High-precision quantum algorithms

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What can we do with a quantum computer?

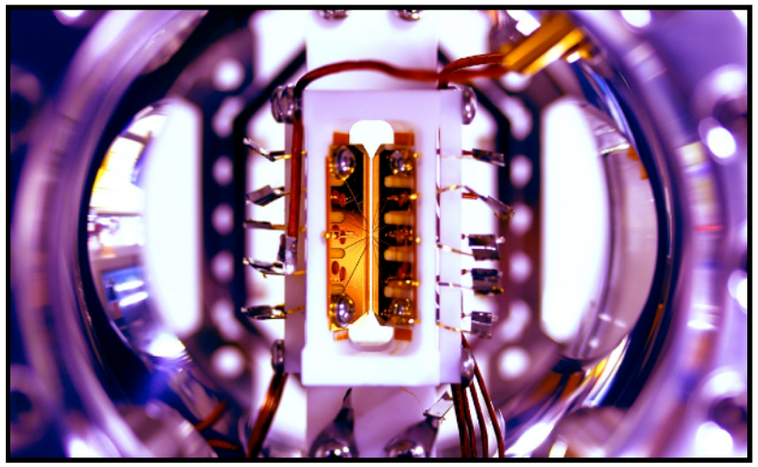
- Factoring
- Many problems with polynomial speedup (combinatorial search, collision finding, graph properties, Boolean formula evaluation, …)
- Simulating quantum mechanics
- Linear systems
- And more: computing discrete logarithms, decomposing abelian groups, computing properties of algebraic number fields, approximating Gauss sums, counting points on algebraic curves, approximating topological invariants, finding isogenies between elliptic curves…

Quantum algorithm zoo: math.nist.gov/quantum/zoo/

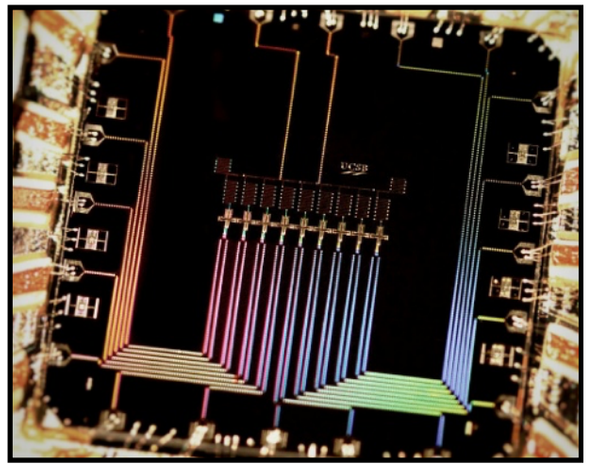
When can I have one?

State of the art: well-characterized qubits with well-controlled interactions and long coherence times.

Leading candidate systems:



trapped ions



superconducting qubits

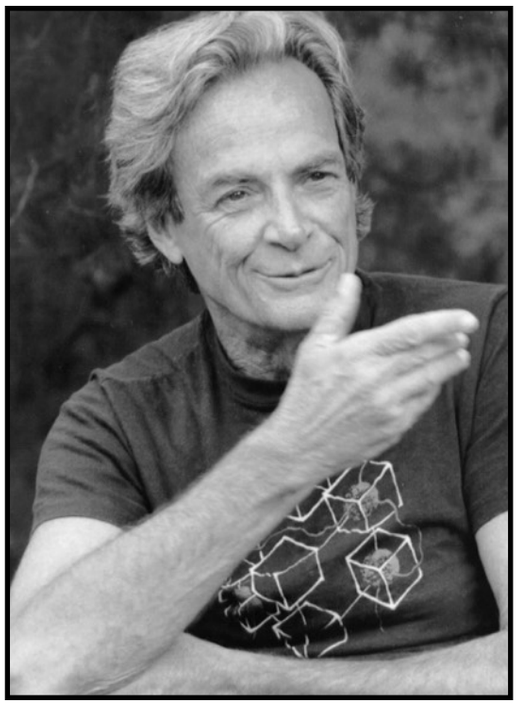
Several large experimental groups (Maryland/IonQ, UCSB/Google, IBM, Delft/Intel, …) have serious efforts underway to consider scaling up to a larger device—a major engineering challenge!

Why else should you care?

- Studying the power of quantum computers addresses a basic scientific question: what can be computed efficiently in the real world?

- To design cryptosystems that are secure against quantum attacks, we have to understand what kinds of problems quantum computers can solve.

- Ideas from quantum information provide new tools for thinking about physics (e.g., the black hole information loss problem) and computer science (e.g., quantum algorithm for evaluating Boolean formulas → upper bound on polynomial threshold function degree → new subexponential (classical!) algorithms in computational learning theory)



"… 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
Simulating physics with computers (1981)

Why simulate quantum mechanics?

Computational chemistry/physics

- chemical reactions (e.g., nitrogen fixation)
- properties of materials

Implementing quantum algorithms

- continuous-time quantum walk (e.g., for formula evaluation)
- adiabatic quantum computation (e.g., for optimization)
- linear/differential equations

Quantum dynamics

The dynamics of a quantum system are determined by its *Hamiltonian*.

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle$$
$$\Downarrow$$
$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

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 by performing measurements on the state, it can answer questions that (apparently) a classical computer cannot

Local and sparse Hamiltonians

Local Hamiltonians [Lloyd 96]

$H = \sum_{j=1}^{m} H_j$ where each H_j acts on $k = O(1)$ qubits

Sparse Hamiltonians [Aharonov, Ta-Shma 03]

At most d nonzero entries per row, $d = \mathrm{poly}(\log N)$
(where H is $N \times N$)

In any given row, the location of the jth nonzero entry and its value can be computed efficiently (or is given by a black box)

Note: A k-local Hamiltonian with m terms is d-sparse with $d = 2^k m$

High-precision computing

Suppose we want to perform a computation that must be accurate to within ϵ. What is the cost as a function of ϵ?

Computing n digits of π: $O(n \operatorname{poly}(\log n))$

→ precision ϵ in $O(\log(1/\epsilon) \operatorname{poly}(\log\log(1/\epsilon))$

Boosting success probability of a randomized algorithm:

Suppose we can solve a decision problem with success probability bounded away from 1/2 (say, 51%)

To get higher accuracy, repeat many times and take a majority vote

For error ϵ, need $O(\log(1/\epsilon))$ repetitions

Quantum circuit synthesis: cost of implementing a one-qubit gate with precision ϵ is $\operatorname{poly}(\log(1/\epsilon))$ [Solovay-Kitaev]

What about quantum simulation?

Product formula simulation

Suppose we want to simulate $H = \sum_{i=1}^{m} H_i$

Combine individual simulations with the Lie product formula:

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

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

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

[Lloyd 96]

High-order product formulas

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

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

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

$$\vdots$$

Systematic expansions to arbitrary order are known [Suzuki 92]

Using the kth order expansion, the number of exponentials required for an approximation with error at most ϵ is at most

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

[Berry, Ahokas, Cleve, Sanders 07]

High-precision simulation

We have recently developed a novel approach that directly implements the Taylor series of the evolution operator

New tools:

- Implementing linear combinations of unitary operations
- Oblivious amplitude amplification

Dependence on simulation error is $\mathrm{poly}(\log(1/\epsilon))$, an exponential improvement over previous work

Algorithms are also simpler, with less overhead

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

Linear combinations 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:

- Using controlled-V_j operations, implement U with some amplitude:

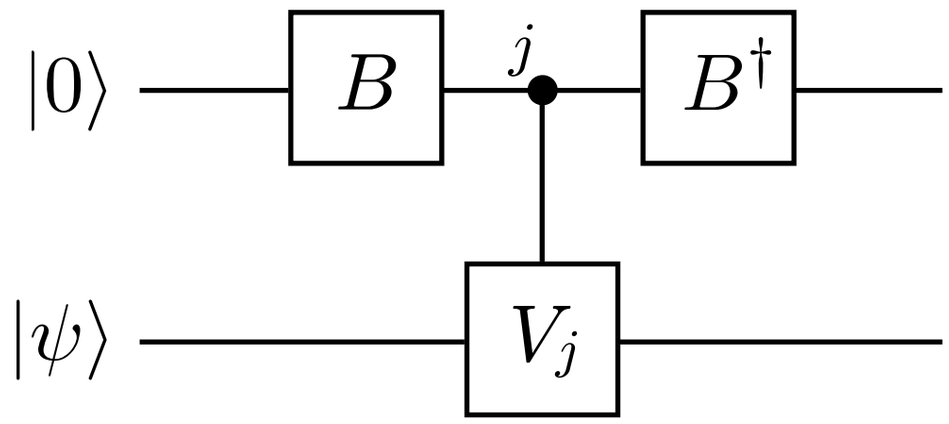
$$|0\rangle|\psi\rangle \mapsto \sin\theta|0\rangle U|\psi\rangle + \cos\theta|\Phi\rangle$$

- Boost the amplitude for success by oblivious amplitude amplification

Implementing U with some amplitude

$$U = \sum_j \beta_j V_j \qquad \text{(WLOG } \beta_j > 0\text{)}$$

Ancilla state: $B|0\rangle = \frac{1}{\sqrt{s}} \sum_j \sqrt{\beta_j}|j\rangle$ $\qquad s := \sum_j \beta_j$



$$\frac{1}{s}|0\rangle U|\psi\rangle + \sqrt{1 - \frac{1}{s^2}}\,|\Phi\rangle$$

with $\langle 0|\Phi\rangle = 0$

Oblivious amplitude amplification

Suppose W implements U with amplitude $\sin\theta$:

$$W|0\rangle|\psi\rangle = \sin\theta|0\rangle U|\psi\rangle + \cos\theta|\Phi\rangle$$

To perform U with amplitude close to 1: use amplitude amplification?

But the input state is unknown!

Using ideas from [Marriott, Watrous 05], we can show that a $|\psi\rangle$-independent reflection suffices to do effective amplitude amplification.

With this *oblivious amplitude amplification*, we can perform the ideal evolution with only about $1/\sin\theta$ steps.

We also give a robust version that works even when U is not exactly unitary.

Simulating the Taylor series

Taylor series of the dynamics generated by H:

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

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

Write $H = \sum_\ell \alpha_\ell H_\ell$ where each H_ℓ is unitary

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

is a linear combination of unitaries

Why $\mathrm{poly}(\log(1/\epsilon))$?

Lowest-order product formula:

$$(e^{-iA/r}e^{-iB/r})^r = e^{-i(A+B)} + O(1/r)$$

so we must take $r = O(1/\epsilon)$ to achieve error at most ϵ

Higher-order formulas exist, but they only improve the power of ϵ

The approximation $e^{-iHt} \approx \sum_{k=0}^{K} \frac{(-iHt)^k}{k!}$ has error ϵ provided

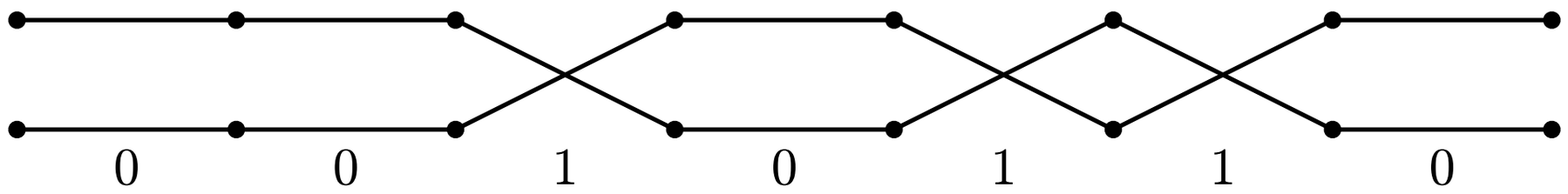
$$K = O\left(\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$$

Lower bounds

No-fast-forwarding theorem [BACS 07]: $\Omega(t)$

Main idea:

- Query complexity of computing the parity of n bits is $\Omega(n)$.
- There is a Hamiltonian that can compute parity by running for time $O(n)$.



New lower bound: $\Omega(\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)})$

Main idea:

- Query complexity of parity is $\Omega(n)$ even for *unbounded error*.
- The same Hamiltonian as above computes parity with unbounded error by running for any positive time. Running for constant time gives the parity with probability $\Theta(1/n!)$.

Linear combination of quantum walk steps

Suppose the Hamiltonian is d-sparse.

Query complexity of the Taylor series approach is quadratic in d.

Another approach:
- Define a quantum walk related to the Hamiltonian
- Express the evolution operator as a linear combination of walk steps
- Implement this with the LCU Lemma

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

$$\tau := d\|H\|_{\max} t$$

[Berry, Childs, Kothari FOCS 15]

Tradeoff between t and ϵ

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

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

Very recent work [Low, Chuang 16], using an alternative method for implementing linear combinations of quantum walk steps, gives an optimal tradeoff.

Quantum algorithm for linear systems

Consider an $N \times N$ linear system $Ax = b$.

Classical (or quantum!) algorithms need time $\mathrm{poly}(N)$ to determine x.

What if we change the model?

- A is sparse (at most $\mathrm{poly}(\log N)$ nonzeros in any row or column) and well-conditioned (condition number κ)
- We have a black box that specifies the nonzero entries in any given row or column
- Can efficiently prepare a quantum state $|b\rangle$

Then we can prepare a quantum state ϵ-close to $|x\rangle \propto A^{-1}|b\rangle$ in time $\mathrm{poly}(\log N, 1/\epsilon, \kappa)$ [Harrow, Hassidim, Lloyd 09].

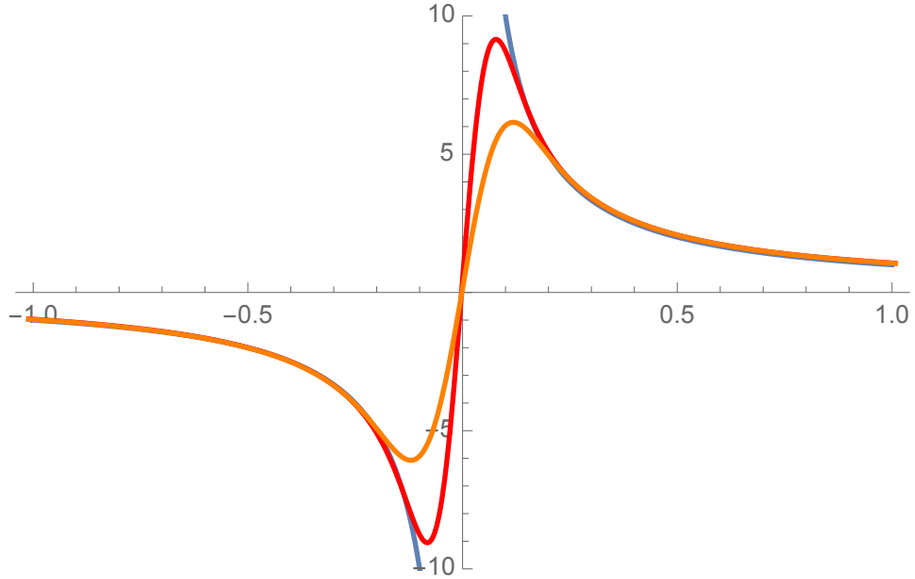
Possible applications: radar scattering cross sections [Clader, Jacobs, Sprouse 13], effective resistance [Wang 13], machine learning (?), …

High-precision quantum linear systems

We give an improved quantum algorithm for linear systems with running time $\mathrm{poly}(\log N, \log(1/\epsilon), \kappa)$, an exponential improvement.

Main idea: Write $\frac{1}{A} \approx \sum_t c_t e^{-iAt}$ and use the LCU Lemma.

(or an analogous Chebyshev expansion, using a quantum walk related to A)



only need a good approximation over $[-1, -\frac{1}{\kappa}] \cup [\frac{1}{\kappa}, 1]$

[Childs, Kothari, Somma 16]

Quantum algorithms for ODEs

Consider a system of differential equations $\frac{\mathrm{d}x}{\mathrm{d}t} = Ax + b$ where A is $N \times N$. Suppose we can prepare states proportional to $x(0)$ and b and would like to prepare a state proportional to $x(T)$.

Linear multistep methods approximate a system of ODEs by a system of linear equations.

$$x(t+\epsilon) \approx x(t) + \epsilon\big(Ax(t) + b\big)$$

Complexity of a quantum algorithm based on linear multistep methods is $\mathrm{poly}(1/\epsilon)$ [Berry 14], even using a quantum linear systems algorithm with complexity $\mathrm{poly}(\log(1/\epsilon))$.

(Note: To have an efficient algorithm, we must avoid regions of exponential growth or decay, since postselection is computationally intractable.)

High-precision quantum ODEs

Can we reduce the complexity to $\mathrm{poly}(\log(1/\epsilon))$?

Directly implementing $\exp(At)$ as a linear combination of unitaries does not seem to work.

Instead we encode this series into a linear system:

$$\begin{pmatrix}
I & & & & & & & & & & \\
-A\epsilon & I & & & & & & & & & \\
 & -A\epsilon/2 & I & & & & & & & & \\
 & & -A\epsilon/3 & I & & & & & & & \\
-I & -I & -I & -I & I & & & & & & \\
 & & & & -A\epsilon & I & & & & & \\
 & & & & & -A\epsilon/2 & I & & & & \\
 & & & & & & -A\epsilon/3 & I & & & \\
 & & & & -I & -I & -I & -I & I & & \\
 & & & & & & & & -I & I & \\
 & & & & & & & & & -I & I
\end{pmatrix} |x\rangle = \begin{pmatrix}
|x_{\mathrm{in}}\rangle \\ \epsilon|b\rangle \\ 0 \\ 0 \\ 0 \\ \epsilon|b\rangle \\ 0 \\ 0 \\ 0 \\ 0 \\ 0
\end{pmatrix}$$

With a careful analysis of this approach, we give an algorithm with complexity $\mathrm{poly}(\log(1/\epsilon))$.

[Berry, Childs, Ostrander, Wang 17]

Open questions

Applications beyond simulating physics

- Algorithms: Scattering cross sections [Clader, Jabobs, Sprouse 13], effective resistance [Wang 13], machine learning?
- Quantum circuit synthesis: "Repeat-until-success" [Paetznick, Svore 14], [Wiebe, Roetteler 14]
- Complexity theory: PreciseQMA=PSPACE [Fefferman, Lin 16]
- More?

Simulations with small quantum computers

Time-dependent ODEs

Time-precision tradeoff for ODEs

High-precision algorithms for PDEs