Algorithmic advances in quantum simulation

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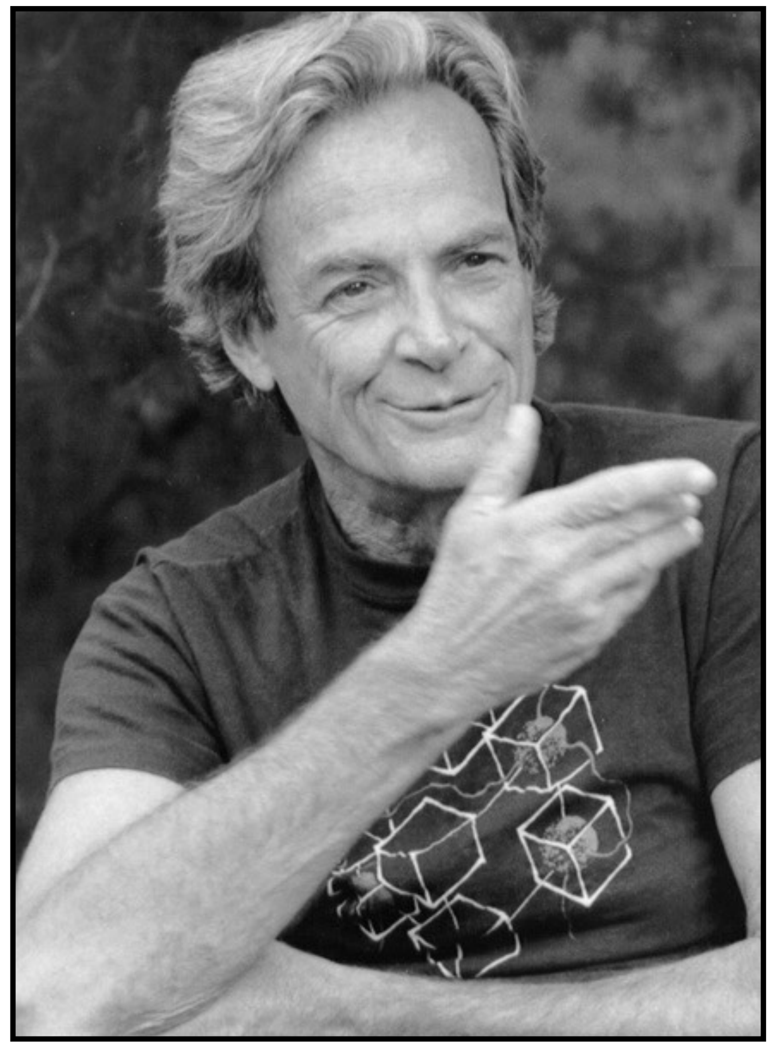
Quantum simulation



"… nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

Richard Feynman (1981)
Simulating physics with computers

Quantum simulation problem: Given a description of the Hamiltonian H, an evolution time t, and an initial state $|\psi(0)\rangle$, produce the final state $|\psi(t)\rangle$ (to within some error tolerance ϵ)

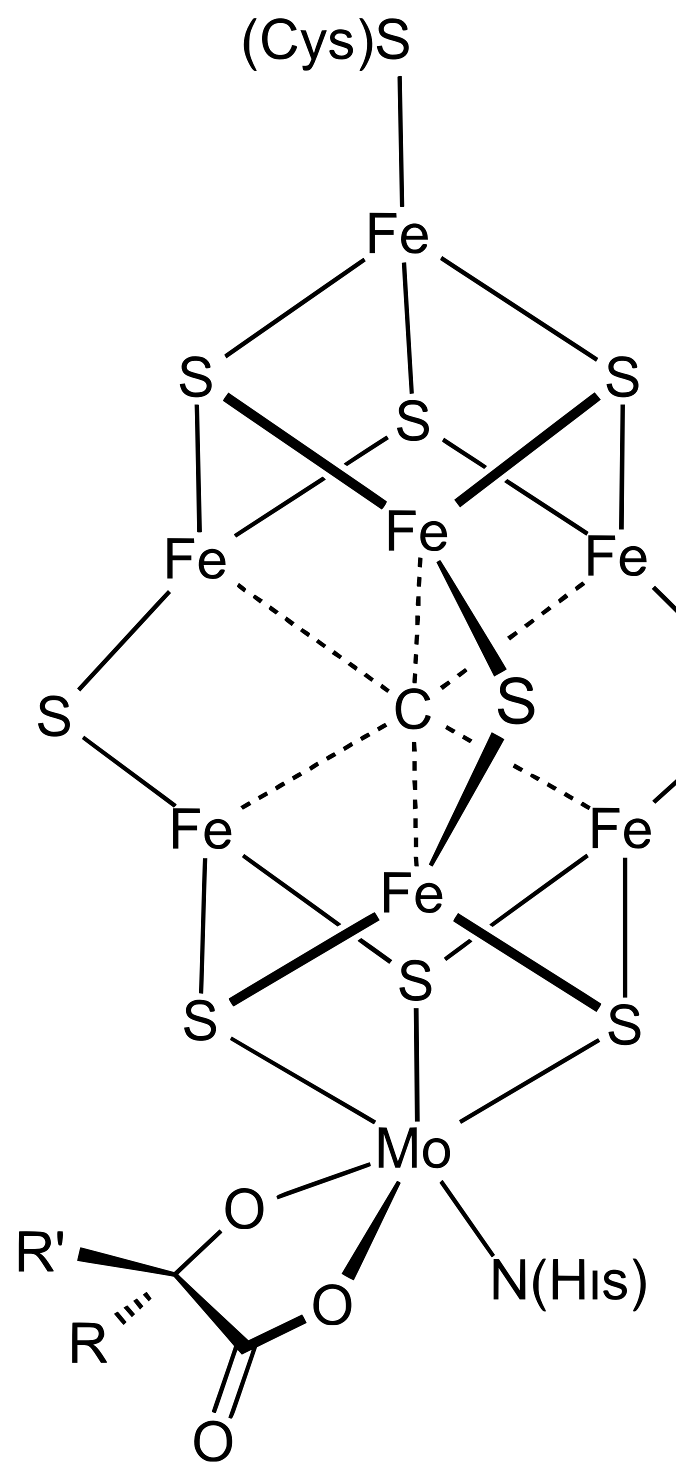
A classical computer cannot even represent the state efficiently.

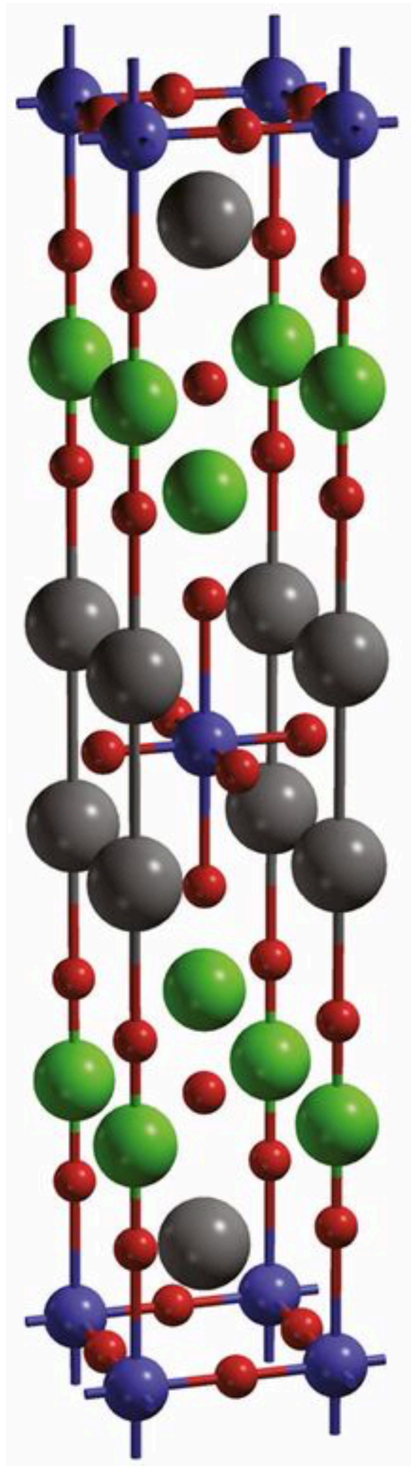
A quantum computer cannot produce a complete description of the state.

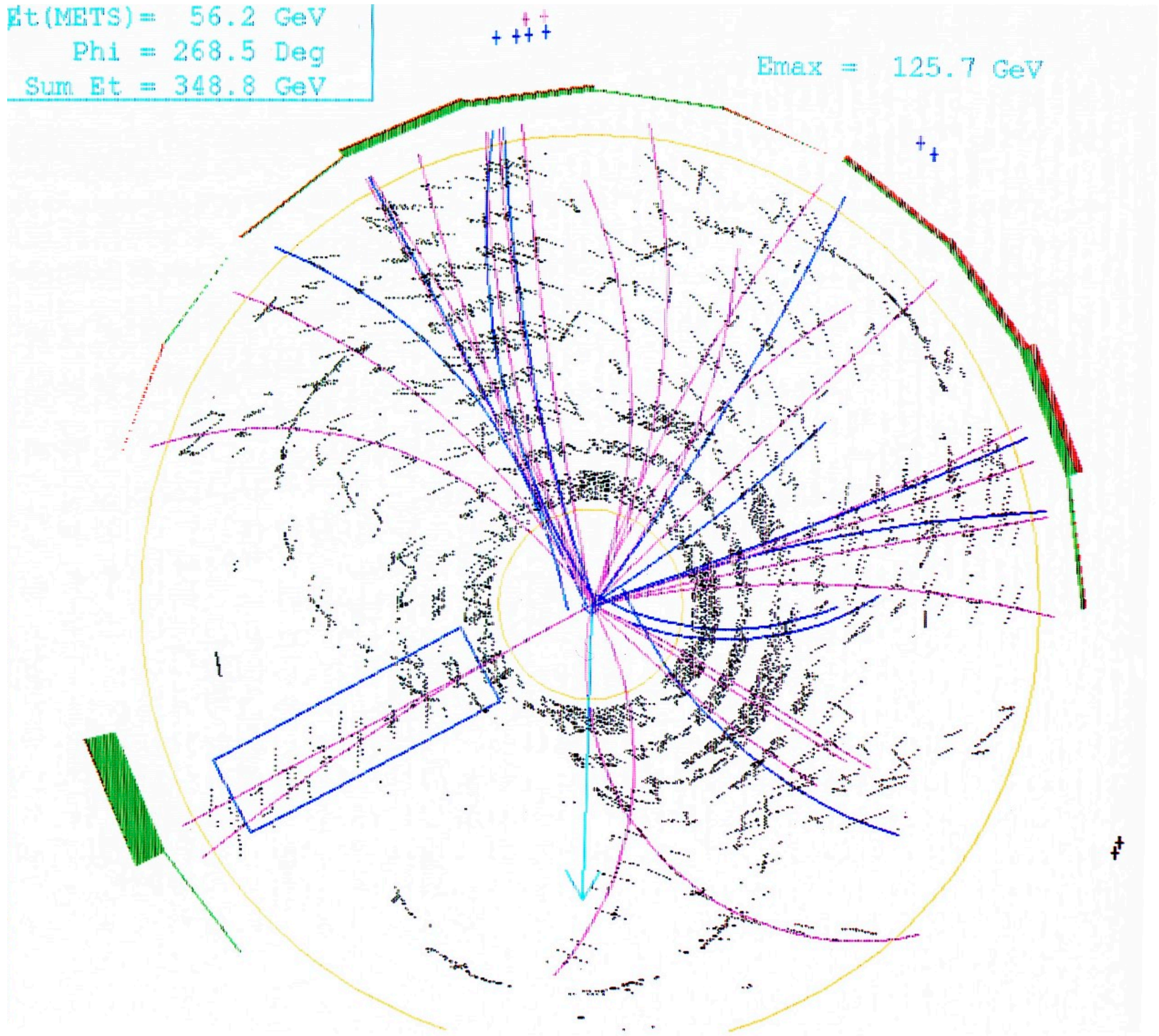
But given succinct descriptions of
- the initial state (suitable for a quantum computer to prepare it efficiently) and
- a final measurement (say, measurements of the individual qubits in some basis),

a quantum computer can efficiently answer questions that (apparently) a classical one cannot.

Computational quantum physics





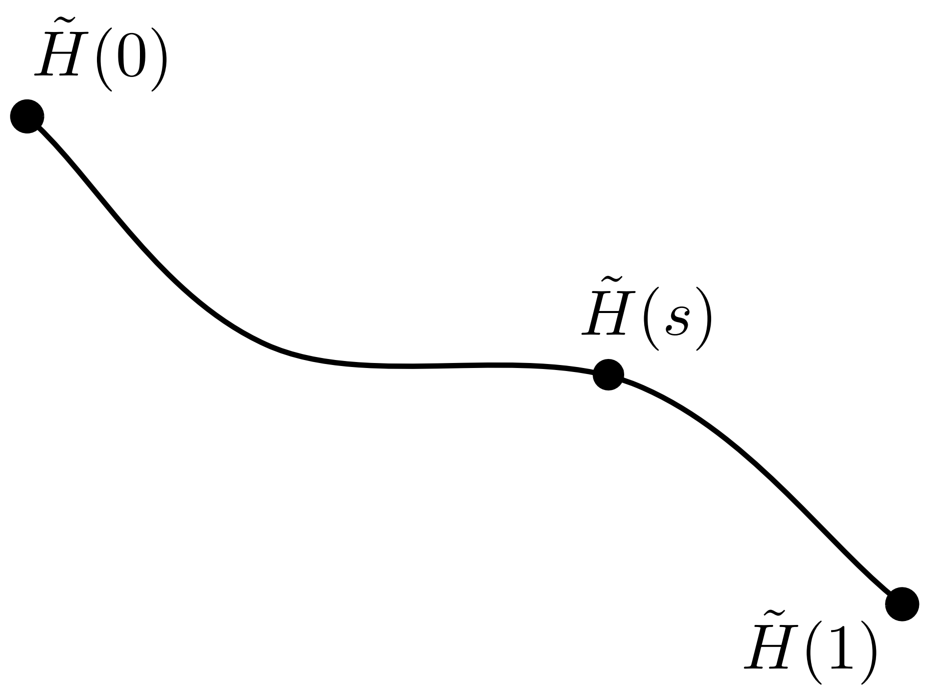


chemical reactions
(e.g., nitrogen fixation)

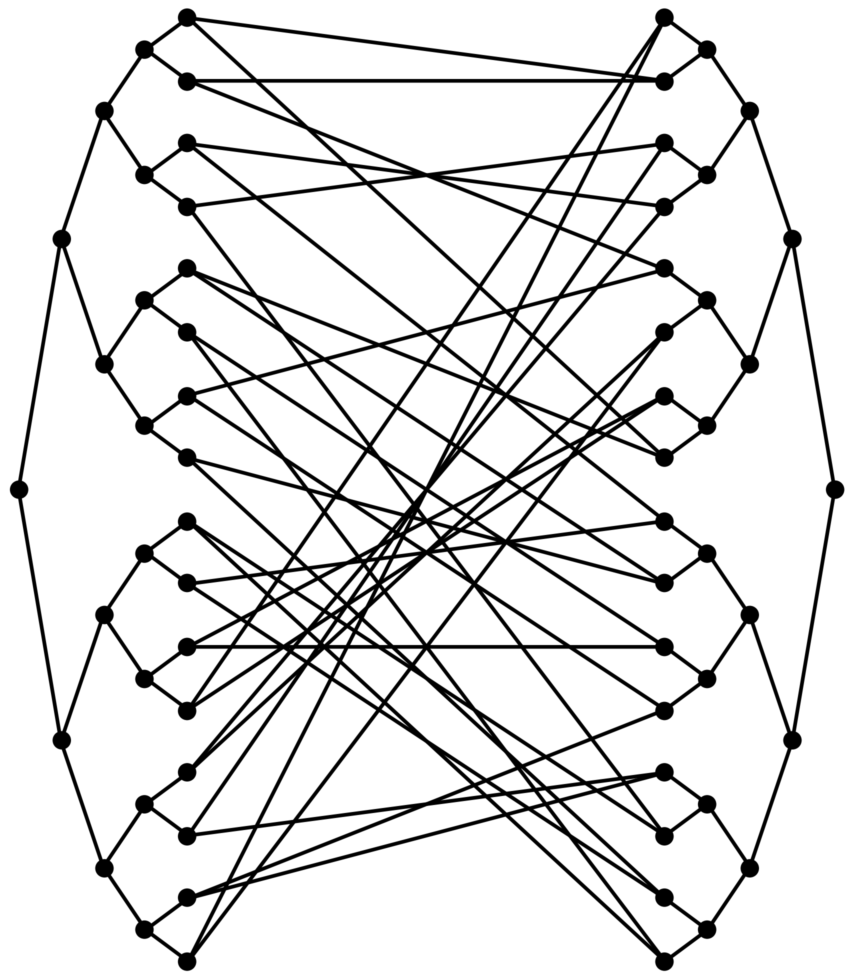
condensed matter physics/
properties of materials

nuclear/particle
physics

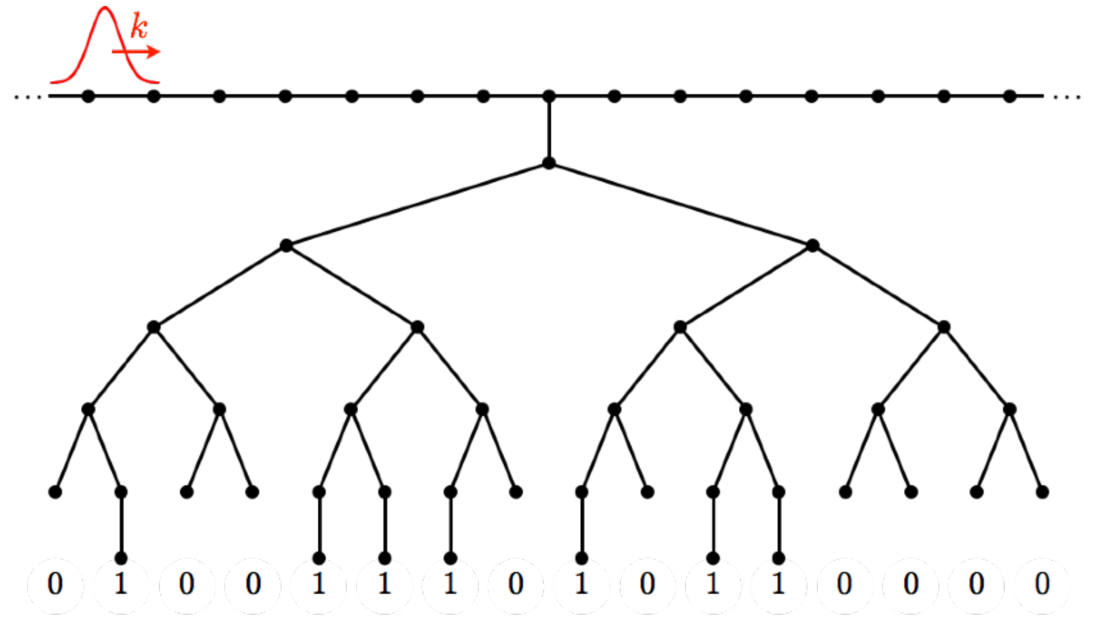
Implementing quantum algorithms



adiabatic optimization



exponential speedup by quantum walk



evaluating Boolean formulas

$$A|x\rangle = |b\rangle$$

linear/ differential equations, convex optimization

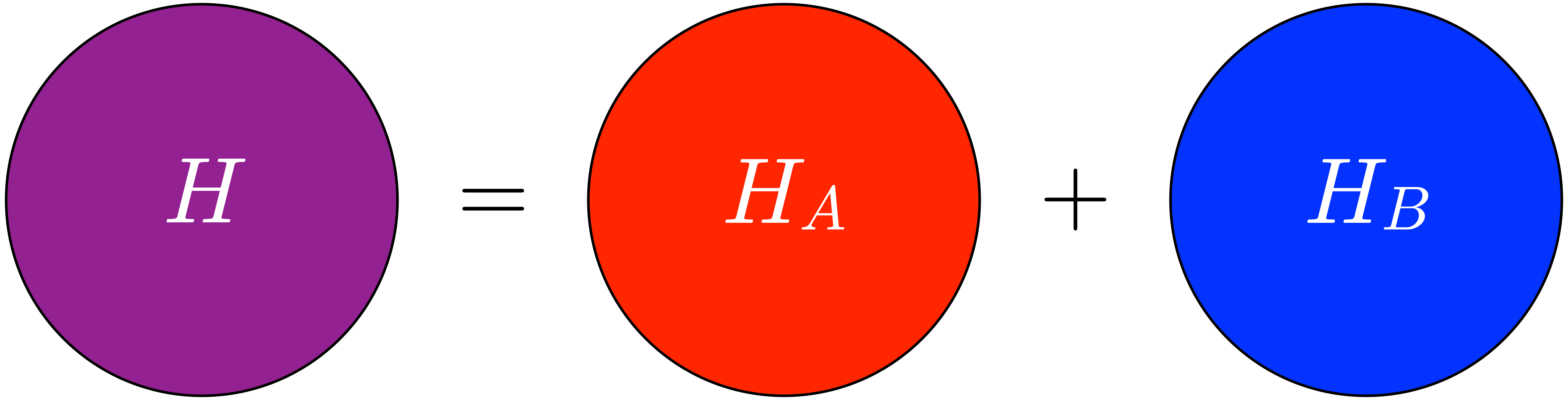
Product formula simulation

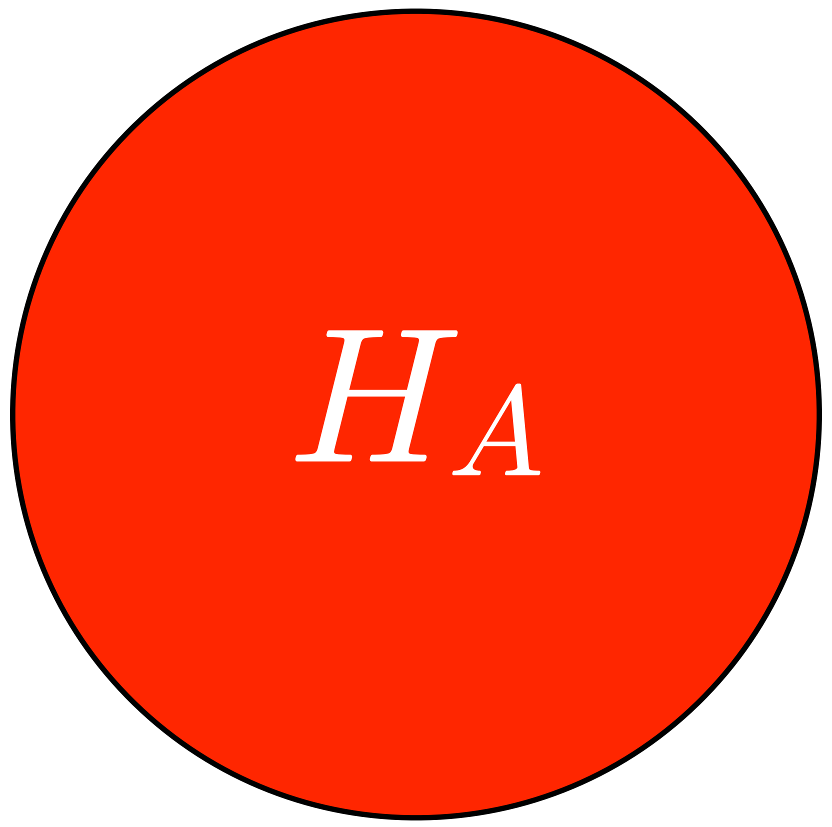
Suppose we want to simulate $H = \sum_{\ell=1}^{L} H_\ell$

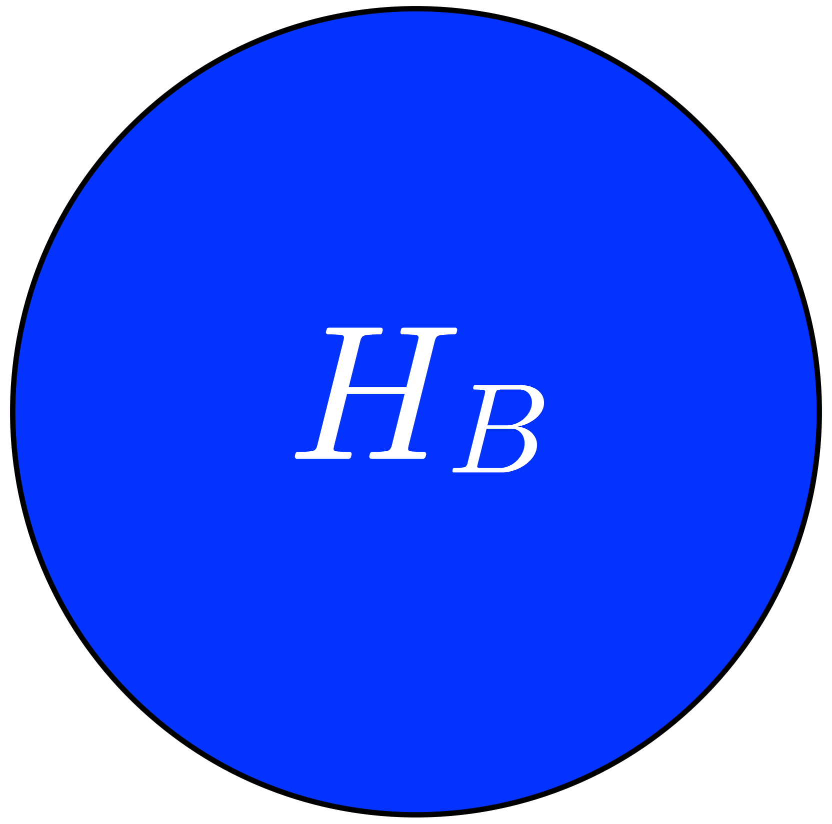
Combine individual simulations with the Lie product formula. E.g., with two terms:

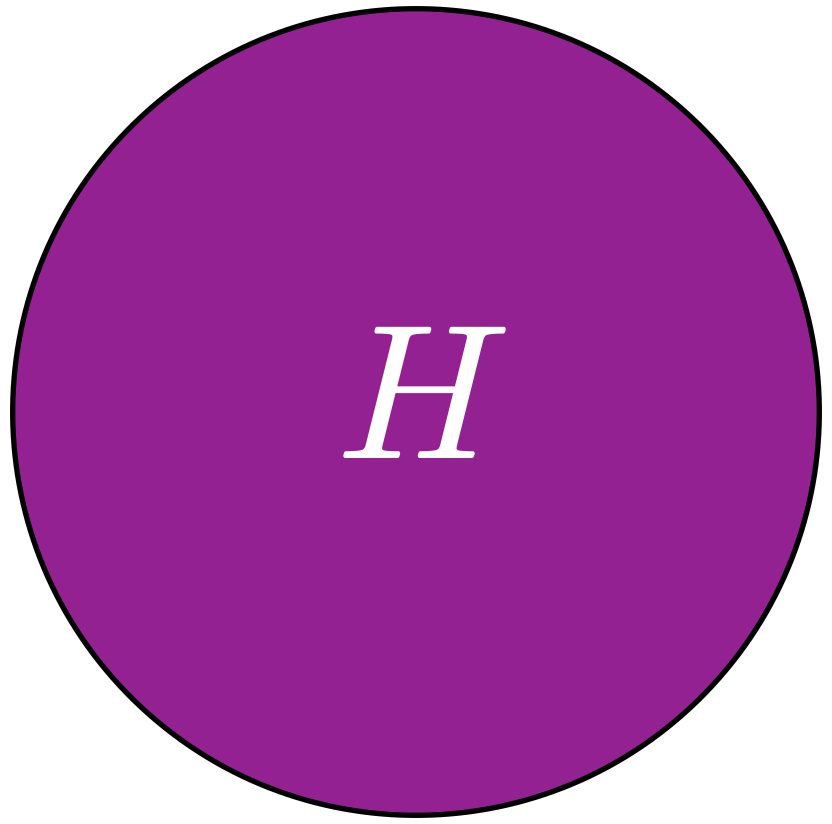
$$\lim_{r\to\infty} \left(e^{-iAt/r} e^{-iBt/r}\right)^r = e^{-i(A+B)t}$$

[Lloyd 96]


H
=
H_A
+
H_B


H_A


H_B


H

Product formula simulation

Suppose we want to simulate $H = \sum_{\ell=1}^{L} H_\ell$

Combine individual simulations with the Lie product formula. E.g., with two terms:

$$\lim_{r\to\infty} \left(e^{-iAt/r} e^{-iBt/r}\right)^r = e^{-i(A+B)t}$$

$$\left(e^{-iAt/r} e^{-iBt/r}\right)^r = e^{-i(A+B)t} + O(t^2/r)$$

To ensure error at most ϵ, take $r = O\big((\|H\|t)^2/\epsilon\big)$

[Lloyd 96]

To get a better approximation, use higher-order formulas.

E.g., second order:

$$(e^{-iAt/2r} e^{-iBt} e^{-iAt/2r})^r = e^{-i(A+B)t} + O(t^3/r^2)$$

Systematic expansions to arbitrary order are known [Suzuki 92]

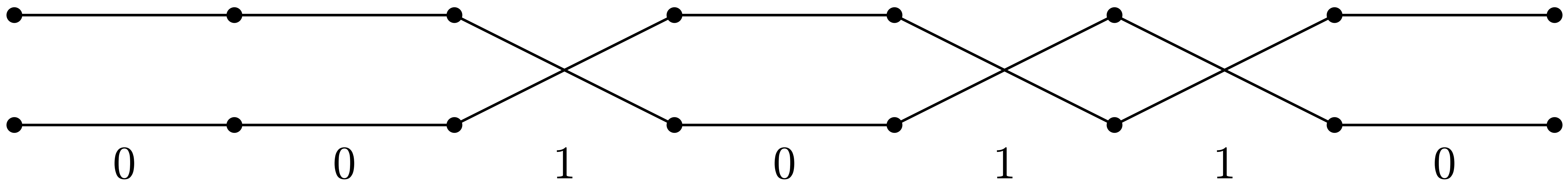
Using the $2k$th order expansion, the number of exponentials required for an approximation with error at most ϵ is at most

$$5^{2k} L^2 \|H\| t \left(\frac{L\|H\|t}{\epsilon}\right)^{1/2k}$$

[Berry, Ahokas, Cleve, Sanders 07]

Simulating quantum mechanics in real time

No fast-forwarding theorem: Simulating Hamiltonian dynamics for time t requires $\Omega(t)$ gates.



[Berry, Ahokas, Cleve, Sanders 05]

Complexity of kth order product formula simulation is $O(5^{2k}t^{1+1/2k})$.

Can we give an algorithm with complexity precisely $O(t)$?

Pro: Systems simulate their own dynamics in real time!
Con: Mismatch between continuous-time dynamics and the discrete-time circuit model.

Hamiltonian simulation by quantum walk

Quantum walk corresponding to H

Alternately reflect about $\mathrm{span}\{|\psi_j\rangle\}_{j=1}^N$,

$$|\psi_j\rangle := |j\rangle \otimes \left(\nu \sum_{k=1}^{N} \sqrt{H_{jk}^*}|k\rangle + \nu_j|N+1\rangle\right),$$

and swap the two registers.

If H is sparse, this walk is easy to implement.

Spectral theorem: Each eigenvalue λ of H corresponds to two eigenvalues $\pm e^{\pm i \arcsin \lambda}$ of the walk operator (with eigenvectors closely related to those of H).

Simulation by phase estimation

$$\begin{aligned} |\lambda\rangle &\mapsto |\lambda\rangle|\widetilde{\arcsin \lambda}\rangle && \text{(phase estimation)} \\ &\mapsto e^{-i\lambda t}|\lambda\rangle|\widetilde{\arcsin \lambda}\rangle \\ &\mapsto e^{-i\lambda t}|\lambda\rangle && \text{(inverse phase est)} \end{aligned}$$

Theorem: $O(t/\sqrt{\epsilon})$ steps of this walk suffice to simulate H for time t with error at most ϵ.

[Childs10; Berry, Childs 12]

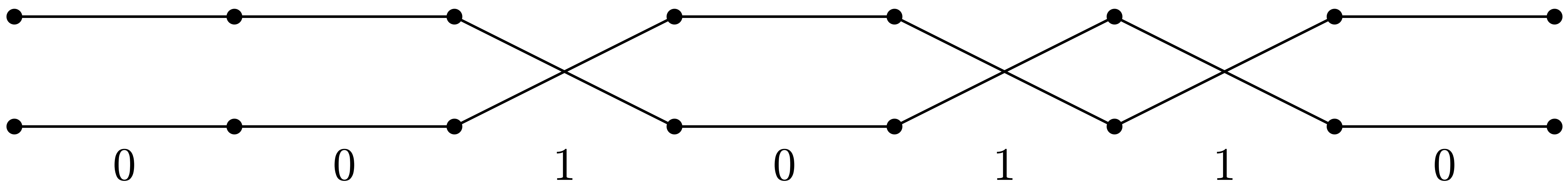
High-precision simulation?

Can we improve the dependence on ϵ?

Many approximate computations can be done with complexity $\mathrm{poly}(\log(1/\epsilon))$:

- computing numerical constants (e.g., π)
- boosting a bounded-error subroutine
- Solovay-Kitaev circuit synthesis
- and more…

Lower bound (based on the *unbounded-error* query complexity of parity): $\Omega\left(\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$



Quantum walk simulation: $O(1/\sqrt{\epsilon})$

Product formulas ($2k$th order): $O(5^{2k}\epsilon^{-2k})$

Can we do better?

Hamiltonian simulation by linear combinations of unitaries

Main idea: Directly implement the series

$$e^{-iHt} = \sum_{k=0}^{\infty} \frac{(-iHt)^k}{k!}$$
$$\approx \sum_{k=0}^{K} \frac{(-iHt)^k}{k!}$$

Write $H = \sum_\ell \alpha_\ell H_\ell$ with H_ℓ unitary.

Then

$$\sum_{k=0}^{K} \sum_{\ell_1,\ldots,\ell_k} \frac{(-it)^k}{k!} \alpha_{\ell_1} \cdots \alpha_{\ell_k} H_{\ell_1} \cdots H_{\ell_k}$$

is a linear combination of unitaries.

LCU Lemma: Given the ability to perform unitaries V_j with unit complexity, one can perform the operation $U = \sum_j \beta_j V_j$ with complexity $O(\sum_j |\beta_j|)$. Furthermore, if U is (nearly) unitary then this implementation can be made (nearly) deterministic.

Main ideas:

- Implement U with some amplitude:
  $$|0\rangle|\psi\rangle \mapsto \sin\theta|0\rangle U|\psi\rangle + \cos\theta|\Phi\rangle$$
- Boost the amplitude for success by *oblivious amplitude amplification*

Query complexity: $O\left(t\frac{\log(t/\epsilon)}{\log\log(t/\epsilon)}\right)$

[Berry, Childs, Cleve, Kothari, Somma 14 & 15]

Tradeoff between t and ϵ

Combining known lower bounds on the complexity of simulation as a function of t and ϵ gives

$$\Omega\Big(t + \frac{\log \frac{1}{\epsilon}}{\log\log \frac{1}{\epsilon}}\Big) \quad \text{vs. upper bound of} \quad O\Big(t \frac{\log \frac{t}{\epsilon}}{\log\log \frac{t}{\epsilon}}\Big)$$

An alternative method for implementing a linear combination of unitary operations, *quantum signal processing*, gives an optimal tradeoff. [Low, Chuang 16, 17]

Main idea: Encode the eigenvalues of H in a two-dimensional subspace; use a carefully-chosen sequence of single-qubit rotations to manipulate those eigenvalues.

Computing the rotation angles is challenging, but can be done efficiently (classically) [Haah 18]. Recent approaches are faster [Dong, Meng, Whaley, Lin 20; Chao, Ding, Gilyén, Huang, Szegedy 20].

Quantum signal processing (and more general *quantum singular value transformation*) gives a powerful framework for designing other quantum algorithms [Gilyén, Su, Low, Wiebe 19].

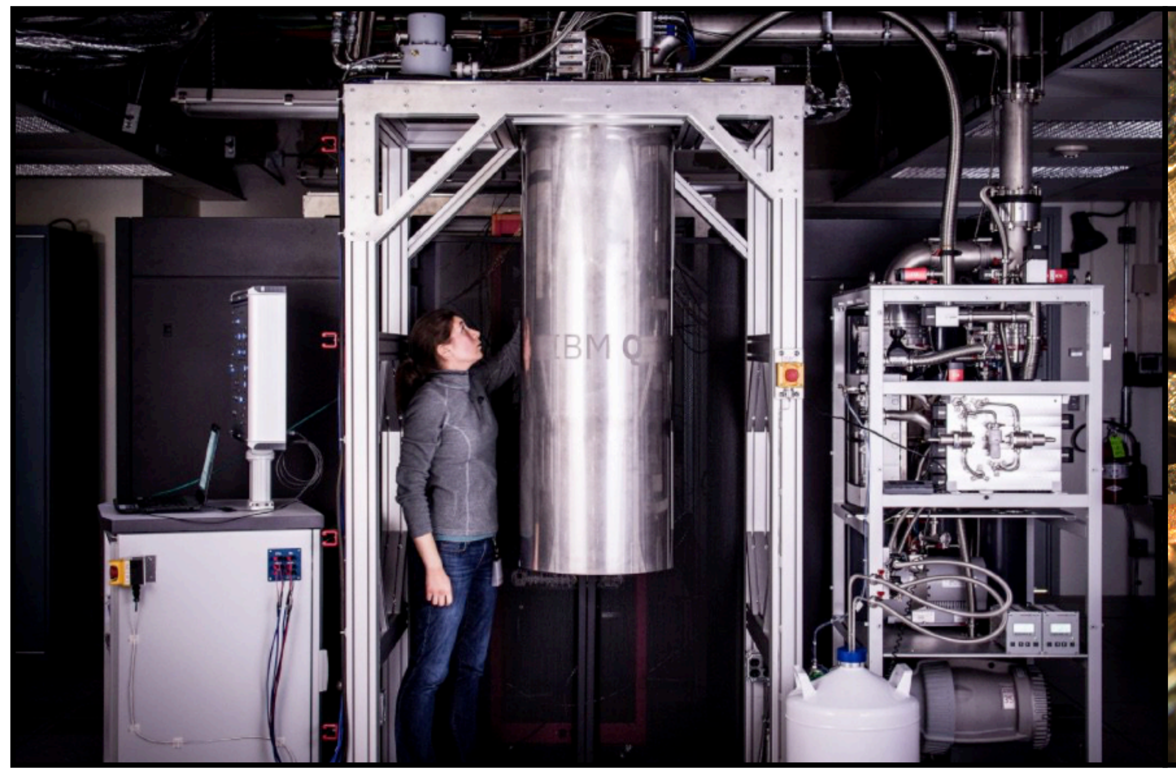
Algorithm comparison

t: evolution time
ϵ: allowed error
d: sparsity

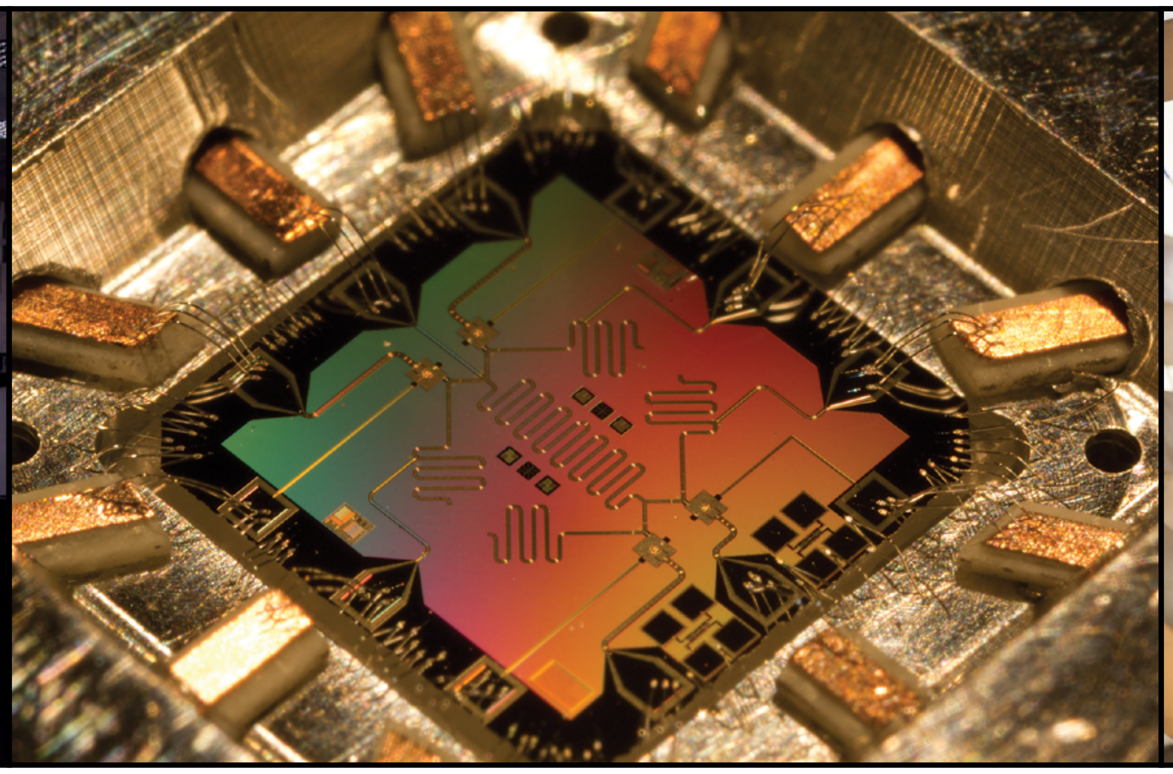
Algorithm	Query complexity	Gate complexity
Product formula, 1st order	$O(d^4t^2/\epsilon)$	$O(d^4t^2/\epsilon)$
Product formula, (2k)th order	$O\left(5^{2k}d^3t(\frac{dt}{\epsilon})^{1/2k}\right)$	$O\left(5^{2k}d^3t(\frac{dt}{\epsilon})^{1/2k}\right)$
Quantum walk	$O(dt/\sqrt{\epsilon})$	$O(dt/\sqrt{\epsilon})$
Fractional-query simulation	$O\left(d^2t\frac{\log(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$	$O\left(d^2t\frac{\log^2(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$
Taylor series	$O\left(d^2t\frac{\log(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$	$O\left(d^2t\frac{\log^2(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$
Linear combination of q. walk steps	$O\left(dt\frac{\log(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$	$O\left(dt\frac{\log^{3.5}(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$
Quantum signal processing	$O\left(dt+\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$	$O\left(dt+\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$

OPTIMAL!

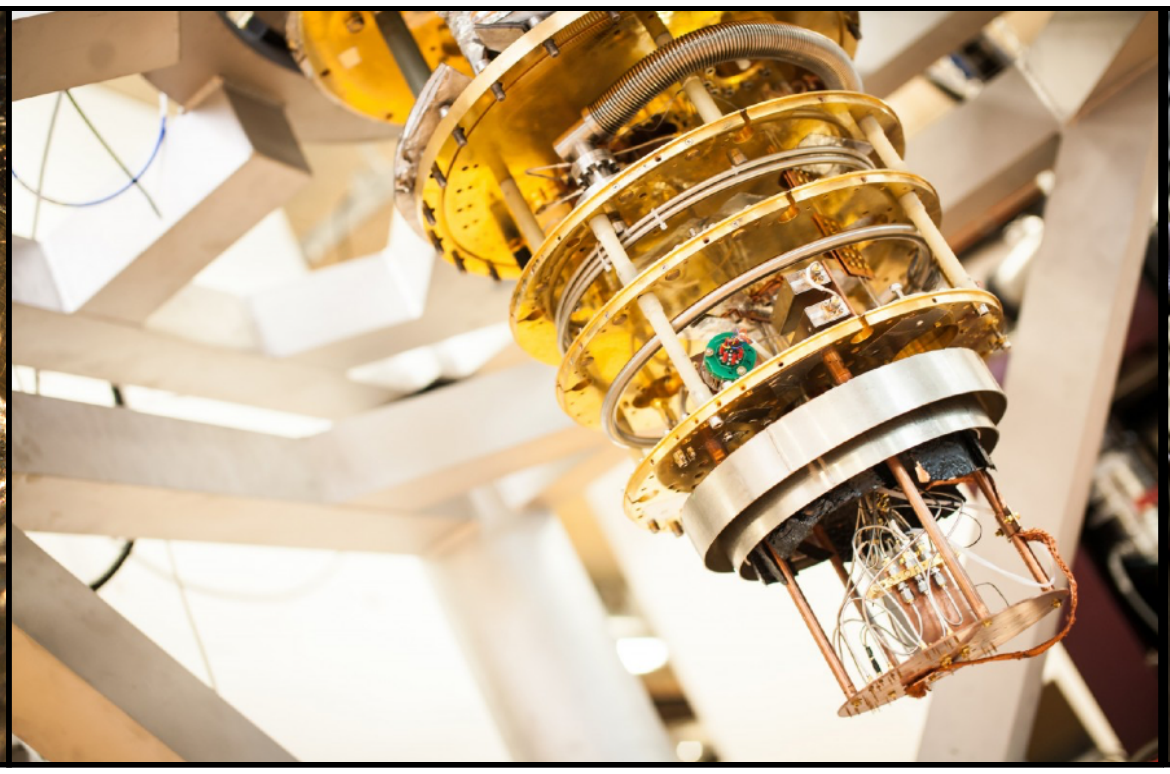
Toward practical quantum speedup



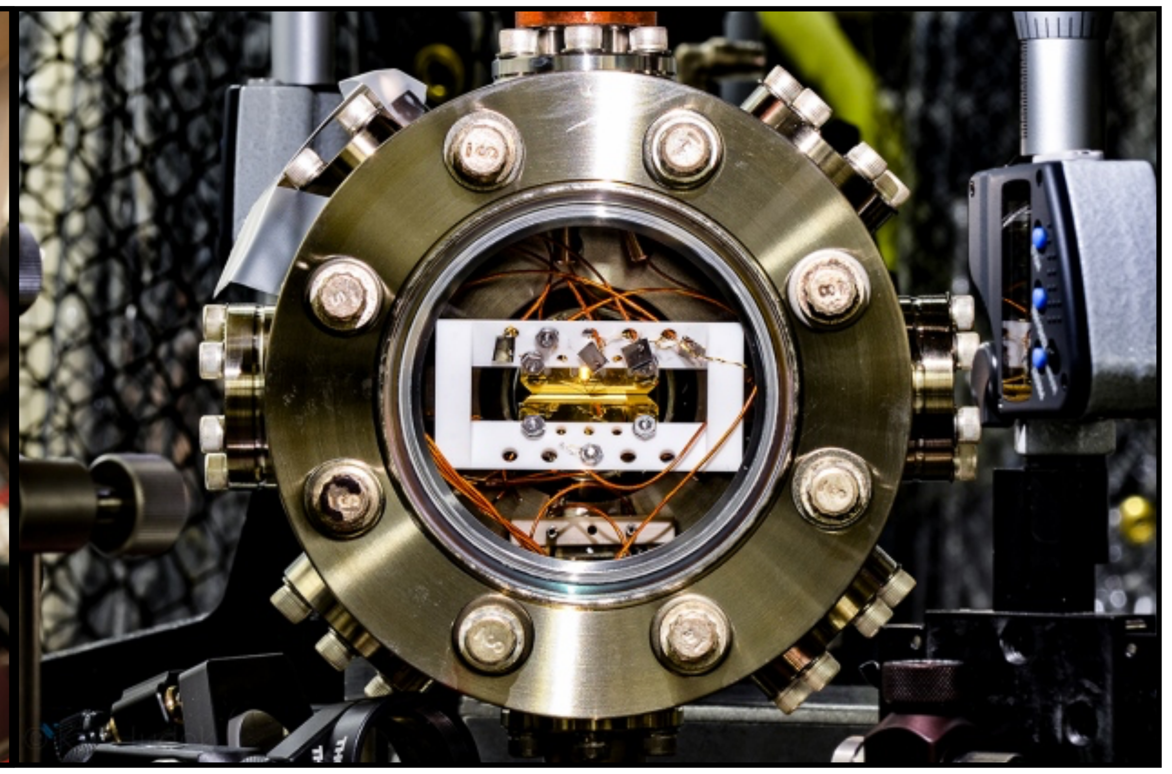
IBM



Google



Delft



Maryland

Important early goal: demonstrate quantum computational advantage

… but can we find a *practical* application of near-term devices?

Challenges

- Improve experimental systems
- Improve algorithms and their implementation, making the best use of available hardware

Goal: Produce concrete resource estimates for the simplest possible practical application of quantum computers

What to simulate?

~~Quantum chemistry?~~ Spin systems!

Heisenberg model on a ring: $H = \sum_{j=1}^{n} (\vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + h_j \sigma_j^z)$ $h_j \in [-h, h]$ uniformly random

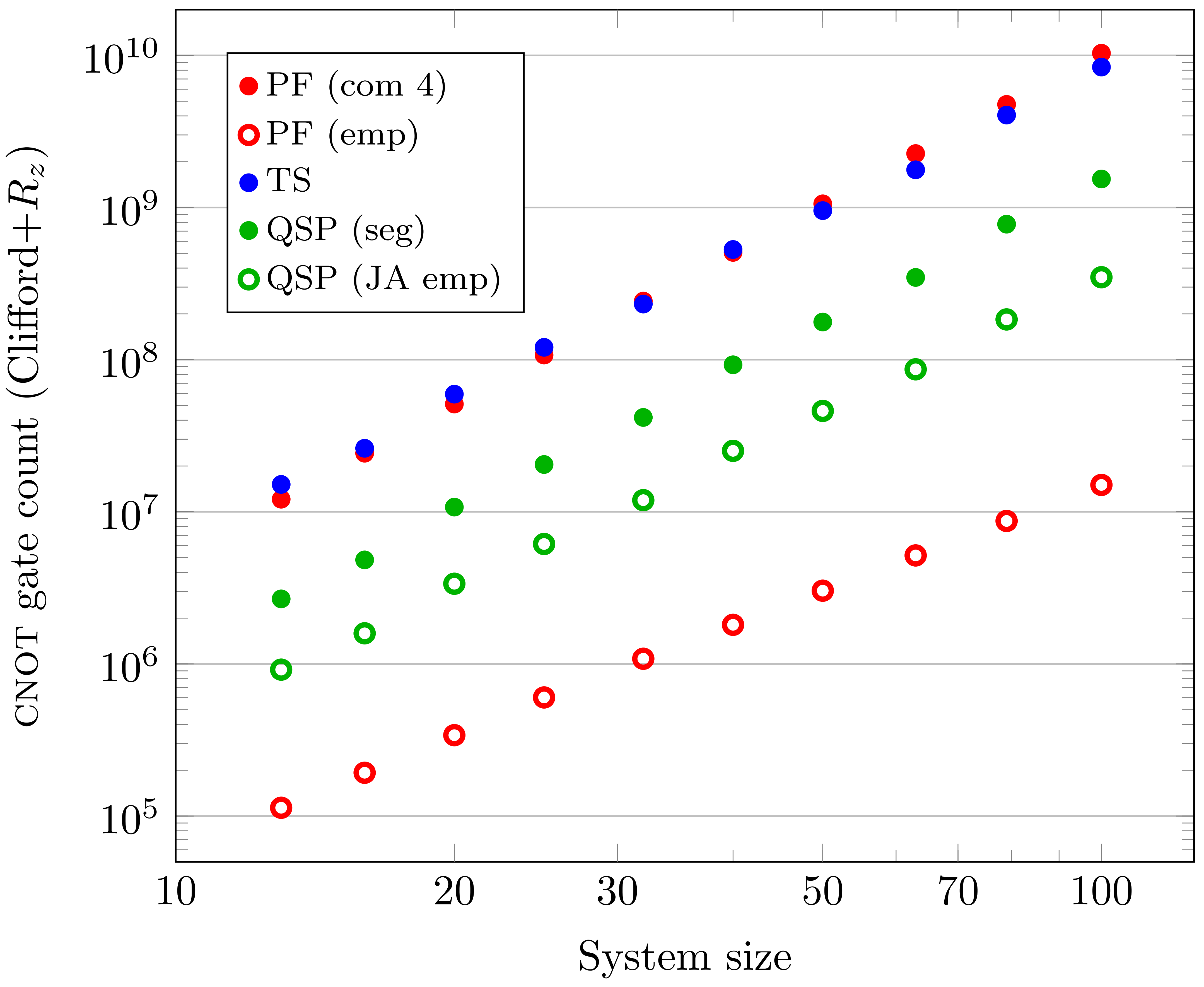
This provides a model of *self-thermalization* and *many-body localization*.

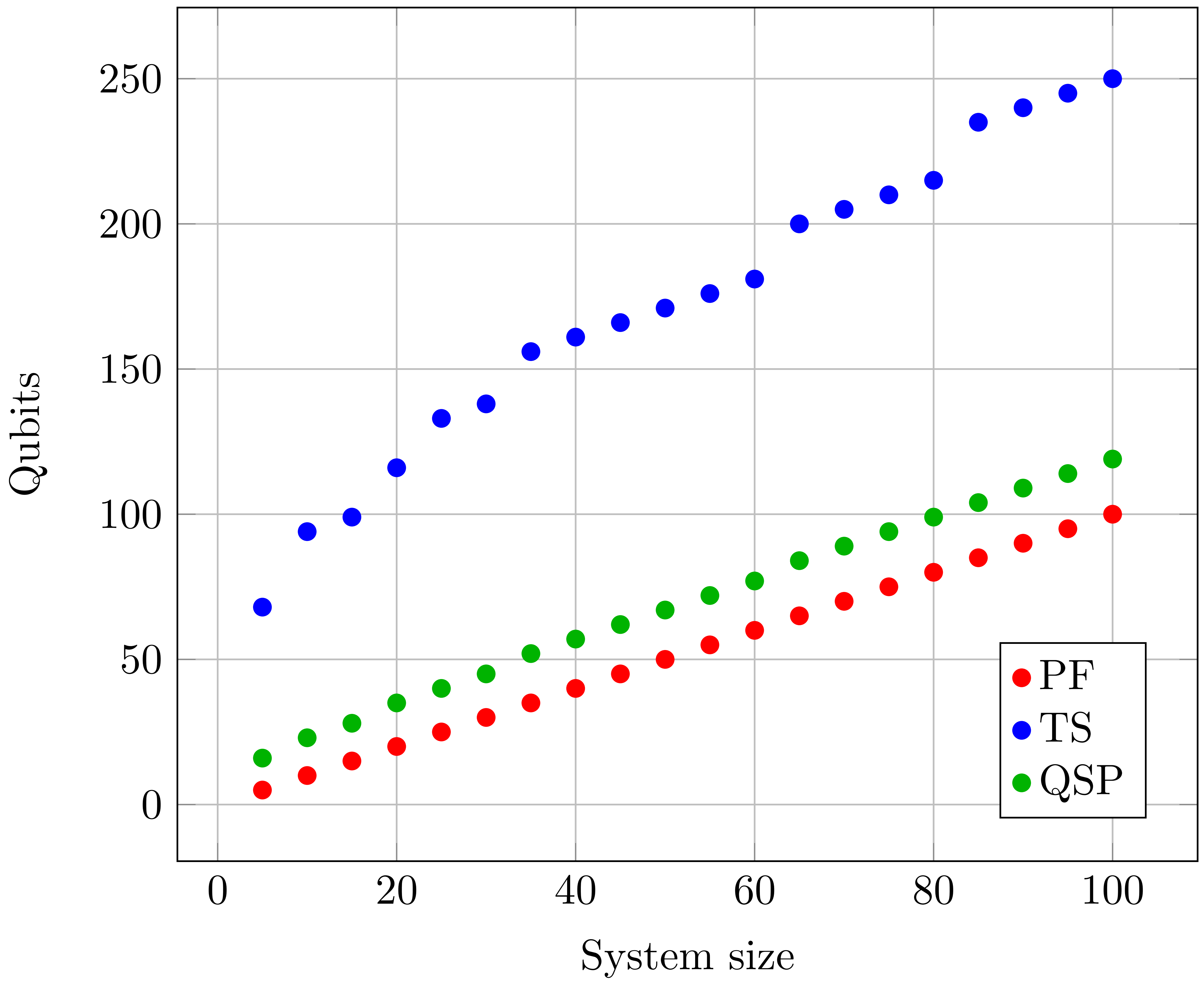
The transition between thermalized and localized phases (as a function of h) is poorly understood. Most extensive numerical study: fewer than 25 spins. [Luitz, Laflorencie, Alet 15]

Could explore the transition by preparing a simple initial state, evolving, and performing a simple final measurement. Focus on the cost of simulating dynamics.

For concreteness: $h = 1, \quad t = n, \quad \epsilon = 10^{-3}, \quad 20 \leq n \leq 100$

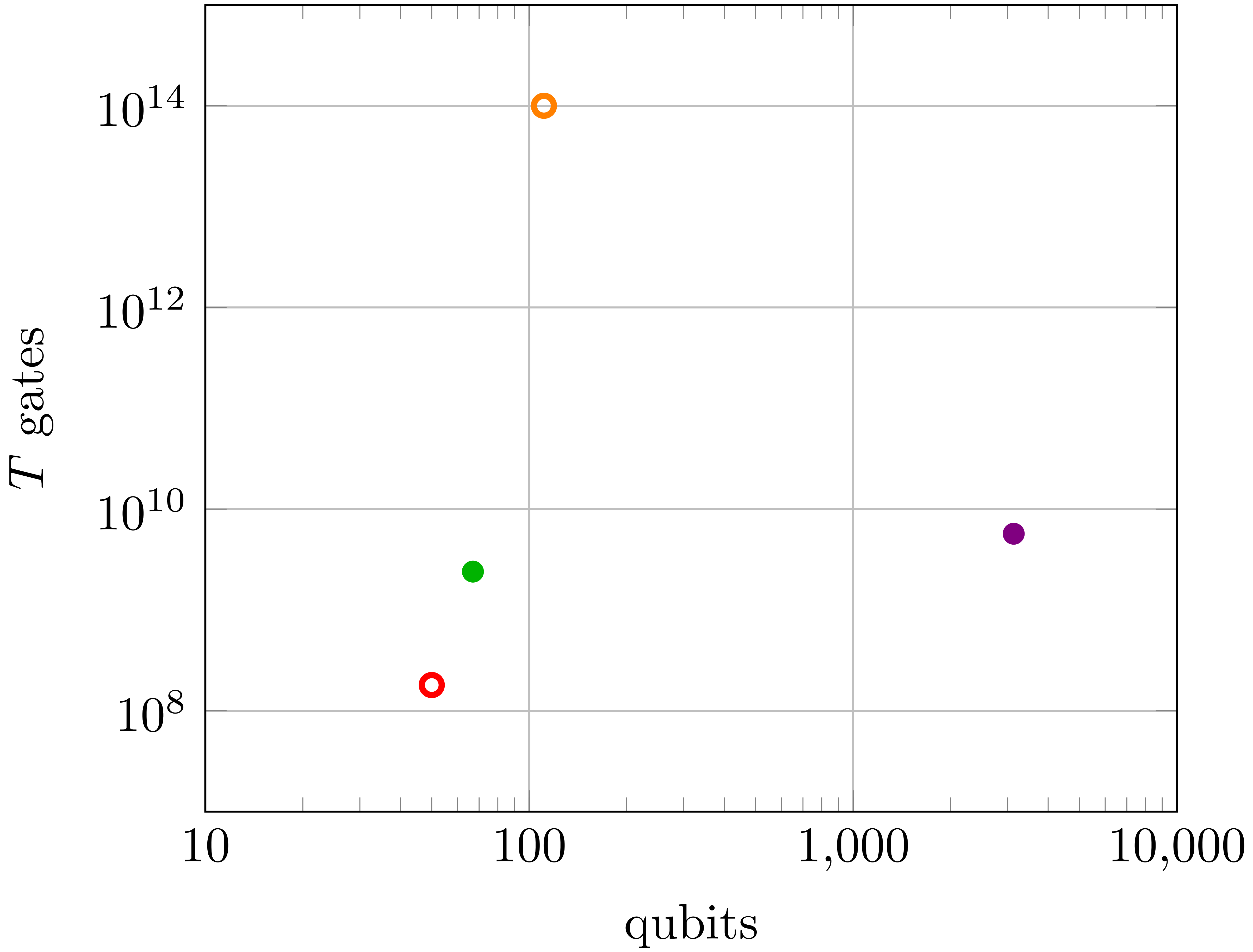
Resource estimates





[Childs, Maslov, Nam, Ross, Su 18]

Comparison



Factoring a 1024-bit number [Kutin 06]

- 3132 qubits
- 5.7×10^9 T gates

Simulating FeMoco [Reiher et al. 16]

- 111 qubits
- 1.0×10^{14} T gates

Simulating 50 spins (segmented QSP)

- 67 qubits
- 2.4×10^9 T gates

Simulating 50 spins (PF6 empirical)

- 50 qubits
- 1.8×10^8 T gates

[Childs, Maslov, Nam, Ross, Su 18]

Lattice Hamiltonians

We've focused on the complexity as a function of t (evolution time) and ϵ (precision).
What about the dependence on system size?

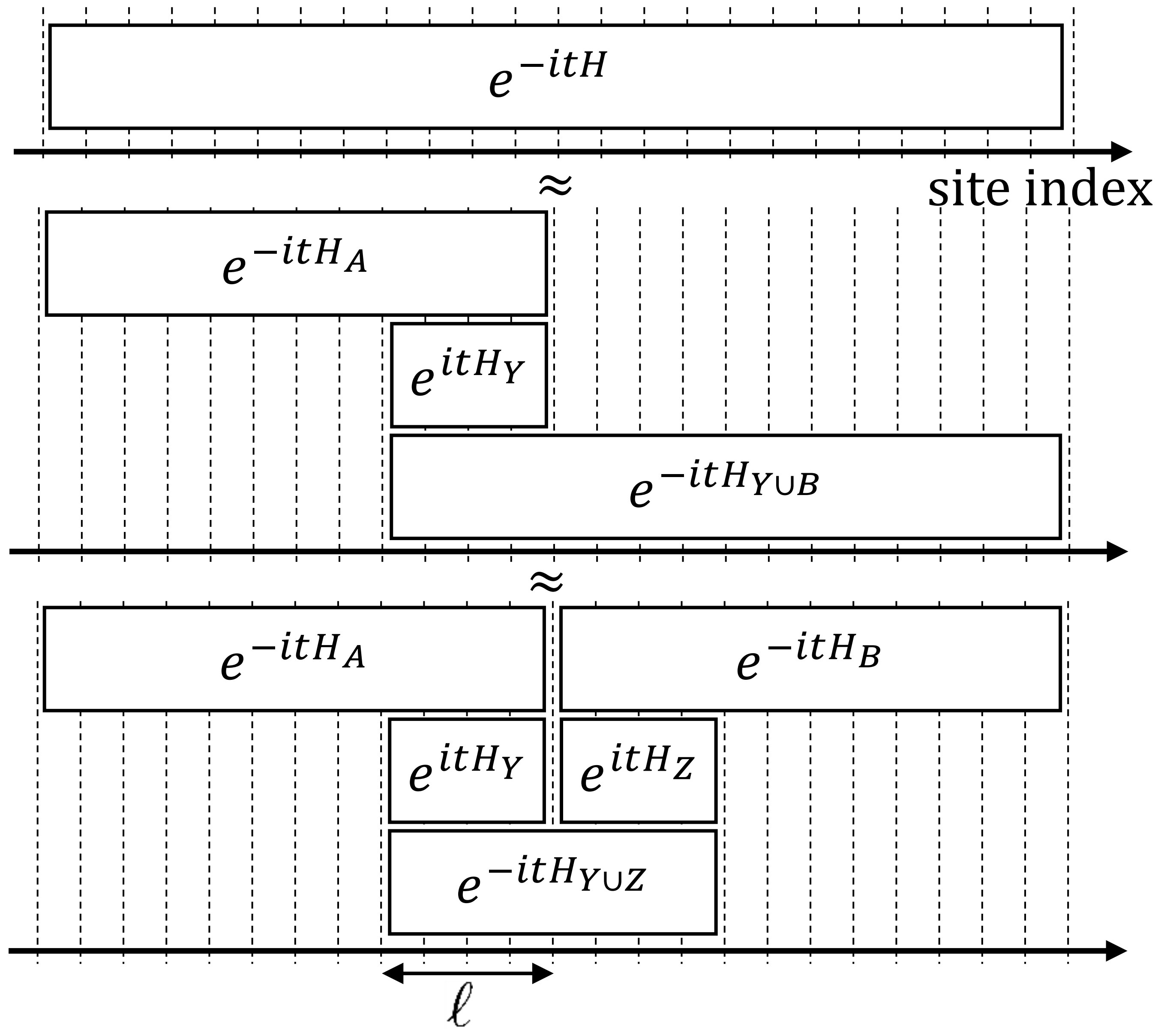
Consider a system of n spins with nearest-neighbor interactions on a grid of fixed dimension. To simulate for constant time, best previous methods (TS, QSP, high-order PF) give:

- total number of gates: $O(n^2)$
- circuit depth (execution time with parallel gates): $O(n)$

Execution time should not have to be extensive!

Recent improvement: simulation with $\tilde{O}(n)$ gates, $\tilde{O}(1)$ depth (optimal!) [Haah, Hastings, Kothari, Low 18]

- Lieb-Robinson bound limits the speed of propagation
- Simulate small regions with negative-time evolutions to correct the boundaries



Local error analysis

In fact, product formulas achieve nearly the same complexity!

Main technique: *local error analysis* provides a convenient integral representation of the error

[Descombes, Thalhammer 10]

Example (first order):

$$e^{-iBt}e^{-iAt} - e^{-i(A+B)t} = \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2\, e^{-i(A+B)(t-\tau_1)} e^{i(\tau_2-\tau_1)B}[A,B]e^{-i\tau_2 B}e^{-i\tau_1 A}$$

For an n-site lattice system, letting A = even terms and B = odd terms, we find a simulation error of $O(nt^2)$, so $O(n^2t^2)$ gates suffice to simulate with constant accuracy (vs. $O(n^3t^2)$ with standard analysis).

Generalizations give similar (though more complicated!) expressions for the error in higher-order product formulas.

Complexity at order p: $O\big((nt)^{1+\frac{1}{p}}\big)$ (vs. $O\big(n(nt)^{1+\frac{1}{p}}\big)$ with standard analysis)

[Childs, Su 19]

A theory of Trotter error

Local error analysis can be generalized to give tight bounds on the error of product formula approximations depending on commutators of the terms.

Theorem. A pth order product formula approximates the evolution of $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$ with additive error $O(\alpha t^{p+1})$ where

$$\alpha := \sum_{\gamma_1,\ldots,\gamma_{p+1}} \left\| [H_{\gamma_{p+1}}, [\cdots, [H_{\gamma_2}, H_{\gamma_1}] \cdots]] \right\|.$$

Therefore $O(\Gamma \alpha^{1/p} t^{1+1/p})$ gates suffice to give a simulation with constant accuracy.

Applications:

- Tighter rigorous analysis of product formulation simulations (e.g., only off by factor of ~5 for 50-qubit Heisenberg model)
- Simpler simulation of plane-wave electronic structure, nearly matching interaction picture simulation
- Simulation of k-local Hamiltonians with better norm scaling than qubitization
- Faster simulation of power-law interactions
- Faster hybrid quantum/classical simulation of clustered Hamiltonians
- Tighter analysis of quantum Monte Carlo methods

[Childs, Su, Tran, Wiebe, Zhu 19; talk at https://ter.ps/trottertalk]

Randomized simulation

Another approach to speeding up simulation: introduce classical randomness

Example:

$$
\begin{aligned}
e^{-i(A+B)t} &= I - i(A+B)t - \tfrac{1}{2}(A^2 + AB + BA + B^2)t^2 + O(t^3) \\
e^{-iAt}e^{-iBt} &= I - i(A+B)t - \tfrac{1}{2}(A^2 + 2AB + B^2)t^2 + O(t^3) \\
e^{-iBt}e^{-iAt} &= I - i(A+B)t - \tfrac{1}{2}(A^2 + 2BA + B^2)t^2 + O(t^3)
\end{aligned}
$$

$$\Downarrow$$

$$\tfrac{1}{2}(e^{-iAt}e^{-iBt} + e^{-iBt}e^{-iAt}) = e^{-i(A+B)t} + O(t^3)$$

[Zhang 12]

Mixing lemma [Campbell 17, Hastings 17]: Error of the average operation is linear in the average error, quadratic in the error of individual operations.

Randomly permuting terms in a higher-order product formula also improves the approximation (though not the order of the formula). [Childs, Ostrander, Su 18]

It can also be advantageous to sample terms of the Hamiltonian nonuniformly. [Campbell 18]
Gives faster simulations of strongly time-dependent Hamiltonians. [Berry, Childs, Su, Wang, Wiebe 20]

Outlook

Develop applications of quantum simulation to physics/chemistry

- Quantum chemistry
- Condensed matter
- Nuclear/particle physics

Improve quantum algorithms for Hamiltonian simulation

- Tighter error bounds for product formulas (improve local error analysis; go beyond the triangle inequality)
- Faster simulation methods for structured Hamiltonians
- More efficient synthesis of the QSP circuit

Explore prospects for near-term implementations

- Resource estimates under realistic hardware constraints
- Can we perform classically hard simulations without invoking fault tolerance?
- Noise-tolerant algorithms

Quantum simulation as an algorithmic tool

- Linear algebra in Hilbert space: linear systems, differential equations, convex optimization, ...
- Find new applications of quantum simulation