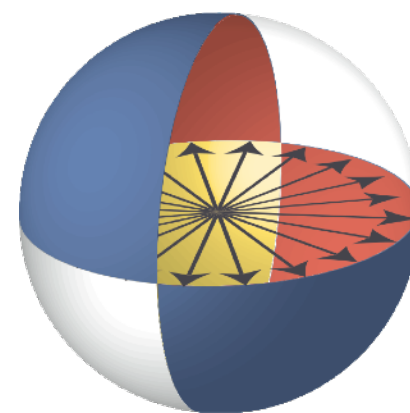


Digital quantum simulation algorithms

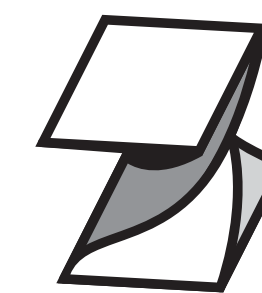
Andrew Childs
University of Maryland



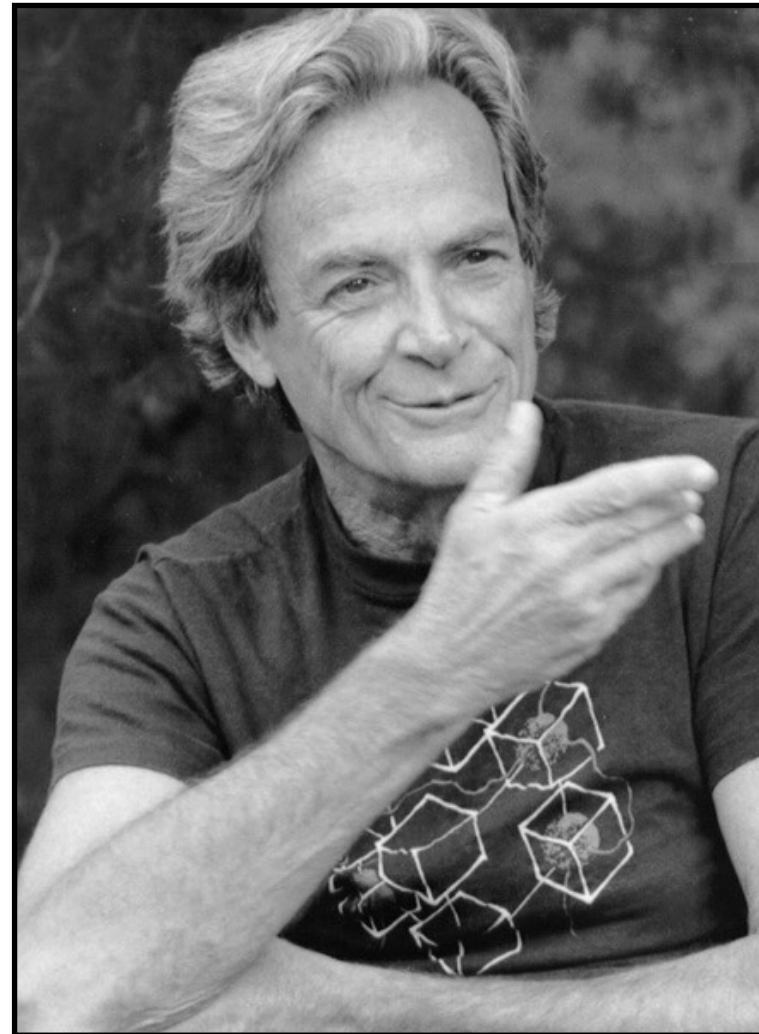
UMIACS
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JOINT CENTER FOR
QUANTUM INFORMATION
AND COMPUTER SCIENCE



Institute for
**Robust 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

Simulating physics with computers (1981)

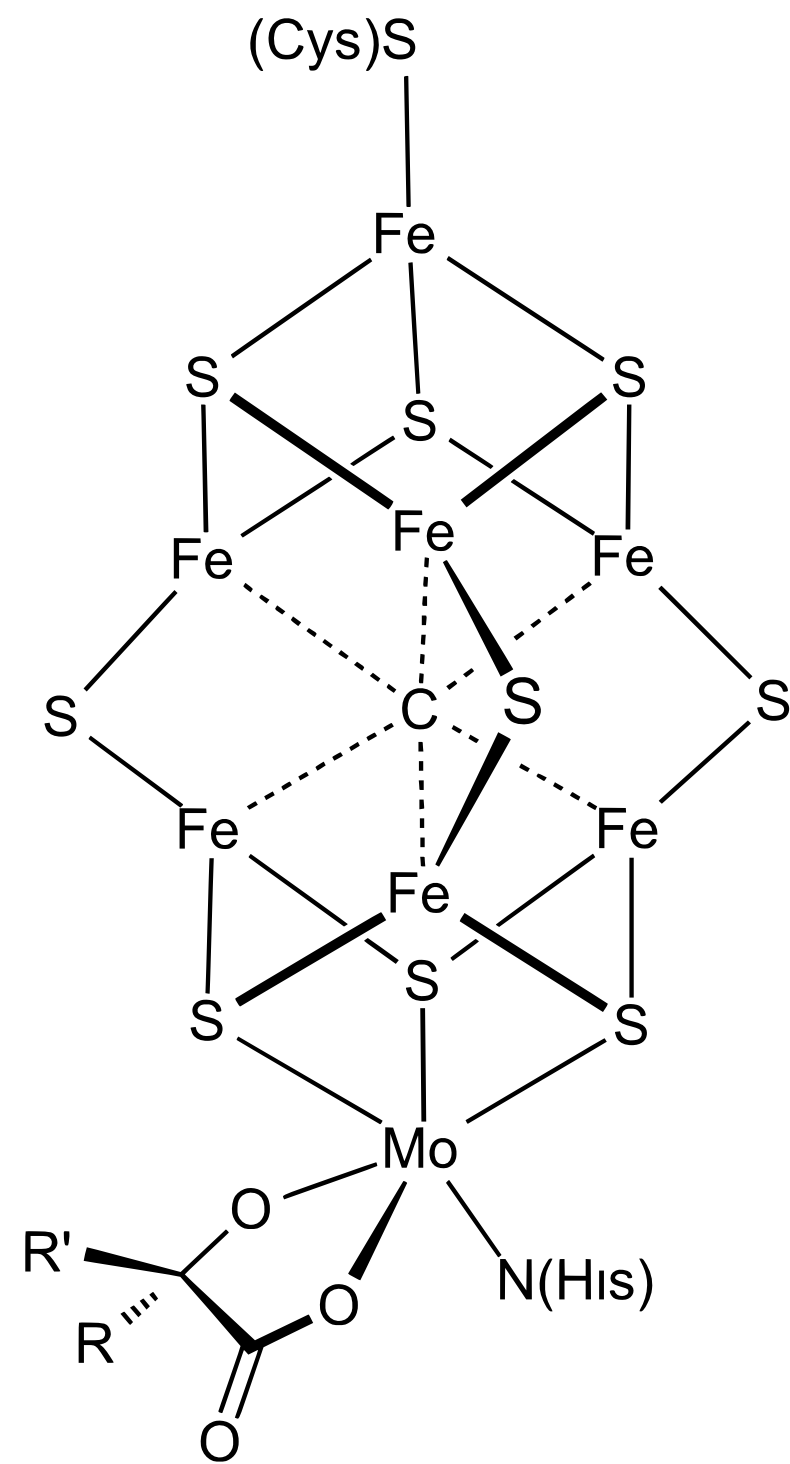
These lectures: Algorithms for simulating quantum dynamics on digital, fault-tolerant quantum computers.

Outline

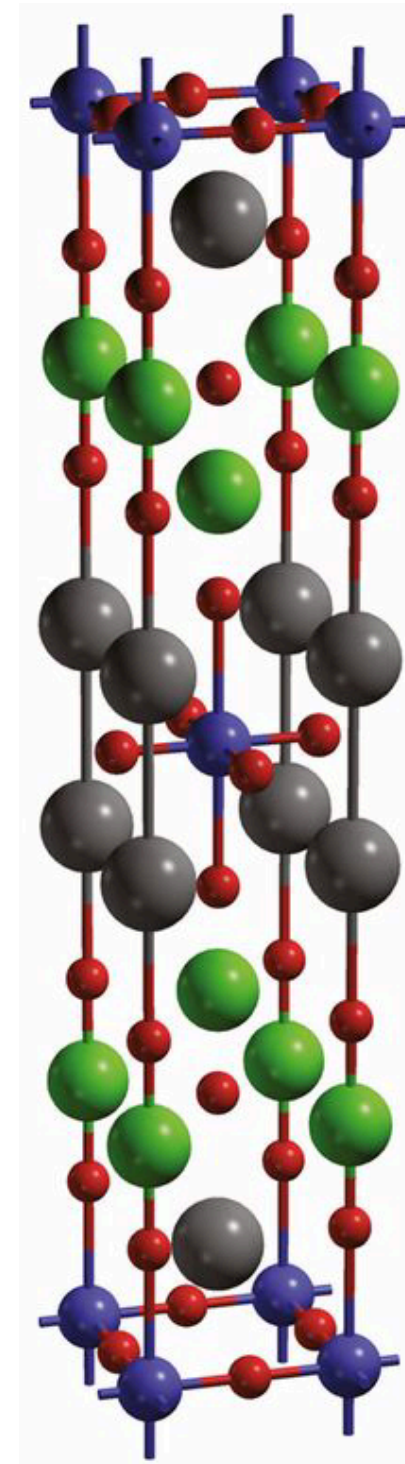
- Background
 - Applications of quantum simulation
 - Problem statement
 - Specifying Hamiltonians
- Complexity
 - BQP-hardness
 - No fast forwarding
- Product formulas
- Post-Trotter methods
- Special topics
 - Spatial locality
 - Interaction picture
 - Randomized simulation
 - Random/entangled states
- Outlook

Background

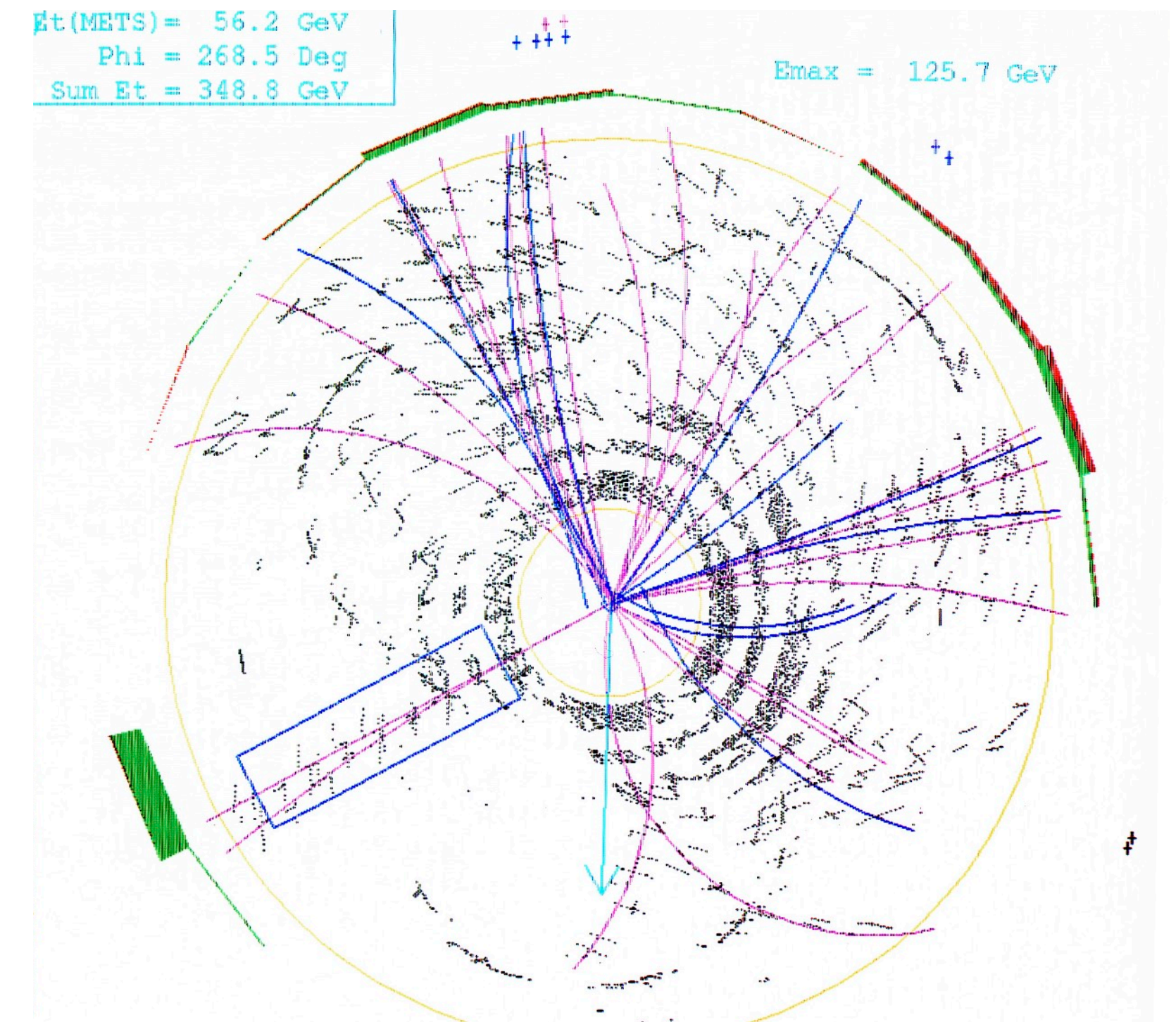
Computational quantum physics



quantum chemistry
(e.g., nitrogen fixation)

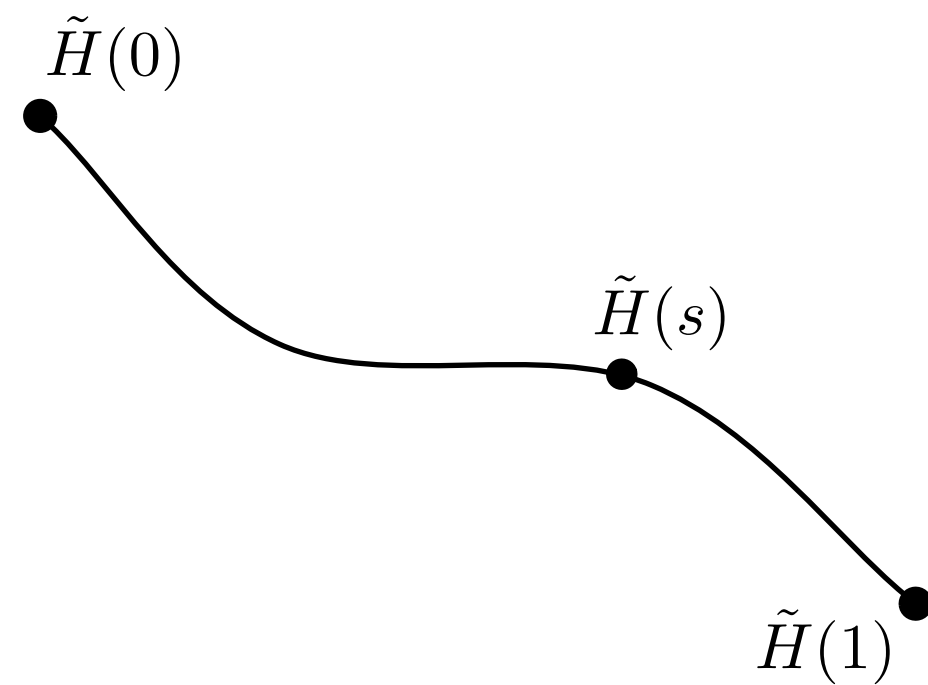


condensed matter physics/
properties of materials

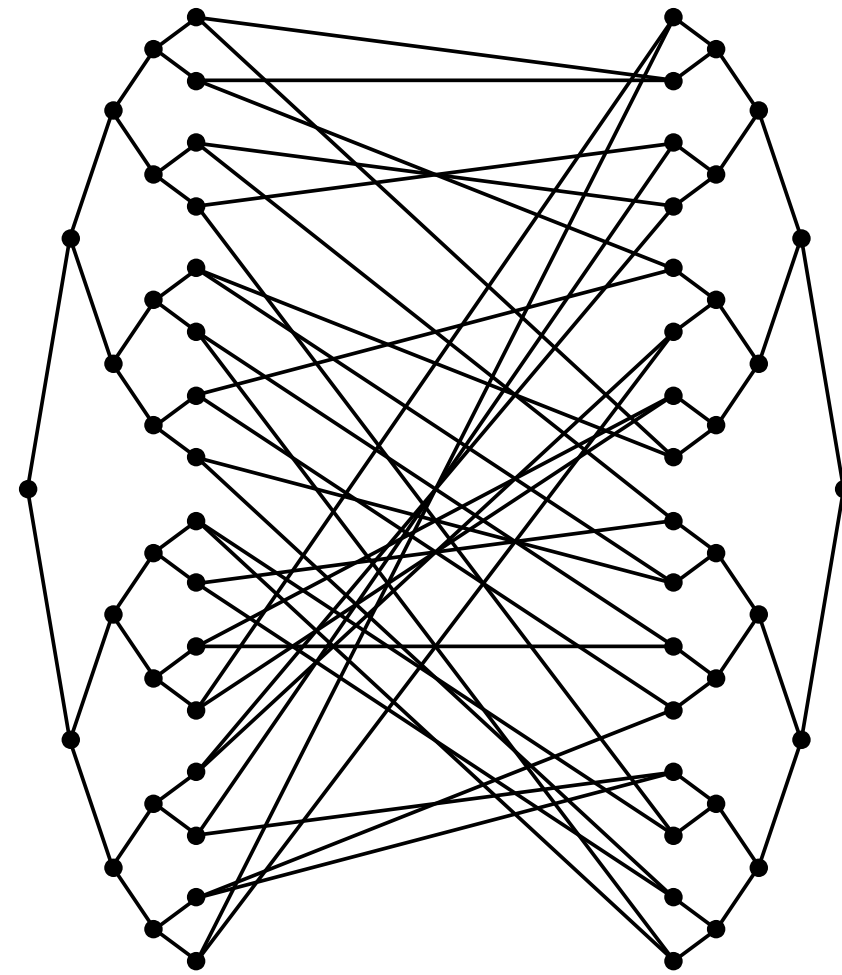


nuclear/particle
physics

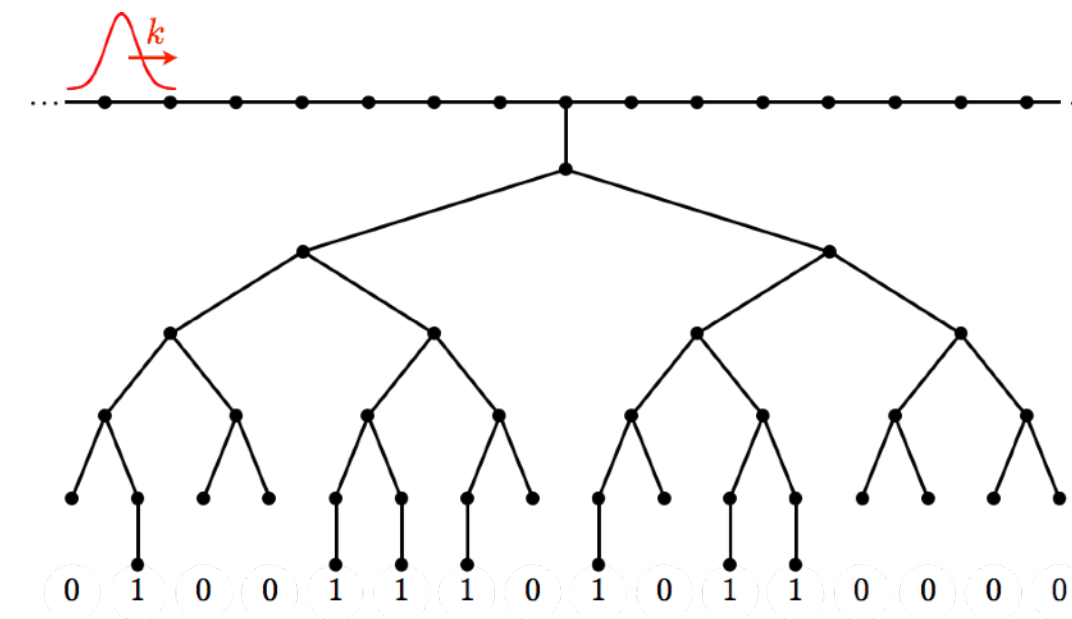
Implementing quantum algorithms



adiabatic
optimization



exponential
speedup by
quantum walk



evaluating
Boolean
formulas

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

linear/
differential
equations,
convex
optimization

Simulation as a theoretical tool

Example: Lieb-Robinson bounds from quantum simulation algorithms

Quantum simulation algorithms provide convenient descriptions of the time evolution operator.

Can we use them as theoretical tools to reason about physics?

PHYSICAL REVIEW X 9, 031006 (2019)

Locality and Digital Quantum Simulation of Power-Law Interactions

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 (Received 25 September 2018; revised manuscript received 21 February 2019; published 10 July 2019)

The propagation of information in nonrelativistic quantum systems obeys a speed limit known as a Lieb-Robinson bound. We derive a new Lieb-Robinson bound for systems with interactions that decay with distance r as a power law, $1/r^\alpha$. The bound implies an effective light cone tighter than all previous bounds. Our approach is based on a technique for approximating the time evolution of a system, which was first introduced as part of a quantum simulation algorithm by Haah *et al.*, FOCS'18. To bound the error of the approximation, we use a known Lieb-Robinson bound that is weaker than the bound we establish. This result brings the analysis full circle, suggesting a deep connection between Lieb-Robinson bounds and digital quantum simulation. In addition to the new Lieb-Robinson bound, our analysis also gives an error bound for the Haah *et al.* quantum simulation algorithm when used to simulate power-law decaying interactions. In particular, we show that the gate count of the algorithm scales with the system size better than existing algorithms when $\alpha > 3D$ (where D is the number of dimensions).

DOI: [10.1103/PhysRevX.9.031006](https://doi.org/10.1103/PhysRevX.9.031006)

Subject Areas: Atomic and Molecular Physics, Condensed Matter Physics, Quantum Information

I. INTRODUCTION

Lieb-Robinson bounds limit the rate at which information can propagate in systems that obey the laws of

Lieb-Robinson bound. Thus, understanding the fundamental limit on the speed of information propagation in these systems holds serious physical implications, including for the applications mentioned above. Despite many efforts in

Quantum dynamics

The dynamics of a quantum system are determined by its *Hamiltonian* H , a Hermitian operator whose spectrum describes the energy levels of the system.

For time-independent H :
$$i \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \quad \Rightarrow \quad |\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle$$

For time-dependent $H(t)$:
$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad \Rightarrow \quad |\psi(t)\rangle = \mathcal{T} e^{-i \int_0^t H(\tau) d\tau} |\psi(0)\rangle$$

The Hamiltonian simulation problem

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

Standard measure of error: worst-case ℓ_2 distance

$$\max_{|\psi(0)\rangle} \| |\psi(t)\rangle - |\psi_{\text{sim}}\rangle \| = \| e^{-iHt} - U_{\text{sim}} \|$$

initial state $\nearrow$ $|\psi(0)\rangle$ $\uparrow$ $e^{-iHt}|\psi(0)\rangle$ $\nwarrow$ simulation output state $\nwarrow$ U_{sim} simulated unitary operation

Alternatives: state-dependent, subspace-dependent, or average-case bounds; diamond norm or other distance measures

Goal: Understand the cost of simulation as a function of t , ϵ , and parameters of H .
(cost could be circuit size, circuit depth, queries, ...)

Also important but not covered in these lectures: state preparation, measurement
(Dynamics are relevant to these too: adiabatic state preparation, energy measurement)

Local Hamiltonians

To make this problem well defined, we must indicate how the Hamiltonian is specified.

One natural model: k -local Hamiltonians

We say H is k -local if it has the form $H = \sum_{j=1}^L H_j$ where each H_j acts on k qubits

Advantages:

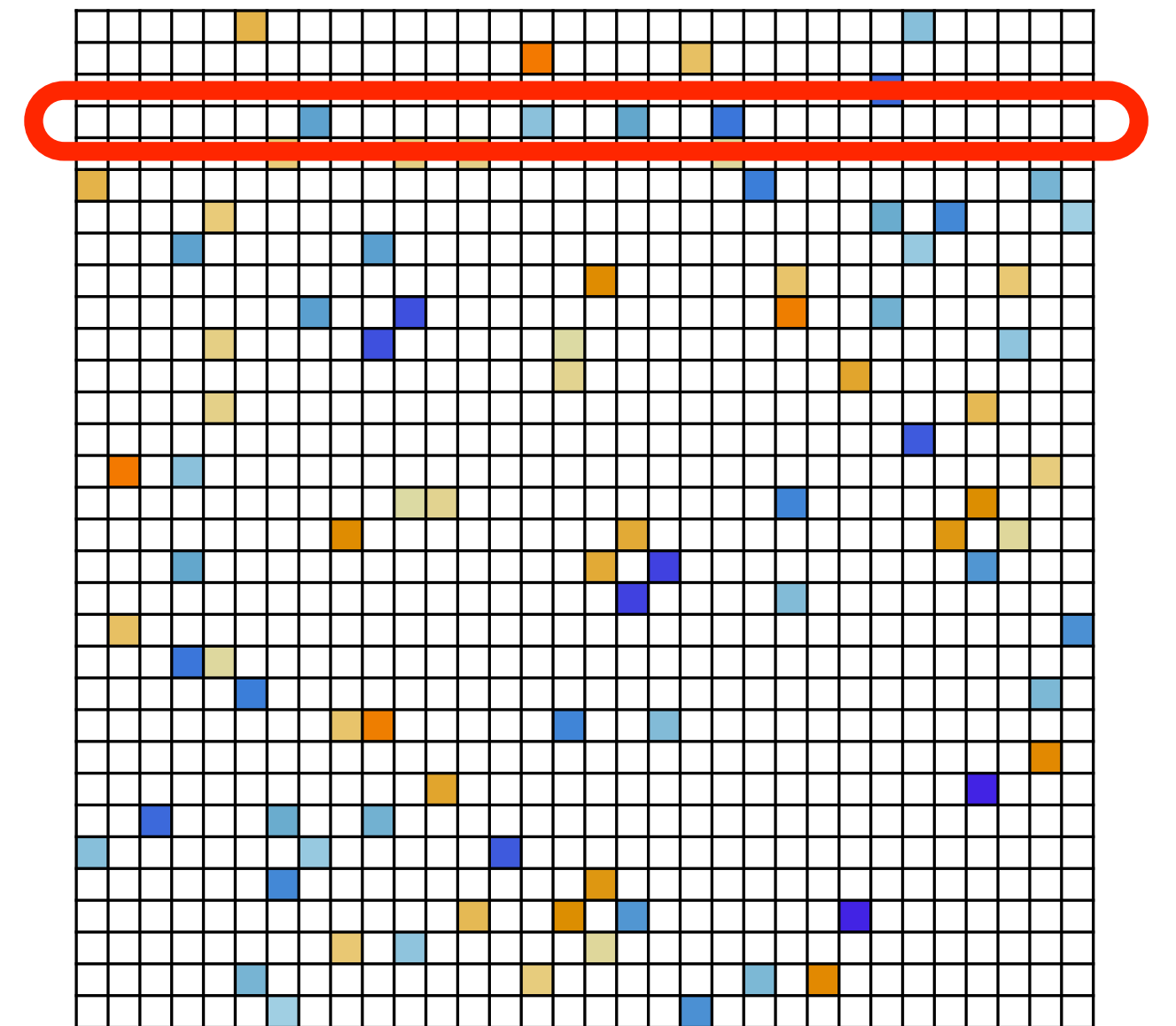
- Physics is local, so many natural Hamiltonians are k -local
- For $k = O(\log n)$, any k -local Hamiltonian has an efficient explicit description (at most $\binom{n}{k}$ terms, each acting on a space of dimension 2^k)
- Provides a decomposition that is useful in simulation algorithms

Sparse Hamiltonians

We say H is d -sparse if it has at most d nonzero entries per row

Suppose it is also row-computable: in any given row, the location of the j th nonzero entry and its value can be computed efficiently (locations and values provided by black boxes)

$$H =$$



Advantages:

- Generalizes local Hamiltonians (a k -local Hamiltonian with L terms is d -sparse with $d = 2^k L$)
- Can still be efficiently simulated
- Describes other Hamiltonians with sparse connectivity graphs (quantum walks, some chemistry simulations, ...)
- Black-box description facilitates query lower bounds

Complexity

How hard is quantum simulation?

A classical computer cannot even represent the state efficiently, so surely general simulation is classically hard.

But a quantum computer cannot produce a complete description of the state. How can we make a fair comparison?

Suppose we provide succinct descriptions of

- the initial state (say, as a small-depth quantum circuit acting on the $|0\rangle$ state),
- the Hamiltonian (say, as a k -local operator), and
- a final measurement (say, measurements of the individual qubits in some basis).

Then a quantum computer can efficiently sample from the output distribution.

How hard is this for a classical computer?

Quantum simulation is BQP-hard

Any quantum circuit can be efficiently implemented by the dynamics of a local Hamiltonian.

[Feynman 85]

Given a circuit $U = U_k \dots U_2 U_1$, append a “clock” register and define

$$H := \sum_{j=1}^k \alpha_j H_j \quad \text{where} \quad H_j := U_j \otimes |j\rangle\langle j-1| + U_j^\dagger \otimes |j-1\rangle\langle j|$$

Advancing the clock from $j-1$ to j corresponds to applying the gate U_j

With an appropriate choice of α_j , we have $e^{-iHk}|\psi\rangle \otimes |0\rangle = U|\psi\rangle \otimes |k\rangle$

However, this uses abstract clock states, not qubits, so it is not a local Hamiltonian

Quantum simulation is BQP-hard: Clock encoding

If we represent the clock state $|j\rangle$ appropriately, then we can implement $|j\rangle\langle j-1|$ with a 2-qubit operation, so if the circuit consists of 2-qubit gates, H is 4-local.

Represent the clock using $k+1$ qubits, with $|j\rangle := |\underbrace{0\dots 0}_j 1 \underbrace{0\dots 0}_{k-j}\rangle$

Represent clock transitions with $|j+1\rangle\langle j| \leftrightarrow \sigma_+^{(j+1)} \sigma_-^{(j)}$, $|j\rangle\langle j+1| \leftrightarrow \sigma_+^{(j)} \sigma_-^{(j+1)}$

$$\text{where } \sigma_+ := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \sigma_- := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

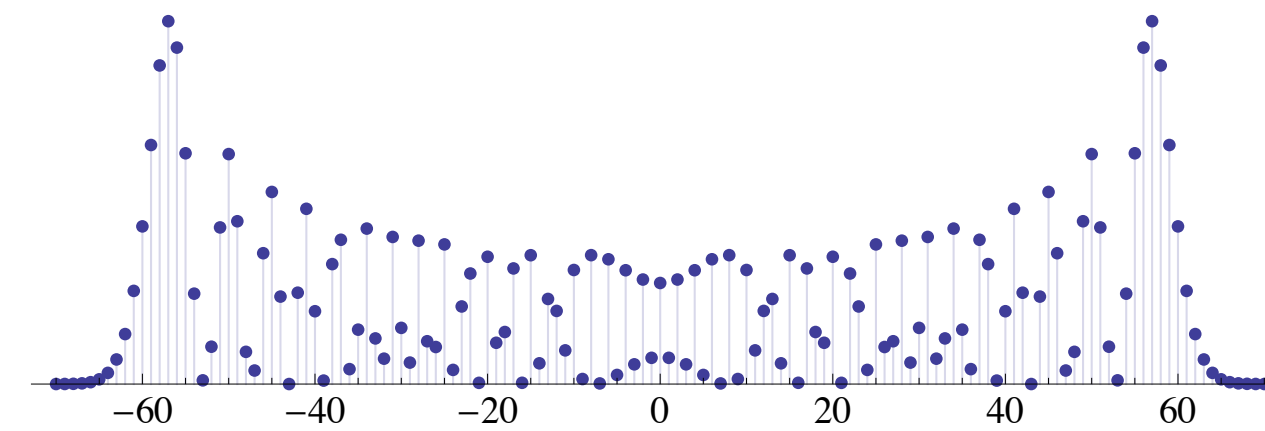
If U_j is a 2-qubit gate, $H_j := U_j \otimes |j\rangle\langle j-1| + U_j^\dagger \otimes |j-1\rangle\langle j|$ is represented by a 4-local term.

Aside: Quantum walk on a (weighted) path

Consider a Hamiltonian describing nearest-neighbor transitions on a path:

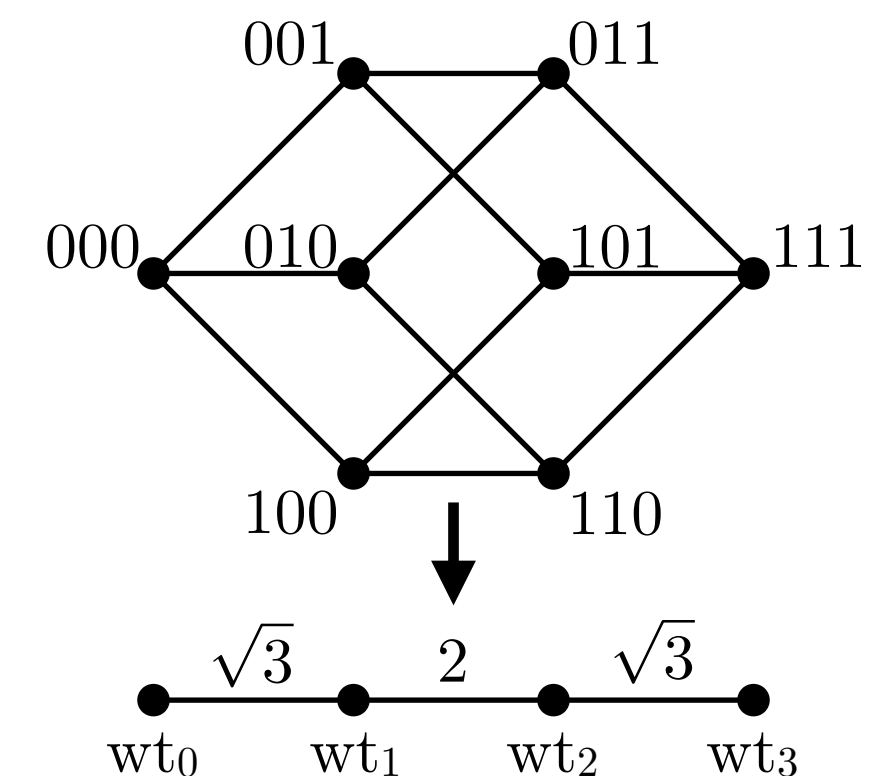


On a long path, waves propagate ballistically, but diffusion reduces the amplitude over time.



On a hypercube, evolution exactly propagates to the opposite corner:

$$H = \sum_{j=1}^n \sigma_x^{(j)} \quad e^{-iH\pi/2} |0 \dots 0\rangle = |1 \dots 1\rangle$$



Consider projection onto a weighted path:

$$|\text{wt}_k\rangle := \binom{n}{k}^{-1/2} \sum_{|x|=k} |x\rangle \quad H|\text{wt}_k\rangle = \sqrt{k(n-k+1)} |\text{wt}_{k-1}\rangle + \sqrt{(k+1)(n-k)} |\text{wt}_{k+1}\rangle$$

So taking bounded amplitudes $\alpha_j = \sqrt{j(n-j+1)}/n$ gives perfect transfer in time $\frac{\pi}{2}n$.

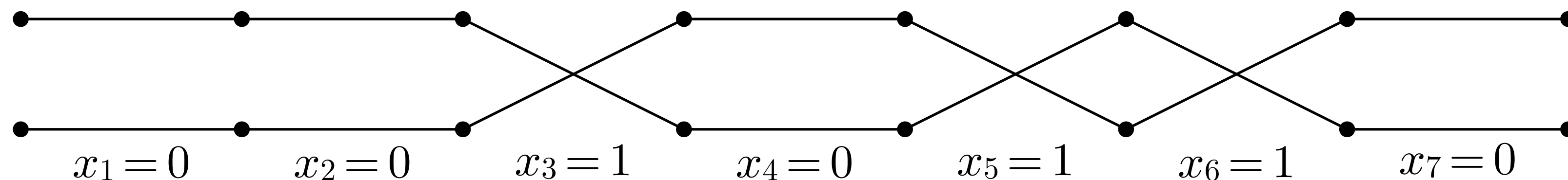
No fast forwarding

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

Proof is based on the hardness of computing parity: given a black box for the bits of a string $x \in \{0, 1\}^n$, computing $x_1 \oplus \cdots \oplus x_n$ requires $\Omega(n)$ quantum queries.

[Beals, Buhrman, Cleve, Mosca, de Wolf 98; Farhi, Goldstone, Gutmann, Sipser 98]

Construct a sparse Hamiltonian that encodes the parity:



Simulation for time $t = O(n)$ can be used to determine the parity (again, choosing weights to ensure perfect transfer), so a general-purpose simulation method must use $\Omega(t)$ gates.

[Berry, Ahokas, Cleve, Sanders 05]

Product formulas

Product formula simulation

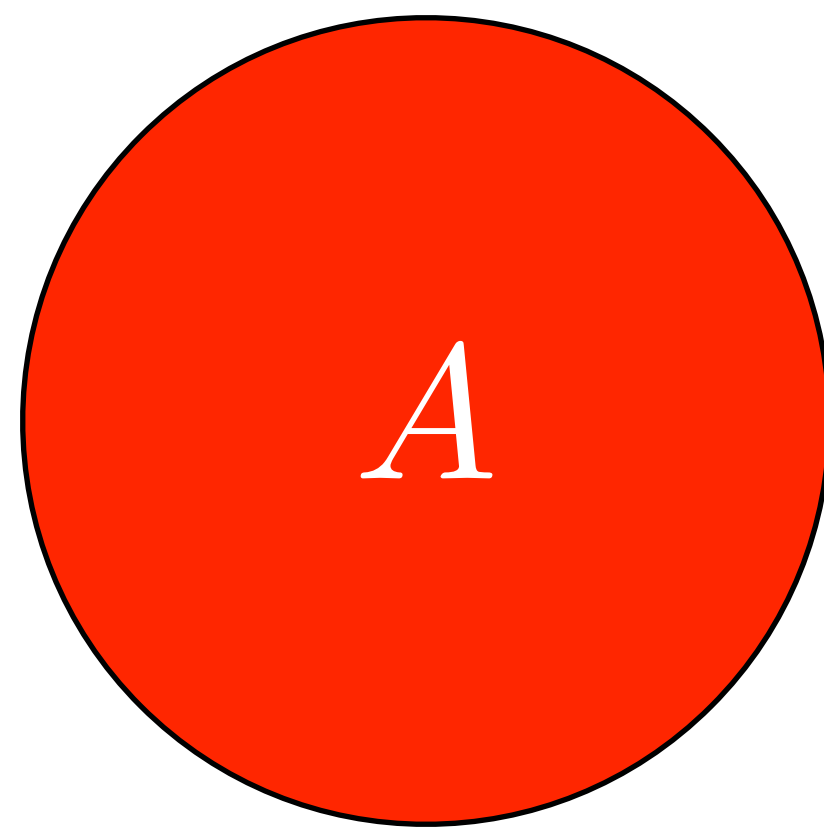
Suppose we want to simulate $H = \sum_{j=1}^L H_j$

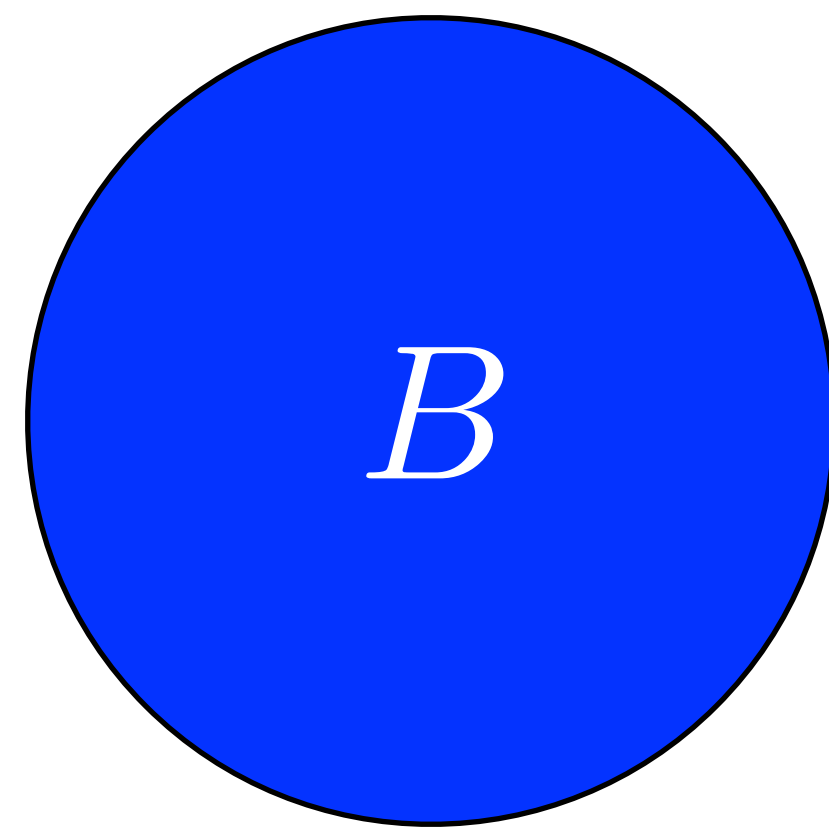
Combine individual simulations with the Lie product formula. E.g., with two terms:

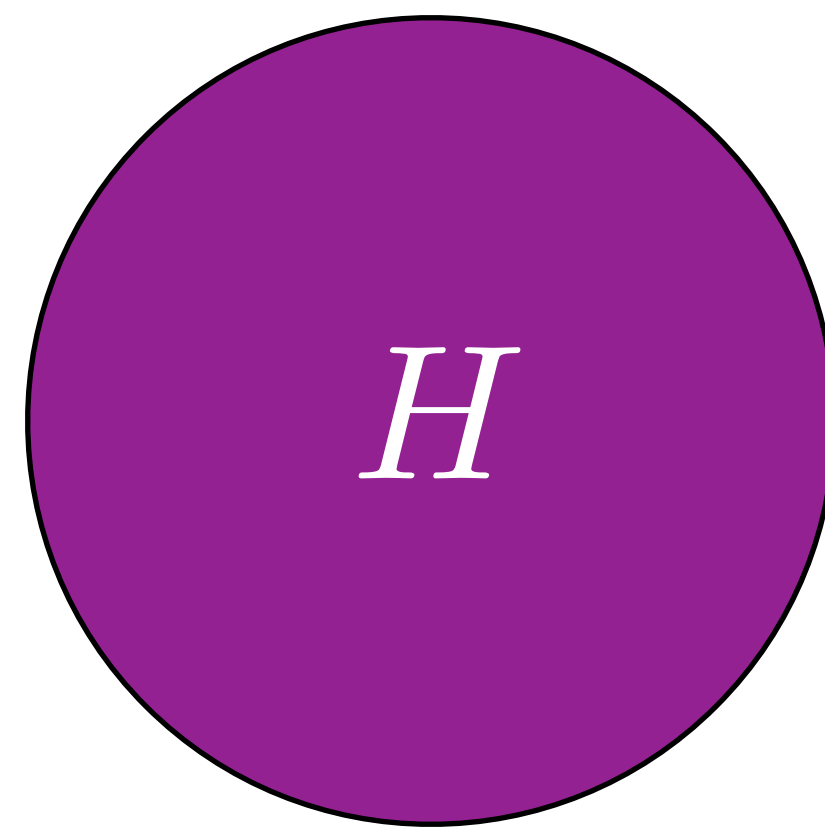
$$\lim_{r \rightarrow \infty} \left(e^{-iAt/r} e^{-iBt/r} \right)^r = e^{-i(A+B)t}$$

A Venn diagram illustrating the relationship between three sets: H , A , and B . The set H is represented by a purple circle on the left. The set A is represented by a red circle in the middle, and the set B is represented by a blue circle on the right. The equation $H = A + B$ is shown between the circles, indicating that H is the union of A and B . The circles are arranged horizontally, and the symbols $=$ and $+$ are placed between them.

$$H = A + B$$







Product formula simulation

Suppose we want to simulate $H = \sum_{j=1}^L H_j$

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

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

$$e^{-i(A+B)t} = 1 - i(A+B)t - \frac{1}{2}(A^2 + AB + BA + B^2)t^2 + O(t^3)$$

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

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

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

Higher-order product formulas

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

E.g., second order:

$$\begin{aligned} S_2(t) &:= e^{-iAt/2} e^{-iBt} e^{-iAt/2} \\ &= (1 - \frac{i}{2}At - \frac{1}{8}A^2t^2 + O(t^3))(1 - iBt - \frac{1}{2}B^2t^2 + O(t^3))(1 - \frac{i}{2}At - \frac{1}{8}A^2t^2 + O(t^3)) \\ &= 1 - i((\frac{1}{2} + \frac{1}{2})A + B)t - ((\frac{1}{8} + \frac{1}{8} + \frac{1}{4})A^2 + \frac{1}{2}AB + \frac{1}{2}BA + \frac{1}{2}B^2)t^2 + O(t^3) \\ &= 1 - i(A + B)t - \frac{1}{2}(A^2 + AB + BA + B^2)t^2 + O(t^3) \end{aligned}$$

Ideal evolution: $e^{-i(A+B)t} = 1 - i(A + B)t - \frac{1}{2}(A^2 + AB + BA + B^2)t^2 + O(t^3)$

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

To ensure error at most ϵ , take $r = O(t^{3/2}/\epsilon^{1/2})$

Suzuki formulas

Recall $S_2(t) := e^{-iAt/2} e^{-iBt} e^{-iAt/2}$

Can use this base case to recursively construct arbitrarily high-order expansions [Suzuki 91]:

$$\text{let } S_{2k}(t) := S_{2k-2}(p_k t)^2 S_{2k-2}(q_k t) S_{2k-2}(p_k t)^2$$

Then you can find numbers p_k and q_k (depending on k) so that

$$S_{2k}(t) = e^{-i(A+B)t} + O(t^{2k+1})$$

Using the order- $2k$ expansion for an L -term Hamiltonian, the number of exponentials required for an approximation with error at most ϵ is at most [Berry, Ahokas, Cleve, Sanders 07]

$$5^{2k} L^2 h t \left(\frac{L h t}{\epsilon} \right)^{1/2k} \quad h := \max_j \|H_j\|$$

Suzuki formula derivation (I/2)

Recall $S_{2k}(t) := S_{2k-2}(p_k t)^2 S_{2k-2}(q_k t) S_{2k-2}(p_k t)^2$.

Let $4p_k + q_k = 1$. Then

$$\exp(-i(A+B)t) = \exp(-ip_k(A+B)t)^2 \exp(-iq_k(A+B)t) \exp(-ip_k(A+B)t)^2 \quad (\star)$$

S_{2k} replaces the terms of the right-hand side of $(\star)$ using S_{2k-2} .

Since $S_{2k-2}(t) = e^{-i(A+B)t} + O(t^{2k-1})$, the terms of order $0, 1, \dots, 2k-2$ in S_{2k} agree with those of the ideal evolution.

The term of order $2k-1$ in $(\star)$ mainly has contributions from products of lower-order terms of the factors, which match the corresponding terms of S_{2k} . However, it also has the contribution $\frac{(-it)^{2k-1}}{(2k-1)!} (4p_k^{2k-1} + q_k^{2k-1})(A+B)^{2k-1}$ coming only from single order- $2k$ terms.

Let $4p_k^{2k-1} + q_k^{2k-1} = 0$. Then this term vanishes, and the corresponding term of S_{2k} also vanishes, so S_{2k} is correct up to order $2k-1$.

Suzuki formula derivation (2/2)

Recall $S_{2k}(t) := S_{2k-2}(p_k t)^2 S_{2k-2}(q_k t) S_{2k-2}(p_k t)^2 = \exp(-it(A+B)) + O(t^{2k})$

Write $\exp(-it(A+B)) = S_{2k}(t) + E_{2k}t^{2k} + O(t^{2k+1})$

Then $I = \exp(-it(A+B)) \exp(it(A+B))$
 $= S_{2k}(t)S_{2k}(-t) + S_{2k}(t)E_{2k}t^{2k} + E_{2k} \cdot (-t)^{2k}S_{2k}(-t) + O(t^{2k+1})$

Since the formula has the symmetry $S_{2k}(t)S_{2k}(-t) = I$, this gives

$$S_{2k}(t)E_{2k} + E_{2k}S_{2k}(-t) = O(t)$$

Taking $t \rightarrow 0$, we find $E_{2k} = 0$, so the formula is in fact correct up to order $2k$.

Solving $\begin{matrix} 4p_k + q_k = 1 \\ 4p_k^{2k-1} + q_k^{2k-1} = 0 \end{matrix}$ gives $\begin{matrix} p_k = \frac{1}{4 - 4^{1/(2k-1)}} \\ q_k = 1 - 4p_k \end{matrix}$

Improved error analysis

Numerics suggest that product formula error bounds based on Taylor series expansion can be very loose in practice.

Alternative: *local error analysis* provides convenient integral representations of the error

[Descombes, Thalhammer 10]

Example (first order):

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

Therefore $\|e^{-iBt}e^{-iAt} - e^{-i(A+B)t}\| \leq \|[A, B]\|t^2$

Advantages:

- no explicit sum over higher-order terms
- commutator scaling
- can offer much better performance, both asymptotically and in practice (more on this later)

[Childs, Su 19]

First-order local error analysis

Let $S(t) := e^{-iAt}e^{-iBt}$

Differentiate:

$$S'(t) = -iAS(t) - iS(t)B = -i(A+B)S(t) + i[B, S(t)] = -i(A+B)S(t) + i[B, e^{-iAt}]e^{-iBt}$$

Use *variation of parameters formula*: the solution of $u'(t) = Lu(t) + f(t)$

$$\text{is } u(t) = e^{Lt}u(0) + \int_0^t e^{L(t-\tau)}f(\tau) \, d\tau$$

$$\text{Therefore } S(t) = e^{-i(A+B)t} + \int_0^t e^{-i(A+B)(t-\tau)} i[B, e^{-iA\tau}] e^{-iB\tau} \, d\tau$$

$$\text{Repeat: } \frac{d}{dt}[B, e^{-iAt}] = -i[B, Ae^{-iAt}] = -iA[B, e^{-iAt}] + i[A, B]e^{-iAt}$$

$$\text{Variation of parameters: } [B, e^{-iA\tau}] = i \int_0^\tau e^{-iA(\tau-\tau')} [A, B] e^{-iA\tau'} \, d\tau'$$

$$\text{Therefore } S(t) = e^{-i(A+B)t} - \int_0^t \int_0^\tau e^{-i(A+B)(t-\tau)} e^{-iA(\tau-\tau')} [A, B] e^{-iA\tau'} e^{-iB\tau} \, d\tau' d\tau$$

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 any number of terms.

Theorem. A p th order product formula approximates the evolution of $H = \sum_{j=1}^L H_j$ with additive error $O(\alpha t^{p+1})$ where

$$\alpha := \sum_{j_1, \dots, j_{p+1}} \left\| [H_{j_{p+1}}, [\dots, [H_{j_2}, H_{j_1}] \dots]] \right\|.$$

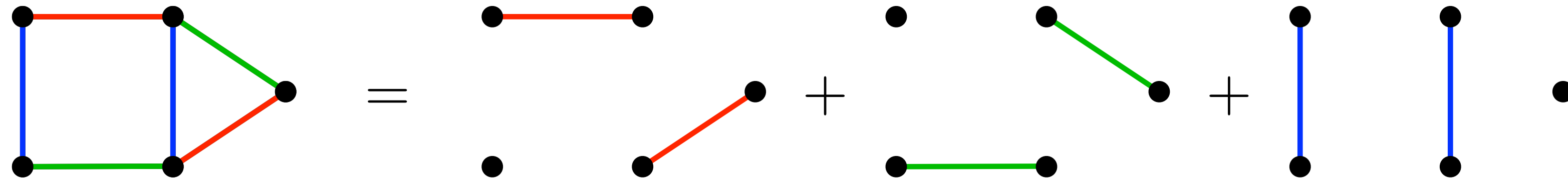
Therefore $O(L\alpha^{1/p} t^{1+1/p})$ gates suffice to simulate H for time t with constant accuracy.

This gives much tighter rigorous analysis of product formulation simulations (e.g., only off by factor of ~ 5 for 4th-order simulation of 50-qubit Heisenberg model), among many other applications.

(However, these bounds are still not tight in all cases, and it can be hard to compute them!)

Sparse Hamiltonians and coloring

Strategy: Color the edges of the graph of H . Then the simulation breaks into small pieces that are easy to handle.



A sparse graph can be efficiently colored using only local information, giving efficient simulations.

Lemma. A bipartite graph with maximum degree d has a locally computable edge coloring using at most d^2 colors.

Proof: For any vertex u , let $\text{idx}(u, v)$ be the index of v in the neighbor list of u . For edge (u, v) with u on the left side of the bipartition and v on the right, assign color $(\text{idx}(u, v), \text{idx}(v, u))$. This uses at most d^2 colors. It is a valid coloring since if (u, v) and (u, w) have the same color, then $\text{idx}(u, v) = \text{idx}(u, w)$, so $v = w$. An analogous argument handles (v, u) vs. (w, u) .

Sparse Hamiltonians and coloring: Bipartiteness is WLOG

Consider the Hamiltonian $\sigma_x \otimes H = \begin{pmatrix} 0 & H \\ H & 0 \end{pmatrix}$.

The graph of this Hamiltonian is bipartite.

Furthermore, there is an invariant subspace in which the expanded Hamiltonian acts like H :

$$(\sigma_x \otimes H)(|+\rangle \otimes |\psi\rangle) = |+\rangle \otimes H|\psi\rangle$$

Thus a simulation of $\sigma_x \otimes H$ can be used to perform a simulation of H .

Post-Trotter methods

Linear-time simulation

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

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 $\text{span}\{|\psi_j\rangle\}_{j=1}^N$,

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

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

$$|\lambda\rangle \mapsto |\lambda\rangle |\widetilde{\arcsin \lambda}\rangle \quad (\text{phase estimation})$$

$$\mapsto e^{-i\lambda t} |\lambda\rangle |\widetilde{\arcsin \lambda}\rangle$$

$$\mapsto e^{-i\lambda t} |\lambda\rangle \quad (\text{inverse phase est})$$

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

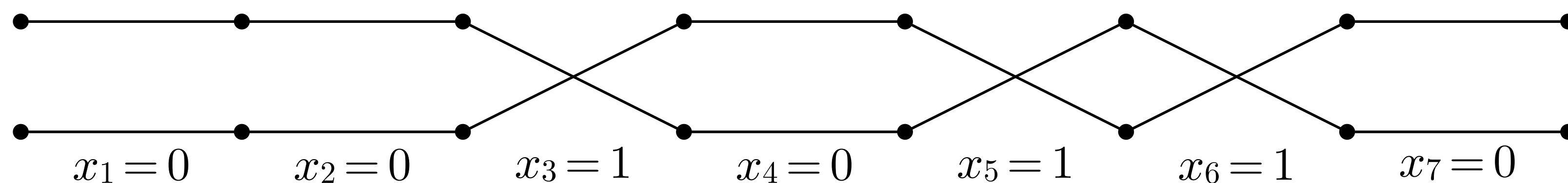
High-precision simulation?

Can we improve the dependence on ϵ ?

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

- 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): $O(5^{2k} \epsilon^{-1/2k})$

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

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

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

Partially implementing U

Given $U = \sum_j \beta_j V_j$

Let B be an operation that maps $|0\rangle$ to $\frac{1}{\sqrt{s}} \sum_j \sqrt{\beta_j} |j\rangle$, where $s := \sum_j |\beta_j|$

Let $W := B^\dagger \text{select}(V) B$ where $\text{select}(V) := \sum_j |j\rangle\langle j| \otimes V_j$

$$\begin{aligned} \text{Then } (\langle 0| \otimes I) W (|0\rangle \otimes |\psi\rangle) &= \frac{1}{\sqrt{s}} (\langle 0| \otimes I) B^\dagger \text{select}(V) \sum_i \sqrt{\beta_j} |j\rangle |\psi\rangle \\ &= \frac{1}{\sqrt{s}} (\langle 0| \otimes I) B^\dagger \sum_j \sqrt{\beta_j} |j\rangle V_j |\psi\rangle \\ &= \frac{1}{s} \sum_j \beta_j V_j |\psi\rangle = \frac{1}{s} U |\psi\rangle \end{aligned}$$

$$\text{so } W|0\rangle|\psi\rangle = \frac{1}{s}|0\rangle \otimes U|\psi\rangle + \sqrt{1 - \frac{1}{s^2}}|\Phi\rangle \text{ for some state } |\Phi\rangle$$

Obvious amplitude amplification

We would like to boost the amplitude of the $U|\psi\rangle$ piece.

This is like amplitude amplification, but with an unknown initial state.

Define $P := |0\rangle\langle 0|$ and $R := (I - 2P) \otimes I$

$$\begin{aligned} \text{Then } (\langle 0| \otimes I)WRW^\dagger RW(|0\rangle \otimes I) \\ &= (\langle 0| \otimes I)(WW^\dagger W - 2WW^\dagger PW - 2WPW^\dagger W + 4WPW^\dagger PW)(|0\rangle \otimes I) \\ &= (\langle 0| \otimes I)(-3W + 4WPW^\dagger PW)(|0\rangle \otimes I) \\ &= -\frac{3}{s}U + \frac{4}{s^3}UU^\dagger U \\ &\approx -\left(\frac{3}{s} - \frac{4}{s^3}\right)U \quad \text{since } U \text{ is approximately unitary} \end{aligned}$$

For $s = 2$, the amplitude is boosted from $1/2$ to 1 , as in 1-out-of-4 search.

End-to-end error dependence

We can produce the final state of a quantum simulation with error ϵ in time $O(\log(1/\epsilon))$.

For an end-to-end problem, we need to extract classical information. What is the cost to estimate the expectation value of an observable with precision ϵ ?

Simple approach: take the average of $O(1/\epsilon^2)$ measurement outcomes.

Using amplitude amplification/estimation, this can be improved to $O(1/\epsilon)$. This is optimal!

With this overhead taken into account, the end-to-end simulation complexity cannot be $\text{poly}(\log(1/\epsilon))$. The simulation cost and the sampling overhead compose multiplicatively, so algorithms with logarithmic error dependence polynomially improve the overall complexity (e.g., using first-order product formula simulation, $O(1/\epsilon^2)$; using LCU, $O(\frac{1}{\epsilon} \log \frac{1}{\epsilon})$).

Tradeoff between t and ϵ

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

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

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].

Block encoding

We say U is a block encoding of a matrix A if

$$U = \begin{pmatrix} A & \cdot \\ \cdot & \cdot \end{pmatrix} = |\mathbf{0}\rangle\langle\mathbf{0}| \otimes A + \dots \quad (\text{requires } \|A\| \leq 1)$$

where $|\mathbf{0}\rangle$ denotes the first computational basis state of an ancilla register.

Example: In the LCU approach, $W := B^\dagger \text{select}(V)B$ is a block encoding of U/s .

Can directly give an efficient block encoding of a sparse matrix A . If

$$R: |0\rangle|0\rangle|i\rangle \mapsto |0\rangle \frac{1}{\sqrt{d}} \sum_{k=1}^N \sqrt{A_{ik}^*} |i\rangle|k\rangle + |1\rangle|i\rangle|\mu_i\rangle$$
$$C: |0\rangle|0\rangle|j\rangle \mapsto |0\rangle \frac{1}{\sqrt{d}} \sum_{\ell=1}^N \sqrt{A_{\ell j}} |\ell\rangle|j\rangle + |2\rangle|j\rangle|\nu_j\rangle$$

then $R^\dagger C$ is a block encoding of A/d .

Quantum signal processing

Problem: Given a block encoding of A , produce a block encoding of $f(A)$.

Block encoding of a scalar, $A = x$: $W(x) := \begin{pmatrix} x & i\sqrt{1-x^2} \\ i\sqrt{1-x^2} & x \end{pmatrix} = e^{i \arccos(x) \sigma_x}$.

Consider the gate sequence $W_\Phi(x) := e^{i\phi_0 \sigma_z} W(x) e^{i\phi_1 \sigma_z} W(x) \cdots W(x) e^{i\phi_k \sigma_z}$

What functions of W can we realize by some choice of $\Phi = (\phi_0, \dots, \phi_k)$?

Lemma. *There exists $\Phi \in \mathbb{R}^{k+1}$ such that*

$$W_\Phi(x) = \begin{pmatrix} f(x) & ig(x)\sqrt{1-x^2} \\ ig^*(x)\sqrt{1-x^2} & f^*(x) \end{pmatrix}$$

if and only if $f, g \in \mathbb{C}[x]$ satisfy

- (i) $\deg(f) \leq k$ and $\deg(g) \leq k-1$,
- (ii) f has parity $k \bmod 2$ and g has parity $k-1 \bmod 2$, and
- (iii) $\forall x \in [-1, 1], |f(x)|^2 + (1-x^2)|g(x)|^2 = 1$.

QSP lemma

Proof: By induction on k .

For $k = 0$, $\deg(f) = 0$, so $f(x) = e^{i\phi_0}$ for some $\phi_0 \in \mathbb{R}$, and $g(x) = 0$.

Since $f(x)f^*(x) + (1 - x^2)g(x)g^*(x)$ is a polynomial, we must have

$\ell := \deg(f) = \deg(g) + 1$ and the leading coefficients must satisfy $|p_\ell| = |q_{\ell-1}|$ to cancel.

Choose $\phi_k \in \mathbb{R}$ so that $e^{2i\phi_k} = p_\ell / q_{\ell-1}$.

$$\begin{aligned} \text{Then } & \begin{pmatrix} f(x) & ig(x)\sqrt{1-x^2} \\ ig^*(x)\sqrt{1-x^2} & f^*(x) \end{pmatrix} e^{-i\phi_k \sigma_z} W^\dagger(x) \\ &= \begin{pmatrix} f(x) & ig(x)\sqrt{1-x^2} \\ ig^*(x)\sqrt{1-x^2} & f^*(x) \end{pmatrix} \begin{pmatrix} xe^{i\phi_k} & -ie^{i\phi_k}\sqrt{1-x^2} \\ -ie^{-i\phi_k}\sqrt{1-x^2} & xe^{-i\phi_k} \end{pmatrix} \\ &= \begin{pmatrix} \bar{f}(x) & i\bar{g}(x)\sqrt{1-x^2} \\ i\bar{g}^*(x)\sqrt{1-x^2} & \bar{f}^*(x) \end{pmatrix} \text{ where } \begin{aligned} \bar{f}(x) &:= xe^{i\phi_k} f(x) + e^{-i\phi_k} (1-x^2)g(x) \\ \bar{g}(x) &:= -e^{i\phi_k} f(x) + e^{-i\phi_k} xg(x) \end{aligned} \end{aligned}$$

Can show that $\bar{f}$ has degree $\ell-1$ and $\bar{g}$ has degree $\ell-2$.

The converse follows by a similar inductive argument.

Lemma. There exists $\Phi \in \mathbb{R}^{k+1}$ such that

$$W_\Phi(x) = \begin{pmatrix} f(x) & ig(x)\sqrt{1-x^2} \\ ig^*(x)\sqrt{1-x^2} & f^*(x) \end{pmatrix}$$

if and only if $f, g \in \mathbb{C}[x]$ satisfy

- (i) $\deg(f) \leq k$ and $\deg(g) \leq k-1$,
- (ii) f has parity $k \bmod 2$ and g has parity $k-1 \bmod 2$, and
- (iii) $\forall x \in [-1, 1], |f(x)|^2 + (1-x^2)|g(x)|^2 = 1$.

Qubitization (1/2)

To perform QSP on a high-dimensional block encoding, we can map it to a qubit by *qubitization*.

Let U be a block encoding of A , so $\Pi U \Pi = |\mathbf{0}\rangle\langle\mathbf{0}| \otimes A$ where $\Pi := |\mathbf{0}\rangle\langle\mathbf{0}| \otimes I$

Let $|\lambda\rangle := |\mathbf{0}\rangle \otimes |\psi_\lambda\rangle$ where $|\psi_\lambda\rangle$ is an eigenvector of A with eigenvalue λ

Then U maps $\text{span}\{|\lambda\rangle, (I - \Pi)U^\dagger|\lambda\rangle\}$ to $\text{span}\{|\lambda\rangle, (I - \Pi)U|\lambda\rangle\}$:

$$\begin{aligned} U|\lambda\rangle &= (\Pi + (I - \Pi))U|\lambda\rangle & U(I - \Pi)U^\dagger|\lambda\rangle &= (I - U\Pi U^\dagger)|\lambda\rangle \\ &= \lambda|\lambda\rangle + (I - \Pi)U|\lambda\rangle & &= |\lambda\rangle - \lambda U|\lambda\rangle \\ & & &= (1 - \lambda^2)|\lambda\rangle - \lambda(I - \Pi)U|\lambda\rangle \end{aligned}$$

Qubitization (2/2)

Therefore, with an appropriate choice of bases, we have

$$U \cong \bigoplus_{\lambda} \begin{pmatrix} \lambda & \sqrt{1 - \lambda^2} \\ \sqrt{1 - \lambda^2} & -\lambda \end{pmatrix}$$

Thus we can perform QSP on A by a sequence

$$e^{i\theta_1(2\Pi-1)}U^\dagger e^{i\theta_2(2\Pi-1)}U e^{i\theta_3(2\Pi-1)}U^\dagger e^{i\theta_4(2\Pi-1)}U \dots e^{i\theta_{k-1}(2\Pi-1)}U^\dagger e^{i\theta_k(2\Pi-1)}U$$

to realize any function of A satisfying the conditions of the QSP lemma.

Hamiltonian simulation by quantum signal processing

Task: Given a block encoding of H , produce a block encoding of e^{-iHt}

Jacobi-Anger formula: $e^{itx} = J_0(t) + 2 \sum_{k=1}^{\infty} i^k J_k(t) T_k(x)$

$\swarrow$ Bessel
 $\nwarrow$ Chebyshev

$$\approx J_0(t) + 2 \sum_{k=1}^K i^k J_k(t) T_k(x)$$

Approximation is within ϵ if we take $K = O\left(t + \frac{\ln(1/\epsilon)}{\ln(e + \ln(1/\epsilon)/t)}\right)$

For technical reasons, QSP can only give a block encoding of $e^{-iHt}/2$, but we can use oblivious amplitude amplification to boost this close to e^{-iHt}

This query complexity achieves the optimal tradeoff between t and ϵ !

Special topics

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?

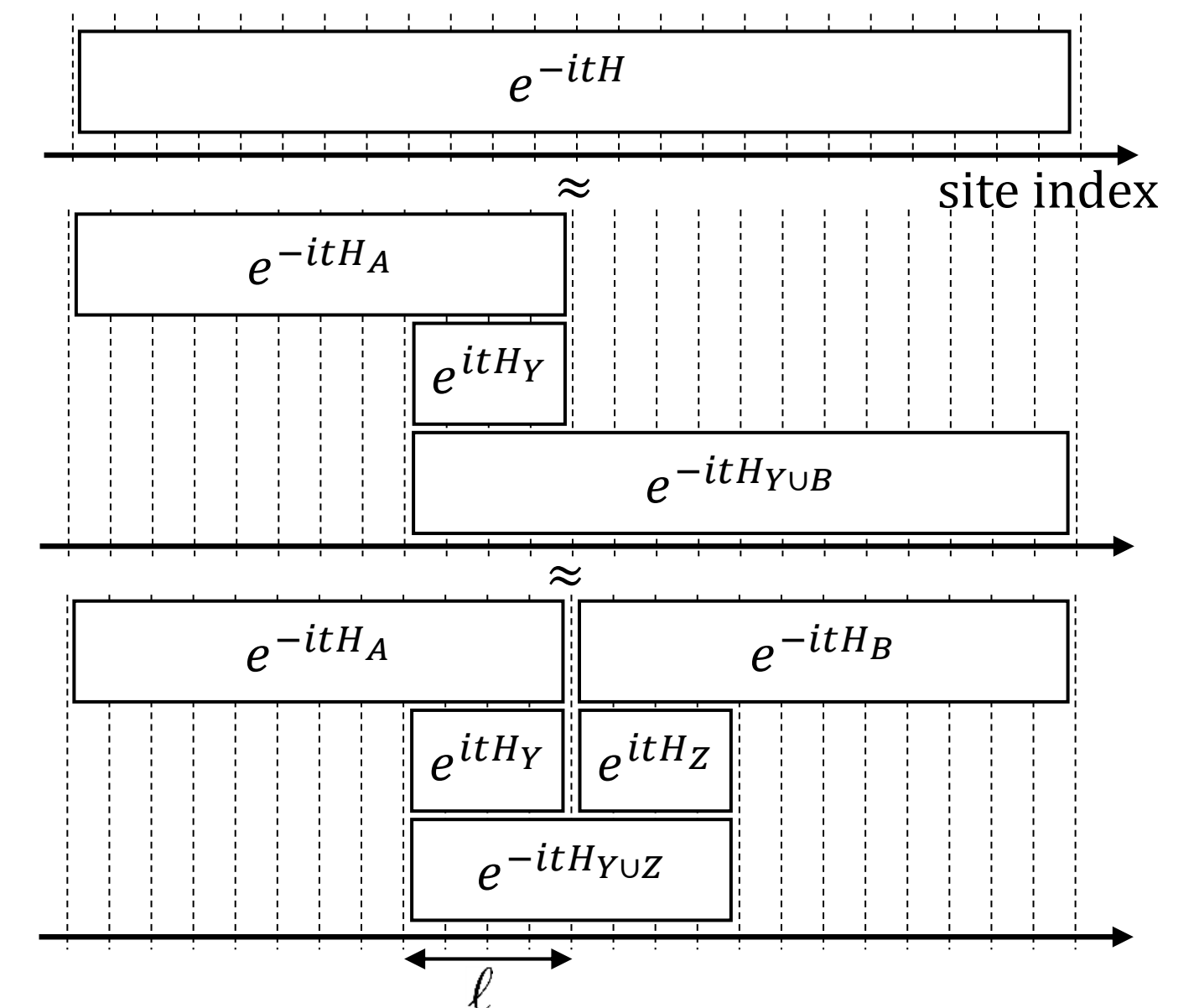
Consider n spins with nearest-neighbor interactions on a grid of fixed dimension. To simulate for constant time, previous methods (LCU, QSP, high-order PF with standard analysis) give:

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

Execution time should not have to be extensive!

Can give a 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



Product formula simulation of lattice Hamiltonians

Using standard error bounds for product formulas, simulation cost is $O\left(5^{2k} L^2 h t \left(\frac{L h t}{\epsilon}\right)^{1/2k}\right)$

For an n -site lattice Hamiltonian of fixed dimension, $L = O(n)$, giving cost at least quadratic in n

Using improved analysis with commutator scaling, cost for an order- p formula is

$$O(L \alpha^{1/p} t^{1+1/p}), \quad \alpha := \sum_{j_1, \dots, j_{p+1}} \left\| [H_{j_{p+1}}, [\dots, [H_{j_2}, H_{j_1}] \dots]] \right\|.$$

For constant p , we have $\alpha = O(n)$ since for any fixed j_1 , there are $O(1)$ nonzero nested commutators

This gives cost $O((n t)^{1+1/p})$, nearly matching the HHKL complexity for large p

Interaction picture simulation

Suppose we want to simulate $H = A + B$ where A is much larger than B , but easy to simulate

Product formula simulation will pay a cost that scales with $\|A\|$

Transform to *interaction picture*: $|\psi_I(t)\rangle := e^{iAt}|\psi(t)\rangle$

$$\begin{aligned} i \frac{d}{dt} |\psi_I(t)\rangle &= -A|\psi_I(t)\rangle + e^{iAt} H |\psi(t)\rangle \\ &= e^{iAt} B e^{-iAt} |\psi_I(t)\rangle \end{aligned}$$

so $|\psi_I(t)\rangle$ evolves according to the interaction picture Hamiltonian $H_I(t) := e^{iAt} B e^{-iAt}$

Simulating time-dependent Hamiltonians is more complicated than the time-independent case...

... but there are methods for doing this, and it can sometimes give a favorable tradeoff

Randomized simulation

Another approach to speeding up simulation: introduce classical randomness

Example: $e^{-i(A+B)t} = I - i(A+B)t - \frac{1}{2}(A^2 + AB + BA + B^2)t^2 + O(t^3)$

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

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

$\Downarrow$

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

[Zhang 12]

Mixing lemma [Campbell 17; Hastings 17; Chen, Huang, Kueng, Tropp 20]: Error of the average operation is linear in the average error.

Randomly permuting terms in a higher-order product formula also improves the approximation (though not the order of the formula), though in practice the improvement is typically small.

[Childs, Ostrander, Su 18]

qDRIFT

Alternative randomized simulation strategy: choose which term to simulate with a probability that depends on its weight

Suppose $H = \sum_j h_j H_j$ with $\|H_j\| = 1$; let $\lambda := \sum_j h_j$

Repeat $\nu = O(\lambda^2 t^2 / \epsilon)$ times: sample H_j with probability h_j / λ and apply $e^{-i\lambda H_j t / \nu}$

Theorem: This gives a simulation that is accurate to within diamond norm distance ϵ .

Cost $O(\lambda^2 t^2 / \epsilon)$, vs. $O(L^3 (\max_j h_j)^2 t^2 / \epsilon)$ for first-order Trotter

Con: Limited to first-order approximation; higher-order methods are better asymptotically

Pro: Simulation cost has no explicit dependence on the number of terms and may outperform deterministic product formulas non-asymptotically, especially when the terms have widely varying size

Random inputs

Worst-case input states could be atypical. Can we give a more efficient simulation with extra information about the input state?

Recall that for a p th-order formula, the worst-case error is $O(\alpha t^{p+1})$ where

$$\alpha := \sum_{j_1, \dots, j_{p+1}} \left\| [H_{j_{p+1}}, [\dots, [H_{j_2}, H_{j_1}] \dots]] \right\|.$$

We can give a tighter bound if the input state is chosen at random from some distribution. For a 1-design ensemble on a d -dimensional system, the average error is $O(\alpha_F t^{p+1})$ where

$$\alpha_F := \frac{1}{\sqrt{d}} \sum_{j_1, \dots, j_{p+1}} \left\| [H_{j_{p+1}}, [\dots, [H_{j_2}, H_{j_1}] \dots]] \right\|_F.$$

This is no worse, but can sometimes give much better performance (for the same algorithm!).

Are random inputs practical?

The random-input analysis suggests that product-formula simulation typically performs much better than the worst case.

The setting is somewhat flexible (only requires a I-design input distribution), but it does require the input to be drawn from some well-behaved distribution.

In applications, we may not have a nice distribution, or may care about a particular input state.

Can we identify specific, typical features that make simulation faster?

State-dependent error bound

The leading-order contribution to the error only depends on the marginals of the state corresponding to the leading-order error terms of the product formula approximation.

Leading-order PF error: $U - \mathcal{U} = \sum_j E_j + \dots$

Annotations for the leading-order PF error equation:

- U : ideal evolution
- $\mathcal{U}$: product formula
- E_j : local terms
- $\dots$: higher-order terms

Simulation error: $\|(U - \mathcal{U})|\psi\rangle\|^2 \approx \sum_{j,j'} \langle \psi | E_j^\dagger E_{j'} | \psi \rangle$

Annotations for the simulation error equation:

- $E_j^\dagger E_{j'} (\rho_{j,j'} - \mathbb{I}/d_{j,j'})$: restricted to j,j'
- $d_{j,j'}$: dimension of the j,j' subsystem

$$\approx \sum_{j,j'} \text{tr} \left(\widetilde{E_j^\dagger E_{j'} (\rho_{j,j'} - \mathbb{I}/d_{j,j'})} \right) + \sum_{j,j'} \text{tr} \left(E_j^\dagger E_{j'} \right) / 2^n$$

$$\lesssim \sum_{j,j'} \|E_j^\dagger E_{j'}\| \text{tr} |\rho_{j,j'} - \mathbb{I}/d_{j,j'}| + \|E\|_F^2$$

If the marginals are maximally mixed, then the error is given by the Frobenius norm of the product formula error (as for a random input state).

More generally, there is a contribution from the spectral norm of the product formula error, but it is small if the marginals are close to maximally mixed.

Entanglement accelerates quantum simulation

Theorem. For a given pure quantum state $|\psi\rangle$ and quantum evolution $U = e^{-iHt}$ with p th-order product formula approximation $\mathcal{U}$,

$$\|(U - \mathcal{U})|\psi\rangle\| = \mathcal{O} \left(\sqrt{\sum_{j,j'} \|E_j^\dagger E_{j'}\| \operatorname{tr} |\rho_{j,j'} - \mathbb{I}/d_{\rho_{j,j'}}|} t^{p+1} + \|E\|_F t^{p+1} + \alpha_{p+2} t^{p+2} \right).$$

where E_j are the leading-order local error terms in the Trotter approximation, $E = \sum_j E_j$, $\rho_{j,j'}$ is the reduced state of $|\psi\rangle$ on the support of $E_j^\dagger E_{j'}$, and α_{p+2} is the next-leading-order spectral-norm commutator sum.

Highly entangled states have marginals that are close to maximally mixed. (Could recast the bound in terms of entropies of the marginals.)

To simulate evolution for long times, divide into short segments such that the total error is small.

Improvement over worst-case simulation

Consider simulating an n -site nearest-neighbor lattice Hamiltonian in constant dimensions with a p th-order product formula.

Worst case: $\alpha := \sum_{j_1, \dots, j_{p+1}} \left\| [H_{j_{p+1}}, [\dots, [H_{j_2}, H_{j_1}] \dots]] \right\| = O(n)$

Number of Trotter steps to evolve for time t with error at most ϵ : $O(t(nt/\epsilon)^{1/p})$

Average case: $\alpha_F := \frac{1}{\sqrt{d}} \sum_{j_1, \dots, j_{p+1}} \left\| [H_{j_{p+1}}, [\dots, [H_{j_2}, H_{j_1}] \dots]] \right\|_F = O(\sqrt{n})$

Number of Trotter steps to evolve for time t with error at most ϵ : $O(t(\sqrt{n}t/\epsilon)^{1/p})$

This analysis sets strictly better parameters for *the same algorithm*.

Outlook

Outlook: Algorithmic questions

Improve quantum algorithms for Hamiltonian simulation

- Tighter error bounds for product formulas (e.g., going beyond the triangle inequality)
- Better product formulas/limitations on improvements to product formulas
- Faster simulation methods for structured Hamiltonians (including cases where fast-forwarding is possible)
- Deeper exploration of alternative metrics: state-dependent simulation, simulation within a subspace, average-case simulation, ...

Quantum simulation as an algorithmic tool

- Linear algebra in Hilbert space: linear systems, differential equations, convex optimization, ...
- Find new quantum algorithms based on Hamiltonian simulation
- Use product formula error bounds to analyze classical algorithms (e.g., quantum Monte Carlo)

Quantum simulation as a theoretical tool

- Lieb-Robinson bounds
- Entanglement area laws
- Scrambling
- ...

Outlook: Applications

Develop applications of quantum simulation to physics/chemistry

- Quantum chemistry
- Materials/condensed matter
- Nuclear physics
- Particle physics

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
- Optimized implementations of near-term fault-tolerant simulations

Major goal: Describe concrete end-to-end applications of quantum simulation with compelling evidence for speedup

Further reading

- Lecture notes on quantum algorithms (part V): <https://www.cs.umd.edu/~amchilds/qa/>
- Lin Lin's lecture notes: <https://math.berkeley.edu/~linlin/qasc/>
- Simulation gate counts: [arXiv:1711.10980](https://arxiv.org/abs/1711.10980)
- Product formula error: [arXiv:1912.08854](https://arxiv.org/abs/1912.08854)
- Martyn-Rossi-Tan-Chuang survey on QSP: [arXiv:2105.02859](https://arxiv.org/abs/2105.02859)

Lectures and seminars

- John Preskill simulation lecture: <https://www.youtube.com/watch?v=t-qUR5kweCE>
- Nathan Wiebe survey talk: <https://www.youtube.com/watch?v=X4gegxlulho>
- Yuan Su on Trotter error: <https://www.youtube.com/watch?v=3AVnKJ3uCrU>
- Robin Kothari on LCU/QSP: <https://www.youtube.com/watch?v=mWg56DxtDy0>
- András Gilyén on QSVT: <https://www.youtube.com/watch?v=SMdLc36ysJE>