Quantum algorithms

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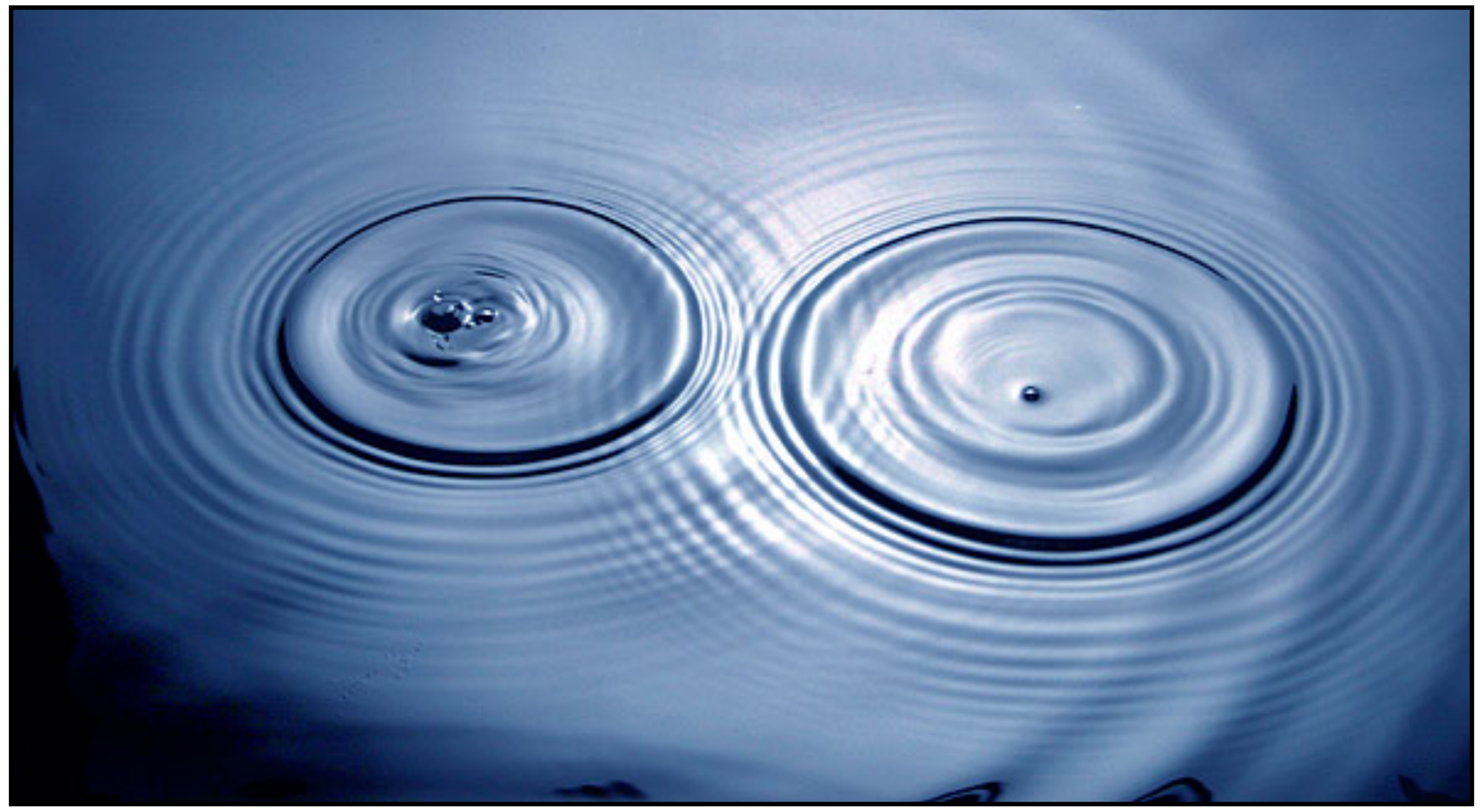
Robust Quantum
Simulation

Overview

0. Introduction

The origin of quantum speedup

Quantum computers allow for *interference between computational paths*



To perform a computation, we should arrange that
- paths to the solution interfere constructively
- paths to non-solutions interfere destructively

Quantum mechanics gives an *efficient representation of high-dimensional interference*

Quantum computing ≠ exponential parallelism

Can we just explore all potential solutions in parallel and pick out the correct one?

No! The linearity of quantum mechanics prohibits this.

Specifically, unstructured search over N items requires $\Omega(\sqrt{N})$ queries. [BBBV 97]

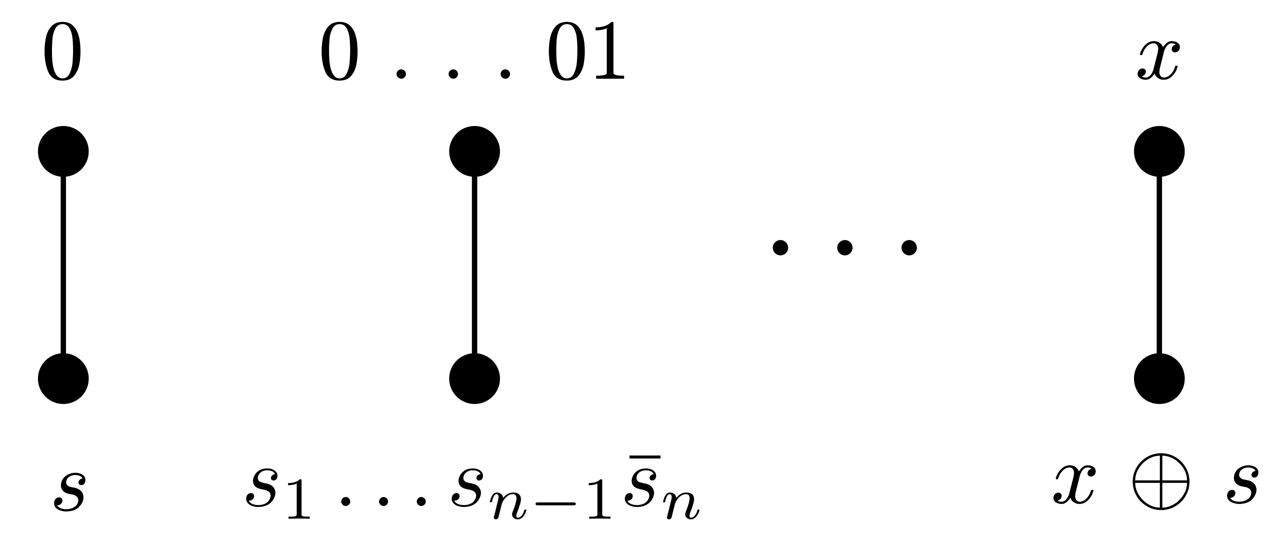
To get significant speedup, quantum computers need to exploit structure.

Key question: What kinds of problems have the right structure for quantum computers to exploit?

Simon's problem

Given a black-box function $f\colon \{0,1\}^n \to R$

Promise: There is some $s \in \{0,1\}^n$ such that $f(x) = f(y)$ if and only if $x = y$ or $x = y \oplus s$



Problem: Find s

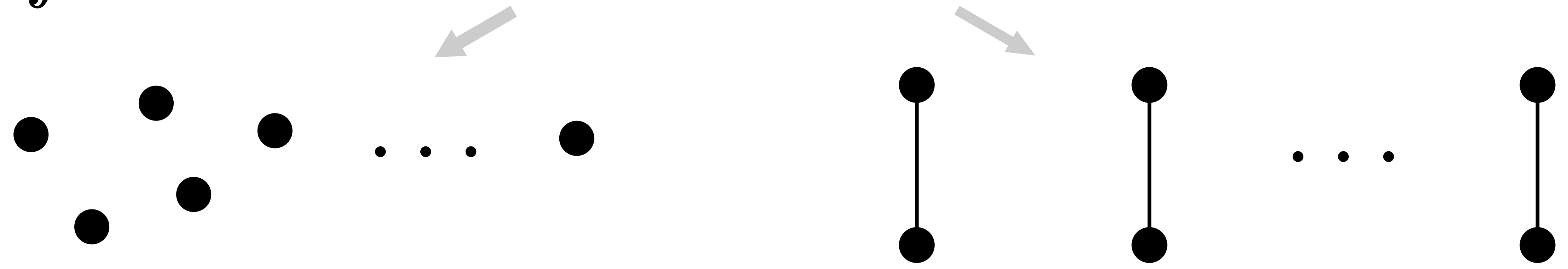
Classically, we can query random inputs until we find a collision. By the birthday problem, this takes about $\sqrt{2^n}$ steps. This is essentially optimal.

But quantumly, there is a 1-query algorithm that learns a random x orthogonal to s. This can be repeated $O(n)$ times to determine s with constant probability.

The collision problem

Given a black-box function $f\colon \{0,1\}^n \to R$ $\qquad N = 2^n$

Promise: f is either 1-to-1 or 2-to-1



Problem: Determine which holds

Can be solved with $O(N^{1/3})$ queries [Brassard, Høyer, Tapp 97]

- query K items
- search through remaining items for a duplicate
- cost $O(K + \sqrt{N/K})$ is minimized with $K = \Theta(N^{1/3})$

This is optimal! No exponential speedup. [Aaronson, Shi 01]

The prospect of quantum speedup

The collision problem does not have enough structure to allow a fast quantum algorithm

Simon's problem is a special case with enough additional structure to give a fast quantum algorithm (but not a fast classical algorithm) $\rightarrow$ exponential speedup

Major questions: What problems have fast quantum algorithms?
What structures enable exponential speedup?

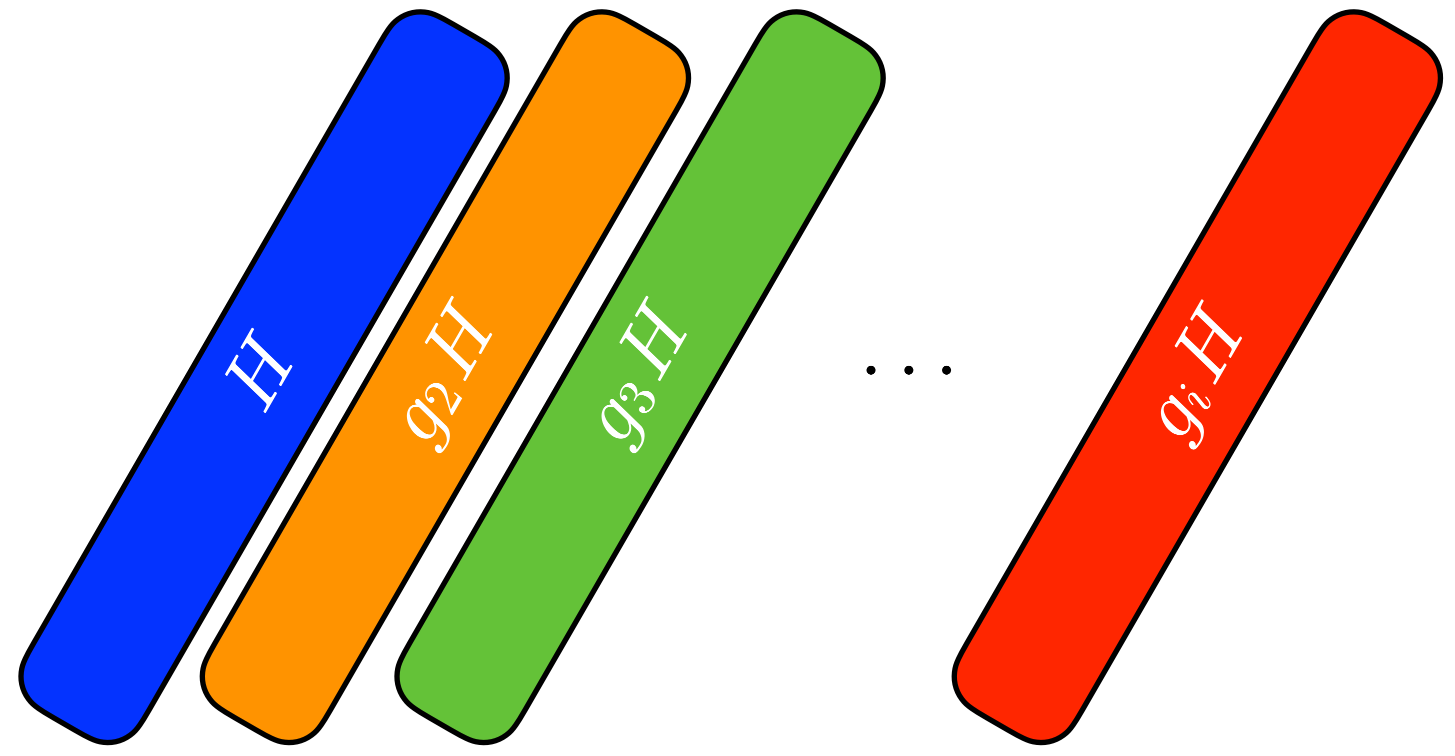
Another important question: When can we get polynomial quantum speedup, and how much is possible?

1. Algebraic problems

Hidden symmetry

Simon's problem exemplifies a more general class of problems with hidden symmetry

Hidden subgroup problem: Given a known group G and a black-box function $f: G \to R$. Promised that f is constant on cosets of some (unknown) subgroup $H \leq G$ and distinct on different cosets. Goal: find (a generating set for) H.



The "standard method" samples a *coset state* $|gH\rangle := \frac{1}{\sqrt{|H|}} \sum_{h \in H} |gh\rangle$ for a uniformly random (unknown) g

Abelian HSP

This problem can be solved efficiently when G is an abelian group.

Finite abelian groups:
- Discrete log [Shor 94]
- Decomposing abelian groups [Cheung, Mosca 01]
- Counting points on algebraic curves [Kedlaya 06]

Infinite abelian groups:
- Factoring [Shor 94]
- Pell's equation ($x^2 - dy^2 = 1$) [Hallgren 02]
- Unit group of a number field [Hallgren 05; Hallgren, Eisenträger, Kitaev, Song 14]
- Principal ideal problem, class groups [Hallgren 05; Biasse, Song 16]
- Ray class groups, Hilbert class fields [Hallgren, Eisenträger 10]

Nonabelian HSP: Examples and applications

When G is a nonabelian group, polynomially many queries suffice.

Efficient algorithms known for specific HSPs: normal subgroups, metacyclic groups, Heisenberg/extraspecial groups, etc.

HSPs with exciting potential applications:
- Symmetric group: graph isomorphism, code equivalence
- Dihedral group: lattice problems [Regev 02]

A standard method algorithm for the symmetric group HSP would require highly entangled measurements [Hallgren, Moore, Rötteler, Russell, Sen, 06]

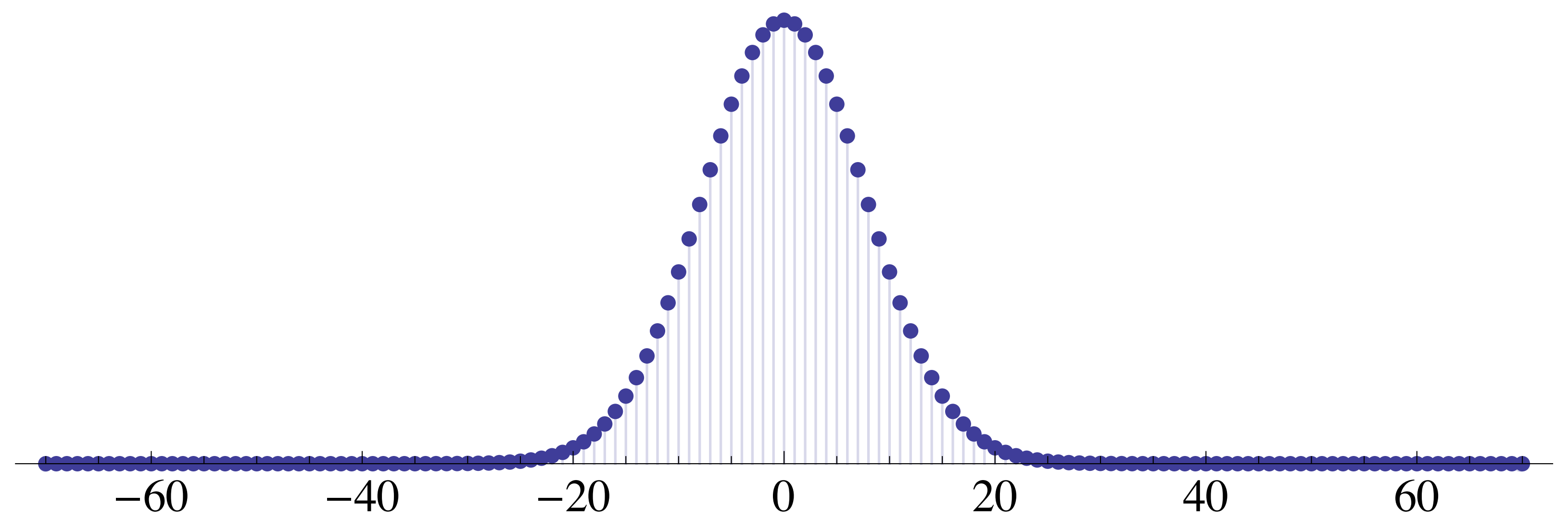
"Kuperberg sieve" solves the dihedral HSP in subexponential time
- No quantum speedup for lattice problems
- Subexponential quantum algorithm for elliptic curve isogenies [Childs, Jao, Soukharev 14]

2. Quantum walk

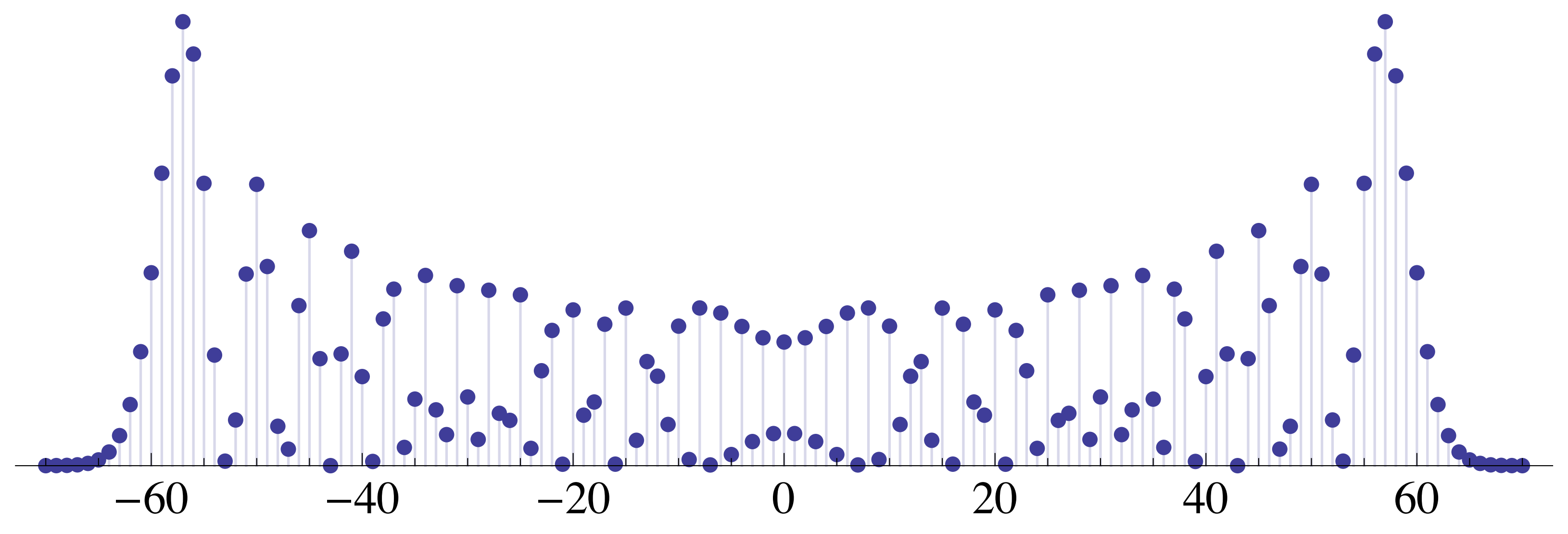
From random to quantum walk

Quantum analog of a random walk on a graph.

Idea: Replace probabilities by quantum amplitudes.
Interference can produce radically different behavior!



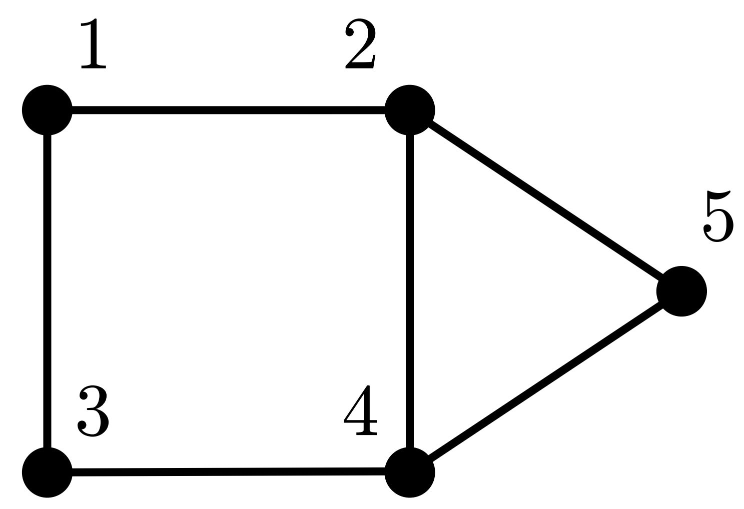
classical



quantum

Continuous-time quantum walk

Graph G:



$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix}$$

adjacency matrix

$$L = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 3 & 0 & -1 & -1 \\ -1 & 0 & 2 & -1 & 0 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{pmatrix}$$

Laplacian

Random walk on G

State: Probability $p_v(t)$ of being at vertex v at time t

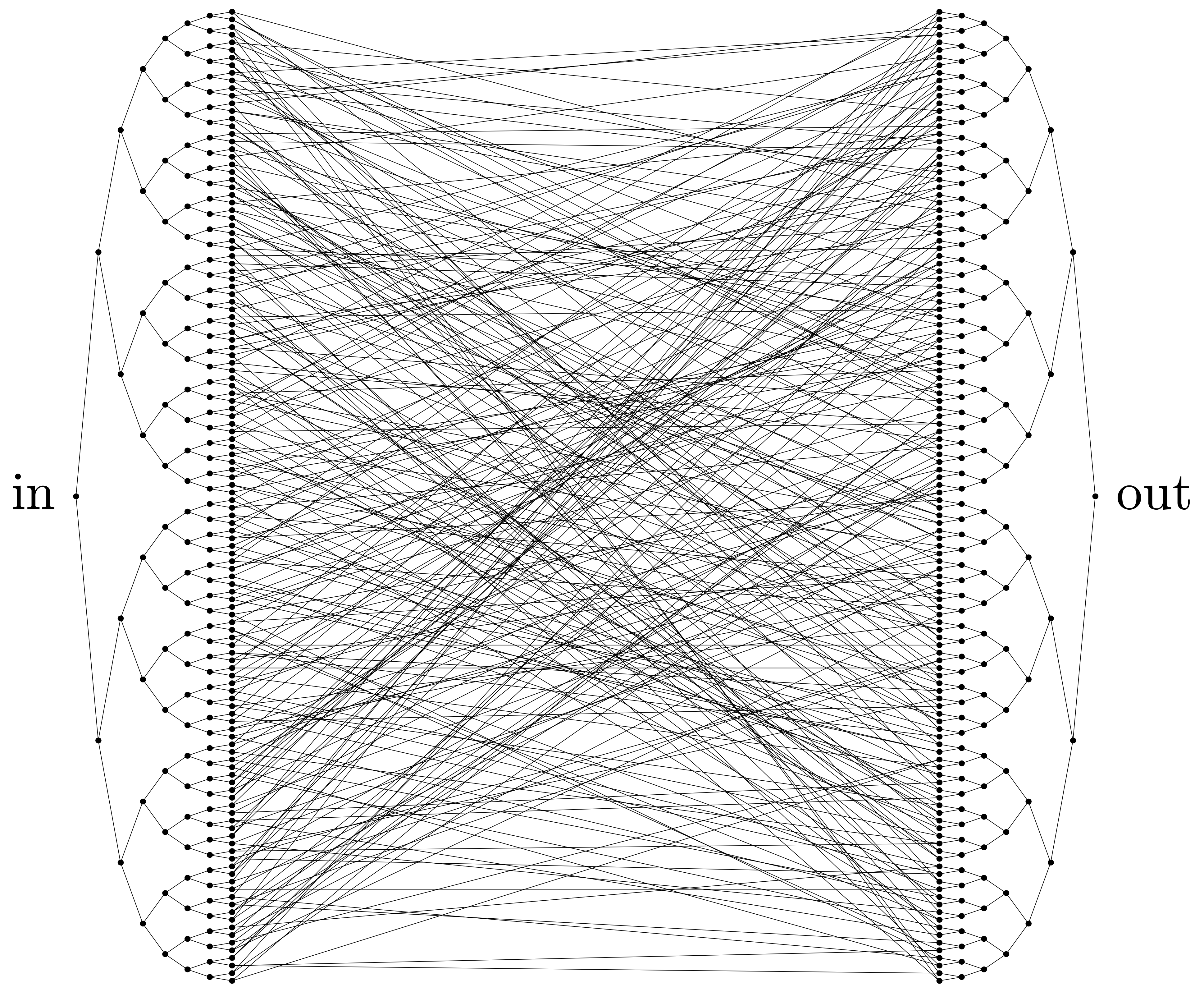
Dynamics: $\frac{\mathrm{d}}{\mathrm{d}t}\vec{p} = L\vec{p}$

Quantum walk on G

State: Amplitude $a_v(t)$ to be at vertex v at time t

Dynamics: $i\frac{\mathrm{d}}{\mathrm{d}t}\vec{a} = L\vec{a}$

Exponential speedup



Problem: Given the label of in and an adjacency-list black box for the graph, find the label of out.

Quantum walk from $|\mathrm{in}\rangle$ stays in the *column subspace* (uniform superpositions over vertices at fixed distance from in).

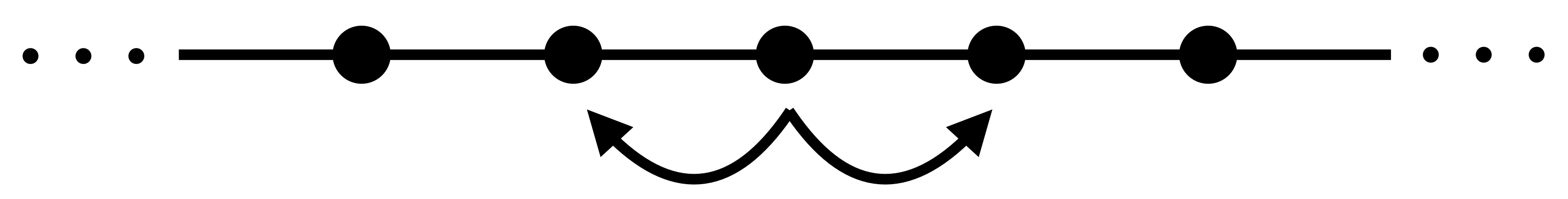
This walk rapidly reaches a state with significant overlap on $|\mathrm{out}\rangle$.

Using polynomially many queries, a classical algorithm cannot distinguish the graph from an infinite binary tree rooted at in.

[Childs, Cleve, Deotto, Farhi, Gutmann, Spielman 03]

Discrete-time quantum walk

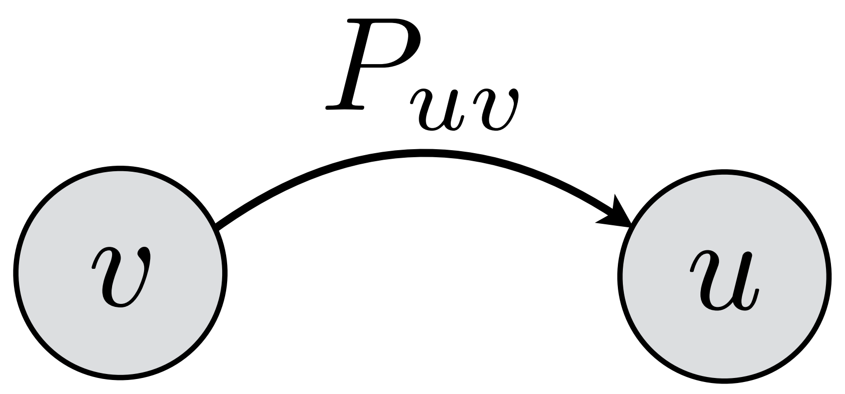
A walk with discrete time steps is a little harder to define.

On a path: $|x\rangle \mapsto \frac{1}{\sqrt{2}}(|x-1\rangle + |x+1\rangle)$?  Not unitary!

Solution: Introduce another register (“coin”) that remembers the previous position

(reduces the potential for interference, but only slightly)

Szegedy walk: For a stochastic transition matrix P,



- Reflect about $\text{span}\{|\psi_v\rangle : v \in V\}$
  where $|\psi_v\rangle := \sum_{u \in V} \sqrt{P_{uv}}|v,u\rangle$
- Swap the edge direction: $S := \sum_{u,v \in V} |u,v\rangle\langle v,u|$

[Szegedy 05]

Quantum walk search

Problem: Given a graph $G = (V, E)$ with a subset $M \subseteq V$ of *marked vertices*. Using an oracle that tells whether a vertex is marked, determine whether M is empty.

Classical strategy: Take a random walk until we reach a marked vertex.

Time to hit a marked vertex is $O(1/\delta\epsilon)$, where

δ = spectral gap of walk $\quad \epsilon = |M|/|V|$

(second-largest magnitude of an eigenvalue of transition matrix is $1 - \delta$)

Quantum strategy: Consider the Szegedization of the *absorbing walk* that remains at a marked vertex

Perform phase estimation on $|\psi\rangle \propto \sum_{x \notin M} |\psi_x\rangle$

This state is invariant if $|M| = 0$ and lives in eigenspaces with phase $\Omega(\sqrt{\delta\epsilon})$ if $|M| \neq 0$, so $O(1/\sqrt{\delta\epsilon})$ steps of the walk suffice to determine whether $|M| = 0$.

Quantum walk search: examples

Unstructured search: $G =$ complete graph on N vertices $\delta = \Theta(1)$ $\epsilon = 1/N$

Classical: $O(N)$ Quantum: $O(\sqrt{N})$

Element distinctness: [Ambainis 04]

Given $f: [N] \to R$, are there distinct $x, y \in [N]$ with $f(x) = f(y)$? $[N] := \{1, \ldots, N\}$

Classical: $\Omega(N)$

Quantum: Consider walk on Hamming graph $H(N, K)$

vertices = $[N]^K$, edges between K-tuples that differ in one coordinate

store function values associated with the K inputs

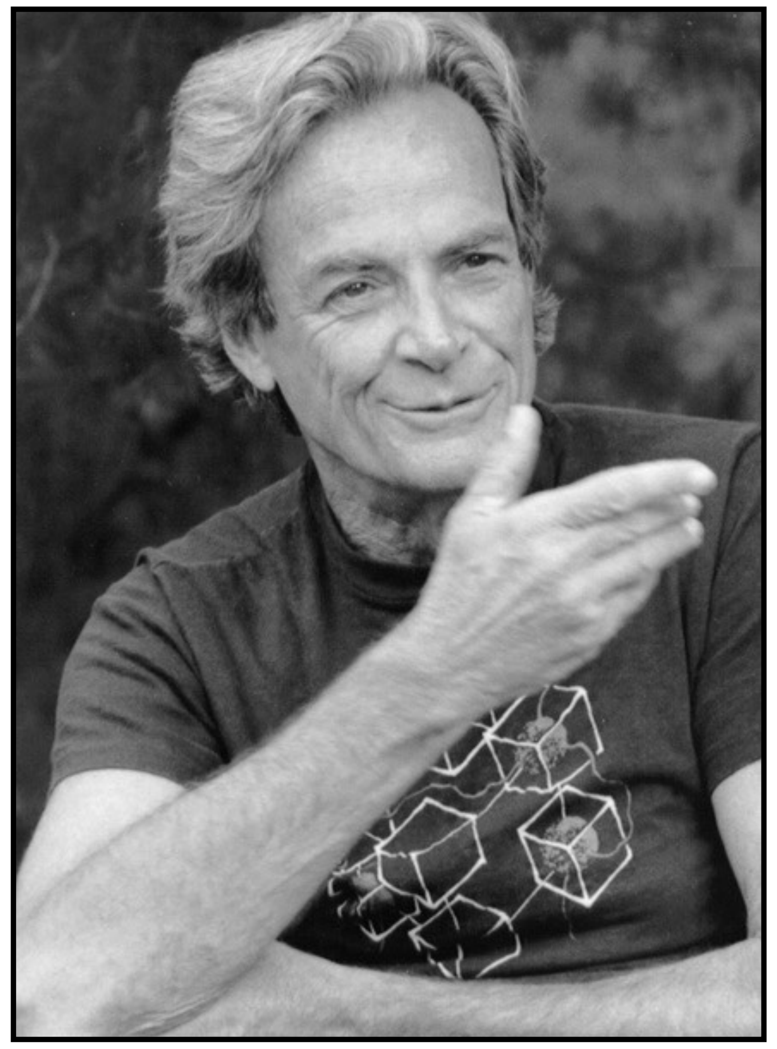
$\delta = \Omega(1/K)$ $\epsilon = \Omega((K/N)^2)$

complexity $K + N/\sqrt{K}$, optimized with $K = N^{2/3}$

This provides a powerful, general tool for search problems

3. Hamiltonian simulation

Simulating Hamiltonian dynamics



"… 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)

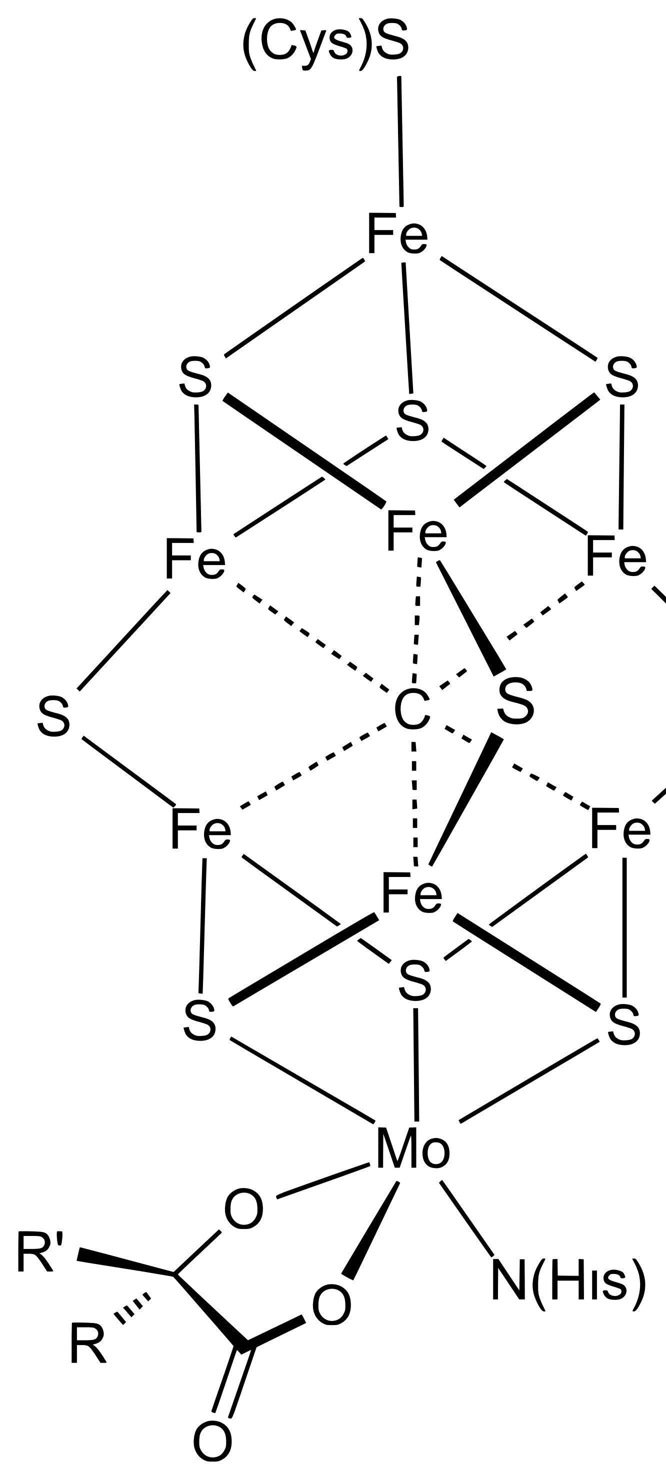
A classical computer cannot even represent the state efficiently.

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

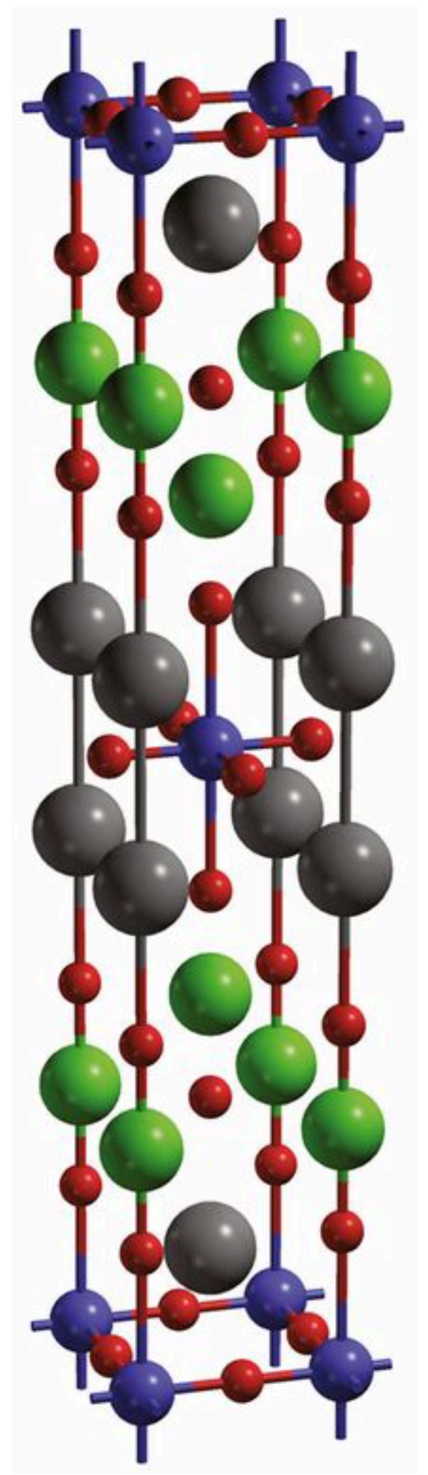
But given succinct descriptions of
- the initial state (suitable for a quantum computer to prepare it efficiently) and
- a final measurement (say, measurements of the individual qubits in some basis),

a quantum computer can efficiently answer questions that (apparently) a classical one cannot. Simulation is BQP-complete!

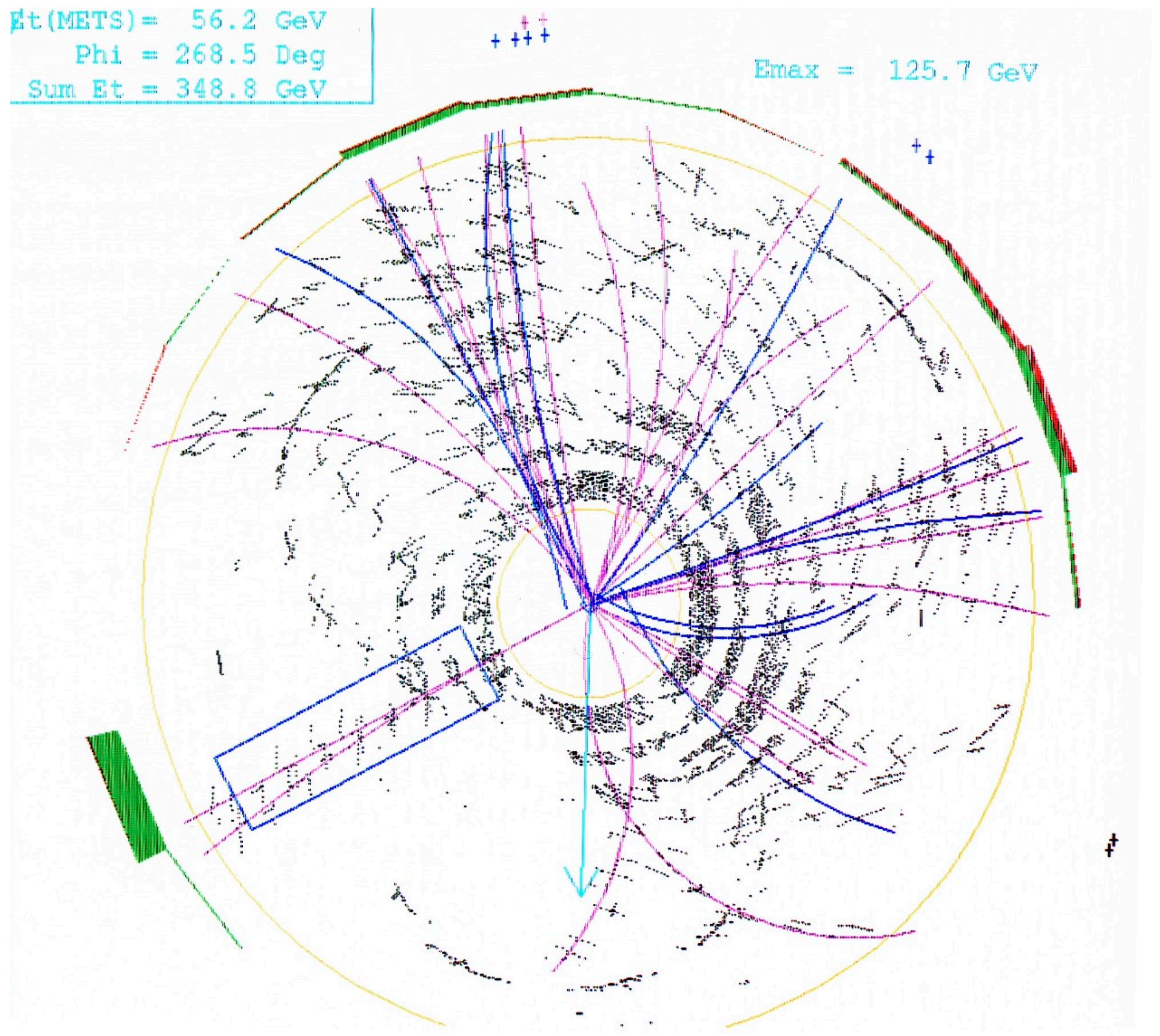
Computational quantum physics



quantum chemistry
(e.g., nitrogen fixation)

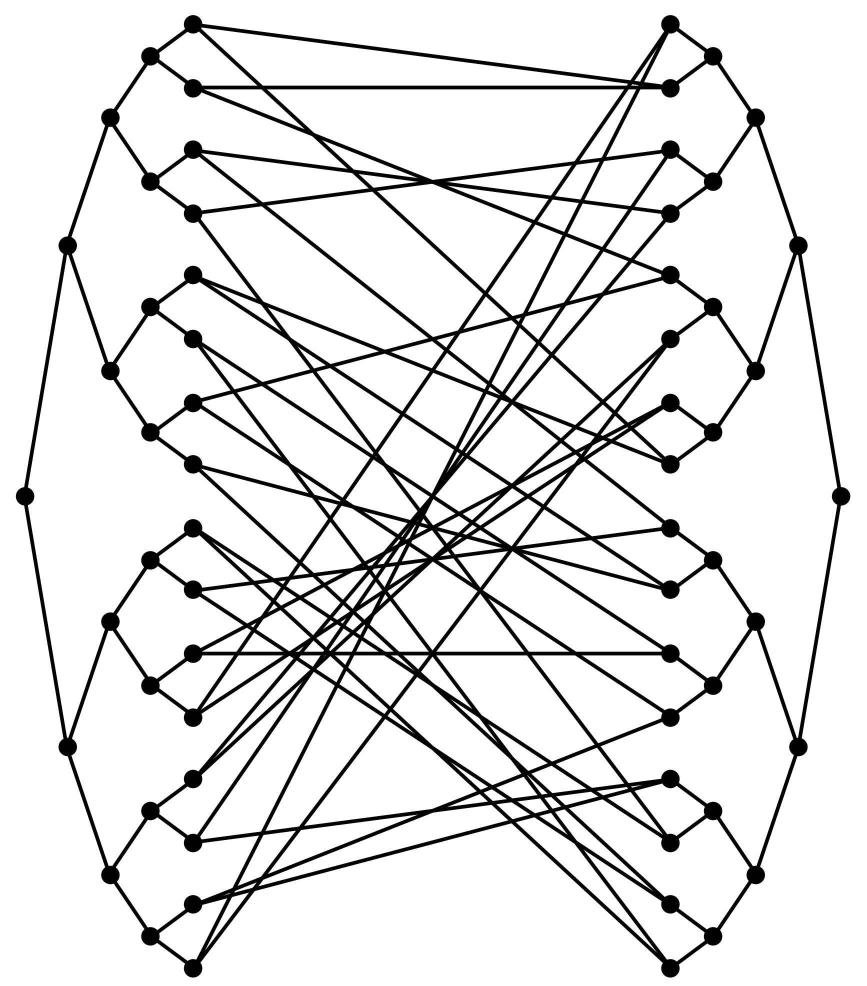


condensed matter physics/
properties of materials

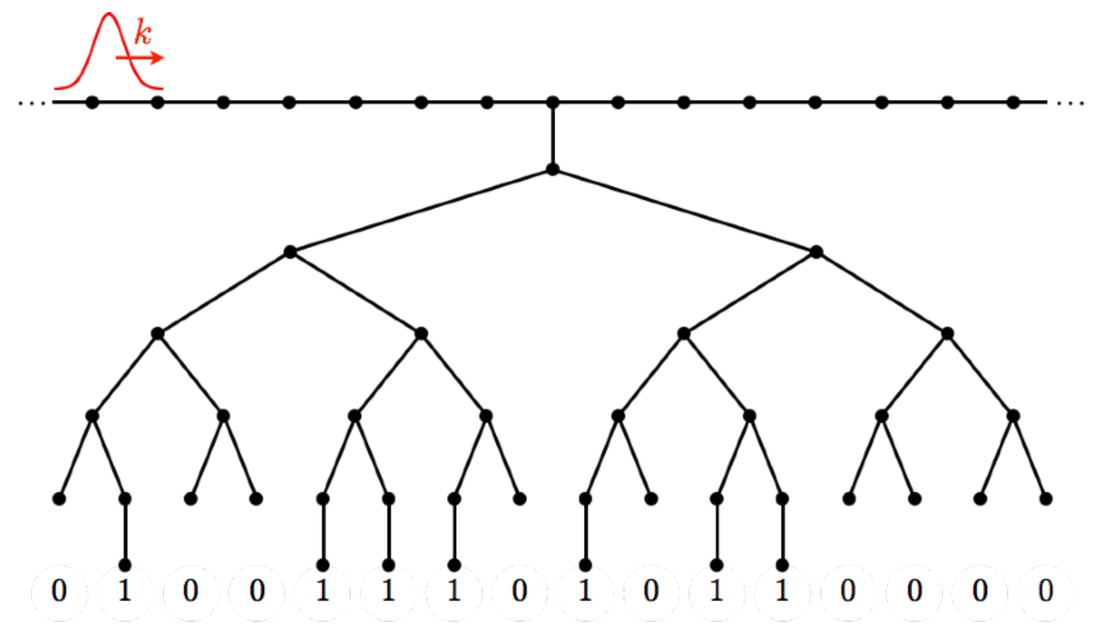


nuclear/particle
physics

Implementing quantum algorithms



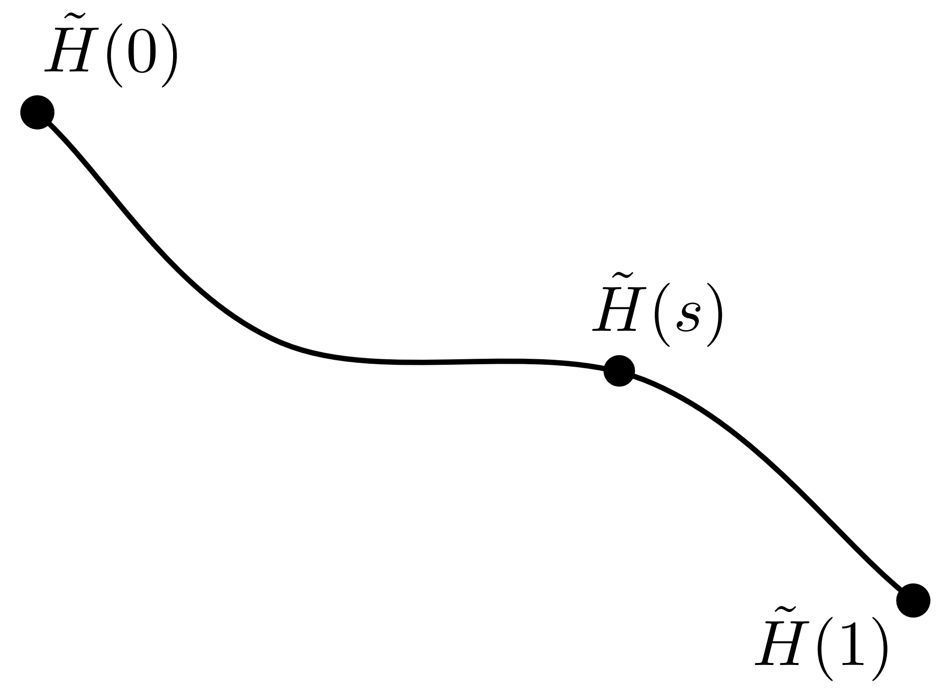
exponential speedup by quantum walk



evaluating Boolean formulas

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

linear/ differential equations, convex optimization



adiabatic optimization

Product formulas

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]

Post-Trotter algorithms I

Linear-time simulation

“No Fast-Fowarding Theorem”: simulation for time t has complexity $\Omega(t)$

[Berry, Ahokas, Cleve, Sanders 07]

Applying phase estimation to a Szegedization of H gives an $O(t)$ simulation

[Childs10; Berry, Childs 12]

High-precision simulation

Directly implement the truncated Taylor series of $\exp(-iHt)$, cost $O(t\frac{\log(t/\epsilon)}{\log\log(t/\epsilon)})$

LCU Lemma: implement $U = \sum_j \beta_j V_j$ with complexity $O(\sum_j |\beta_j|)$

This is the optimal dependence on ϵ

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

Post-Trotter algorithms II

Optimal tradeoff

Quantum signal processing (QSP) implements polynomials of a given "block-encoded" Hamiltonian (or more general matrix)

$$U = \begin{pmatrix} H & \cdot \\ \cdot & \cdot \end{pmatrix}$$

Gives d-sparse Hamiltonian simulation with cost $O(dt + \log(1/\epsilon))$ [Low, Chuang 17]

QSP and "quantum singular value transformation" [Gilyén, Su, Low, Wiebe 19] provide versatile tools for other tasks

Lattice Hamiltonians

Can do even better if the Hamiltonian has spatially local interactions

All above methods use $\Omega(n^2)$ gates to simulate n spins with local interactions for constant time

Combining forward and backward evolution and applying Lieb-Robinson bounds, can improve this to $\tilde{O}(n)$, which is optimal [Haah, Hastings, Kothari, Low 18]

Also other algorithms using multiproduct formulas, interaction picture, randomization, other norms, extrapolation …

Product formulas strike back

Numerical simulations suggest that product formulas can perform much better than straightforward bounds show

Can give tighter bounds using integral representations of the error, e.g.,

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

Provides bounds that can take advantage of small commutators between terms

In particular, shows that product formulas nearly reproduce the complexity of [Haah, Hastings, Kothari, Low 18] for lattice Hamiltonians [Childs, Su, Tran, Wiebe, Zhu 19]

Can give even better bounds if we know the state has low energy [Sahinoglu, Somma 20]

Quantum chemistry

Probably the most-studied application of quantum simulation is the electronic structure problem

Algorithms depend on many choices:

- Often assume nuclei at fixed positions (Born-Oppenheimer approximation)
- Choose a set of electron basis functions (molecular orbitals, plane waves, etc.)

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{ijkl} g_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \qquad \text{fermion operators: } \{a_i, a_j\} = 0,\ \{a_i, a_j^\dagger\} = \delta_{ij}$$

- Convert to spins using a suitable transformation (Jordan-Wigner, Bravyi-Kitaev, etc.)
- Represent in first (locations of electrons) or second (occupation of modes) quantization

Selected asymptotic complexities (N modes, η electrons):

- [Wecker, Bauer, Clark, Hastings, Troyer 14] (2nd quantization, any basis): $O(N^{10})$
- [Babbush, Berry, Kivlichan, Wei, Love, Aspuru-Guzik 16] (2nd quantization, any basis): $O(N^5)$
- [Low, Wiebe 18] (2nd quantization, plane waves): $O(N^2)$
- [Babbush, Berry, McClean, Neven 18] (1st quantization, plane waves): $O(N^{1/3}\eta^{8/3})$

4. Quantum linear algebra

Quantum linear systems algorithm

Given an $N \times N$ system of linear equations $Ax = b$, find $x = A^{-1}b$

Classical (or quantum!) algorithms need time $\Omega(N)$ just to write down x

What if we change the model?

- A is sparse; given a black box that specifies the nonzero entries in any given row or column
- Can efficiently prepare a quantum state $|b\rangle$
- Goal is to prepare a state $|x\rangle \propto A^{-1}|b\rangle$

We can do this in time $\mathrm{poly}(\log N, 1/\epsilon, \kappa)$ where $\kappa := \|A\| \cdot \|A^{-1}\|$

[Harrow, Hassidim, Lloyd 09]

Algorithm estimates the eigenvalues of A (in superposition) and replaces them by their inverse (using postselection)

Subsequent improvements do the same with complexity $\kappa\, \mathrm{poly}(\log(1/\epsilon))$ using variable-time amplitude amplification and LCU [Ambainis 12; Childs, Kothari, Somma 17]

Differential equations

We can apply a similar framework to other linear-algebraic tasks. For example:

Given a system of linear differential equations $\frac{\mathrm{d}}{\mathrm{d}t}x = Ax + b$
with the ability to prepare $|b\rangle$ and $|x(0)\rangle$, and a sparse matrix oracle for A,
prepare $|x(T)\rangle$ for some desired final time T

Approach: apply a finite difference approximation to give a linear system; solve it with the QLSA [Berry 14]

Generalizations give improved performance and also handle time-dependent coefficients, partial differential equations, some nonlinear differential equations, …

Applications?

Linear equations and differential equations are ubiquitous. Surely we can use this for something?

Proposals: electromagnetic scattering, machine learning, finance, …

In general, the input/output requirements impose serious constraints.
So far, there is no compelling end-to-end application with rigorous evidence for speedup.

One significant limitation: quantum finite element analysis in a constant number of spatial dimensions seems limited to polynomial speedup [Montanaro, Pallister 16]

5. Optimization

Discrete optimization

Grover's algorithm ⇒ quadratic speedup for minimization [Dürr, Hoyer 96]

Graph algorithms

- shortest paths [Dürr, Heiligman, Høyer, Mhalla 04]
- minimum spanning trees [Dürr, Heiligman, Høyer, Mhalla 04]
- maximum flows/matchings [Ambainis, Špalek 07]

Speeding up exponential-time algorithms for NP-hard problems (SAT, subset sum, lattice problems, TSP, set cover, …)

Some of these algorithms introduce interesting new tools:

- quantum backtracking using quantum walk [Montanaro 16]
- quantum methods for dynamic programming [Ambainis, Balodis, Iraids, Kokainis, Prusis, Vihrovs 18]

Continuous optimization

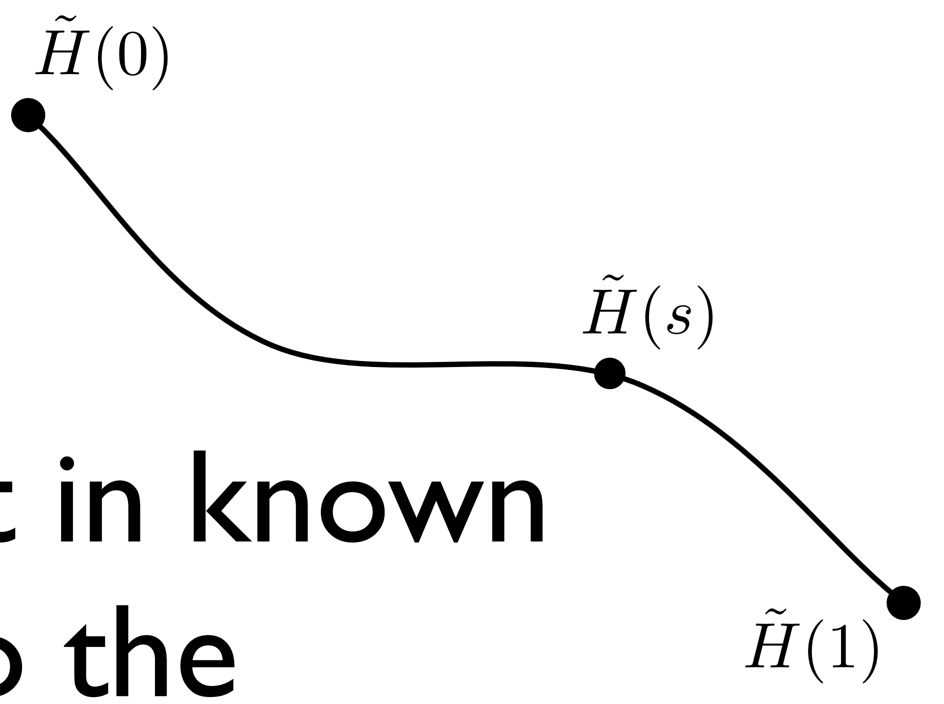
Linear/semidefinite programming

- polynomial speedups based on Gibbs sampling [Brandão, Svore 17; van Apeldoorn, Gilyén 19]
- faster algorithms in a stronger input model [Brandão, Kalev, Li, Lin, Svore, Wu 19]

Gradient-based algorithms

- Fast algorithm for computing gradients [Jordan 05]
- Minimization using gradient descent [Rebentrost, Schuld, Wossnig, Petruccione, Lloyd 19; Kerenidis, Prakash 20]
- Quantum query speedup for convex optimization with membership and evaluation oracles [van Apeldoorn, Gilyén, Gribling, de Wolf 20; Chakrabarti, Childs, Li, Wu 20]
- For high-dimensional non-smooth convex optimization with a gradient oracle, cannot achieve a quantum speedup as a function of the allowed error [Garg, Kothari, Netrapalli, Sherif 20]

Adiabatic optimization and QAOA



Strategy: encode a constraint problem with a diagonal Hamiltonian. Start in known ground state of a simple, non-diagonal Hamiltonian. Slowly interpolate to the problem Hamiltonian to produce its ground state. [Farhi, Goldstone, Gutmann, Sipser 00]

Complexity depends on the minimum spectral gap, but this is hard to estimate.

Often this is done with a Hamiltonian that has all negative off-diagonal entries ("stoquastic"). Then we can in principle apply quantum Monte Carlo (a classical algorithm), but its efficiency is also unclear.

Related strategy: quantum approximate optimization algorithm (QAOA). Alternate between diagonal & off-diagonal evolutions with optimized parameters. [Farhi, Goldstone, Gutmann 14]

6. Machine learning

Quantum machine learning

A challenge: much of the impressive success of classical machine learning is empirical

Quantum algorithms for some ML tasks have been proposed, e.g., recommendation systems [Kerenidis, Prakash 17]

Data structures that enable coherent quantum access can be exploited classically [Tang 19]

Other proposed algorithms for principal component analysis, clustering, etc.
Potential for quantum speedup is unclear.

Another direction: computational learning theory [survey: Arunachalam, de Wolf 17]

Learn a concept given the ability to interact with it quantumly
- query access to a concept $c\colon \{0,1\}^n \to \{0,1\}$
- quantum examples $\sum_x \sqrt{p_x}|x, c(x)\rangle$

Conclusion

Outlook

Finding quantum algorithms is hard!

- Quantum mechanics is nonintuitive
- Classical algorithms are powerful
- We have a limited set of quantum techniques

But we have come a long way in the nearly 30 years since Shor’s algorithm

- New exponential speedups
- New techniques
- Much better understanding of quantum query complexity

Large-scale quantum computers could dramatically change our understanding of quantum algorithms… but we don’t have them yet, and should be careful about extrapolating beyond our limited theoretical understanding.

Further reading

Quantum Algorithm Zoo: quantumalgorithmzoo.org

Lecture notes: cs.umd.edu/~amchilds/qa/

Montanaro survey: arXiv:1511.04206

Gilyén tutorial (QIP 2020): www.koushare.com/video/videodetail/4073
Childs tutorial (QIP 2021, longer version of this talk): youtu.be/M0e5gkf7QSQ

Topical surveys:
- algebraic problems (Childs, van Dam): arXiv:0812.0380
- quantum walk search (Santha): arXiv:0808.0059
- quantum walk (Reitzner, Nagaj, Buzek): arXiv:1207.7283
- optimization (de Wolf): youtu.be/1-2LIopvNIk
- computational learning theory (Arunachalam, de Wolf): arXiv:1701.06806