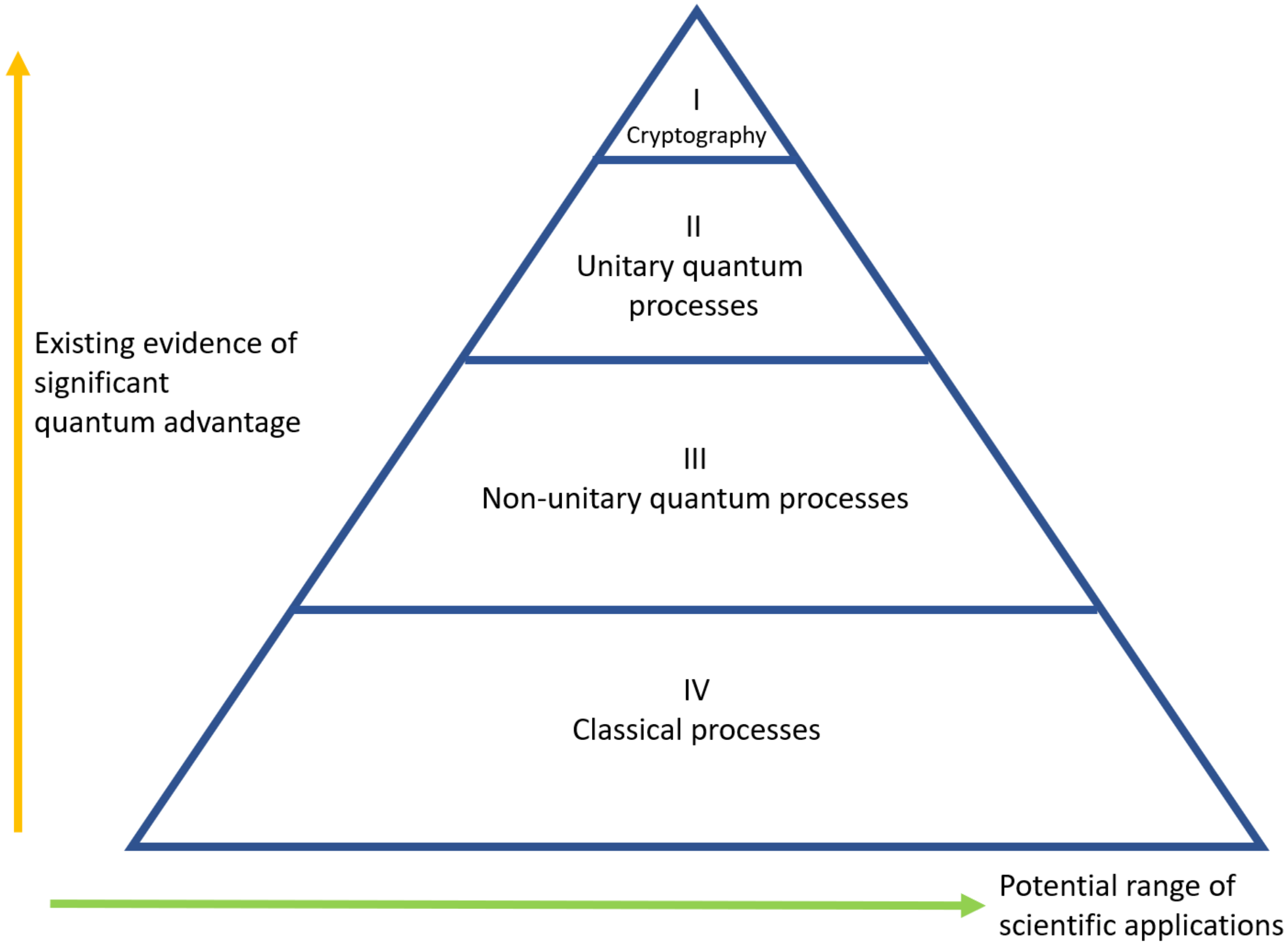
- High dimensional problems ($\mathbb{R}^d, d \gg 3$)
  - Quantum many body system: condensed matter physics, quantum chemistry, materials science, quantum field theory.. (Schrödinger equation, Lindblad equation, Dirac equation..)
  - Control theory, game theory (Hamilton-Jacobi equation)
  - Probability theory, sampling (Fokker-Planck equation)
  - Optimization theory
- Low dimensional problems ($\mathbb{R}^d, d \leq 3$)
  - Molecular dynamics (Newton's equation)
  - Fluid dynamics (Navier-Stokes equation)
  - Electromagnetism (Maxwell equation, Helmholtz equation)
  - Approximate models for high dimensional problems (Kohn-Sham density functional theory, Mean-field games..)

Quantum advantage in scientific computation

Quantumly easy, classically hard

- Low quantum input cost
- Low quantum output cost
- Low quantum running cost
- High classical cost

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

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

Towards quantum advantage for simulating non-unitary quantum processes

- Non-Hermitian quantum dynamics

$$\partial_t u(t) = -Au(t) = -\left(iH + \frac{1}{2}K^+K\right)u(t)$$

- Lindblad dynamics (think $\rho(t) = \mathbb{E}\,|u(t)\rangle\langle u(t)|$)

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

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

How to solve non-Hermitian dynamics

with optimal state preparation cost?

(Reduce input cost)

Linear differential equations

$$\frac{du(t)}{dt} = -A(t)u(t), \quad A(t) \in \mathbb{C}^{N\times N},$$
$$u(0) = U_I \left|0^n\right\rangle = \left|u_0\right\rangle .$$

- Initial state preparation cost: number of queries to U_I.
- $\alpha = \max_t \|A(t)\|$, $q = \max_t \|u_0\|/\|u(t)\|$.
- Previous best algorithm[1]: $\mathcal{O}\left(q\alpha t \log\left(\frac{1}{\epsilon}\right)\right)$.
- Lower bound: $\mathcal{O}(q)$

[1] Berry-Costa, arXiv:2212.03544 (2022)

Linear combination of Hamiltonian simulation (LCHS)

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

Theorem (LCHS)

Suppose $A(t) = L(t) + iH(t)$ and $L(t) \succeq 0$, then

$$u(t) = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} U_k(t) \left|u_0\right\rangle dk.$$

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

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

Reaches lower bound in state preparation cost: $\mathcal{O}(q)$

[An, Liu, **Lin**, Phys. Rev. Lett. 131, 150603, 2023] (QIP24)

Quantum Physics

[Submitted on 6 Dec 2023]

Quantum algorithm for linear non-unitary dynamics with near-optimal dependence on all parameters

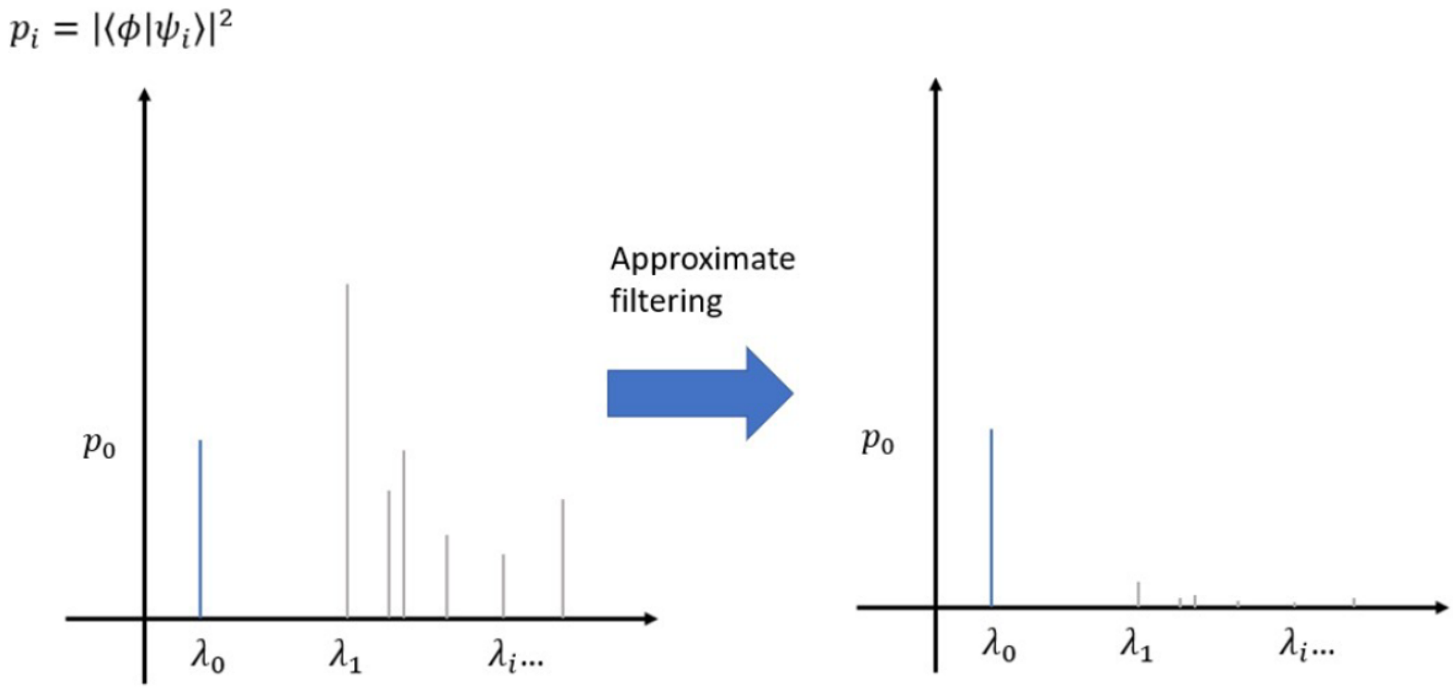
Dong An, Andrew M. Childs, Lin Lin

We introduce a family of identities that express general linear non-unitary evolution operators as a linear combination of unitary evolution operators, each solving a Hamiltonian simulation problem. This formulation can exponentially enhance the accuracy of the recently introduced linear combination of Hamiltonian simulation (LCHS) method [An, Liu, and Lin, Physical Review Letters, 2023]. For the first time, this approach enables quantum algorithms to solve linear differential equations with both optimal state preparation cost and near-optimal scaling in matrix queries on all parameters.

How to prepare ground state

starting from zero initial overlap?

Challenge in quantum phase estimation



They are essentially filtering methods.
Do not work if $p_0 = |\langle\phi|\psi_0\rangle|^2$ is small (# repetition p_0^{-1})

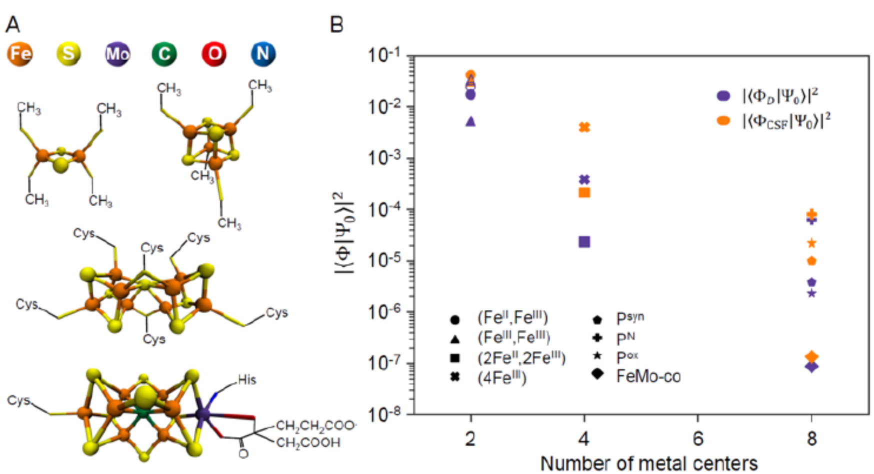
Good initial overlap for strongly correlated systems?

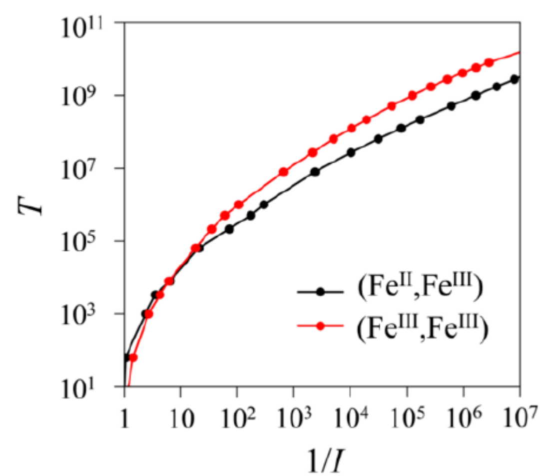
nature communications

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

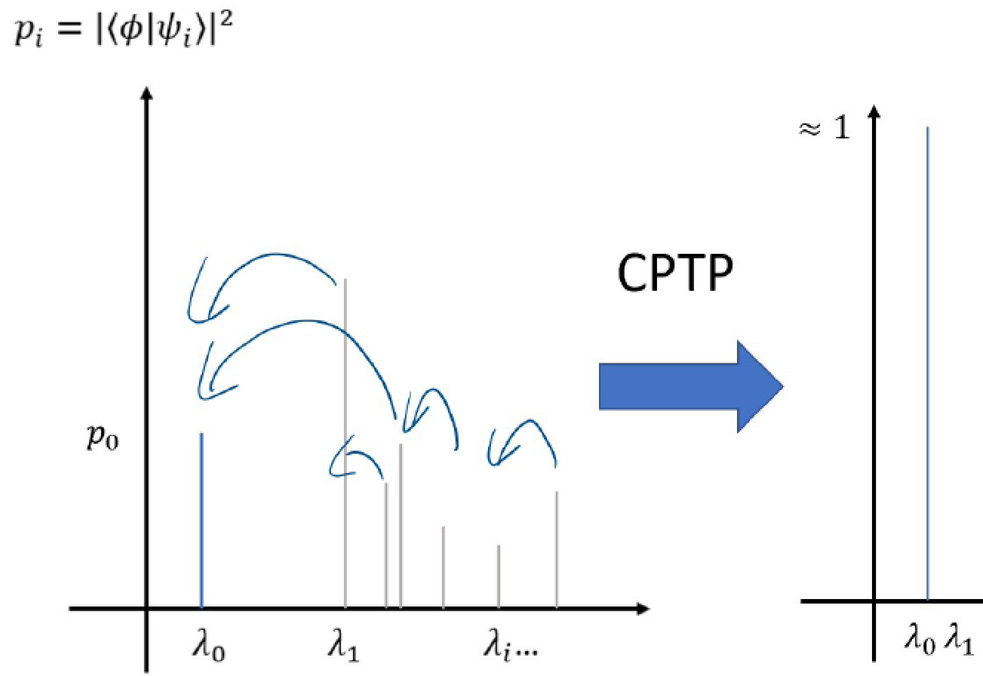
Nature Communications **14**, Article number: 1952 (2023) | Cite this article

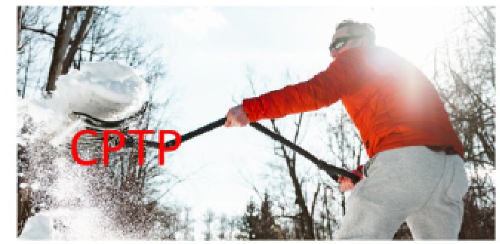




Lindblad idea for ground state preparation

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





From filtering to shoveling.
If works (poly(n) mixing time), succeeds w.p. 1, independent of p_0 (and initial guess in general)!

(Ding, Chen, **Lin**, arXiv:2308.15676)

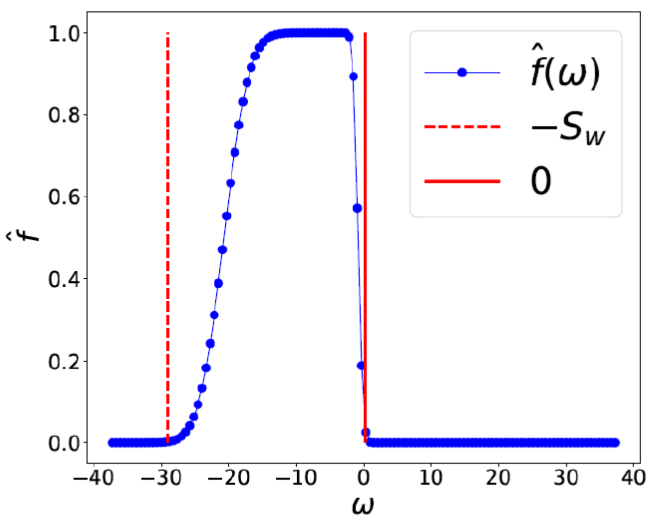
Jump operator: linear combination of Heisenberg evolution

$$\hat{f}(\omega) = 0 \quad \forall \omega \geq 0, \quad \hat{f}(\omega) = \int_{\mathbb{R}} f(s) e^{i\omega s} \mathrm{d}s.$$

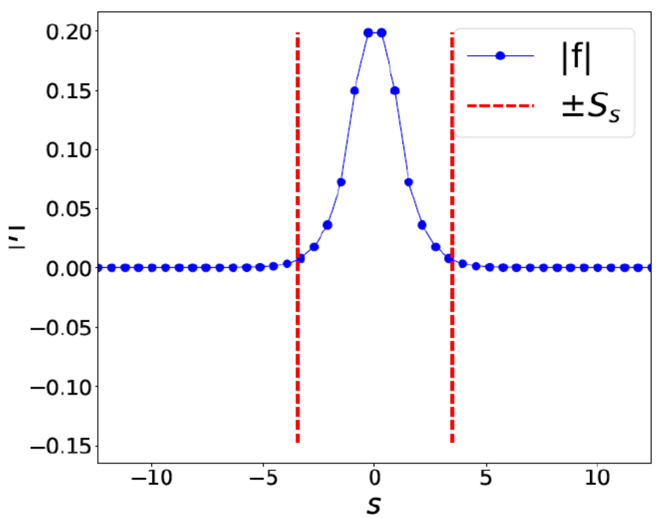
Notice

$$K = \int_{-\infty}^{\infty} f(s) e^{iHs} A e^{-iHs} \,\mathrm{d}s = \sum_{i,j \in [N]} \hat{f}(\lambda_i - \lambda_j) \left|\psi_i\right\rangle \left\langle \psi_i \middle| A \middle| \psi_j \right\rangle \left\langle \psi_j \right|$$

$$= \sum \hat{f}(\lambda_i - \lambda_j) \left|\psi_i\right\rangle \left\langle \psi_i \middle| A \middle| \psi_j \right\rangle \left\langle \psi_j \right|$$

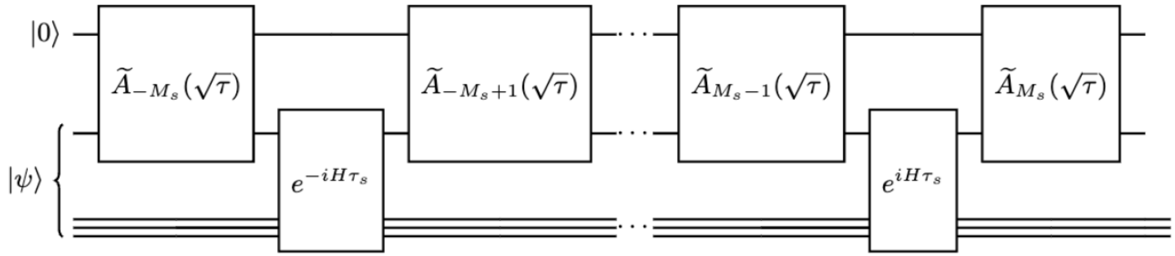


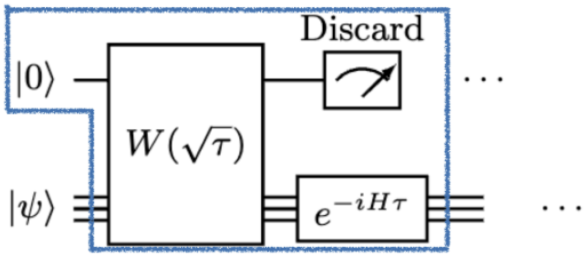
(a) $\hat{f}(\omega)$



(b) $f(s)$

Single ancilla simulation of discrete-time dynamics





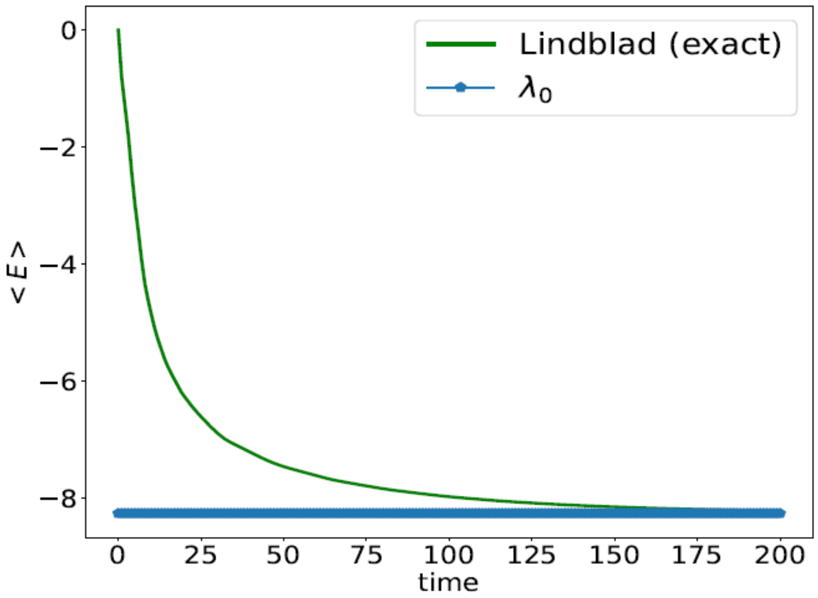
One ancilla qubit, simple gates

Theorem

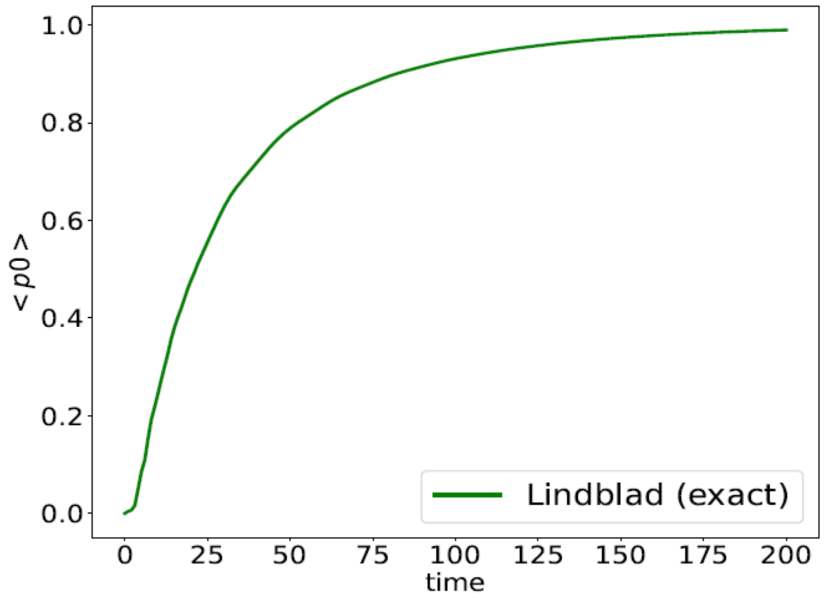
For simulation time $T = N\tau$ and precision ϵ, the total Hamiltonian simulation time is

$$T_{H,\text{total}} = \widetilde{\Theta}\left(T^{1+o(1)}\epsilon^{-o(1)}\right) .$$

TFIM-6 model:



(a) Simulation time vs energy



(b) Simulation time vs overlap

Start from $p_0 = 0$!

Outlook

- Likely to achieve quantum advantage in Level I (cryptography) and Level II (unitary quantum).
- A lot more quantum algorithms may be discovered at Level III (non-unitary quantum) and Level IV (classical).
- Co-design perspective:
  Interplay between algorithmic design, circuit synthesis, error correction, error mitigation
- Find better ways to communicate with the public on what have been achieved and what are achievable!