# Hamiltonian simulation with nearly optimal dependence on all parameters

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Joint work with Dominic Berry (Macquarie) and Robin Kothari (MIT),
building on previous work also with Richard Cleve (Waterloo) and Rolando Somma (Los Alamos)

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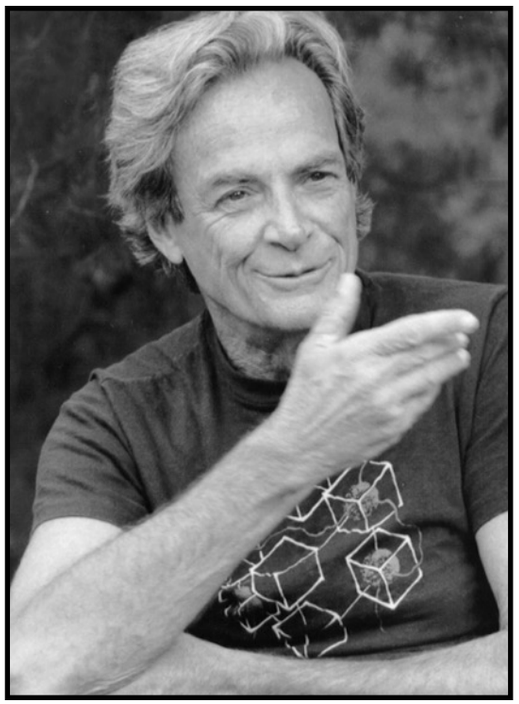


"... nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

Richard Feynman
*Simulating physics with computers* (1981)

# Why simulate quantum mechanics?

Computational chemistry/physics

- chemical reactions
- 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 $\epsilon$)

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]

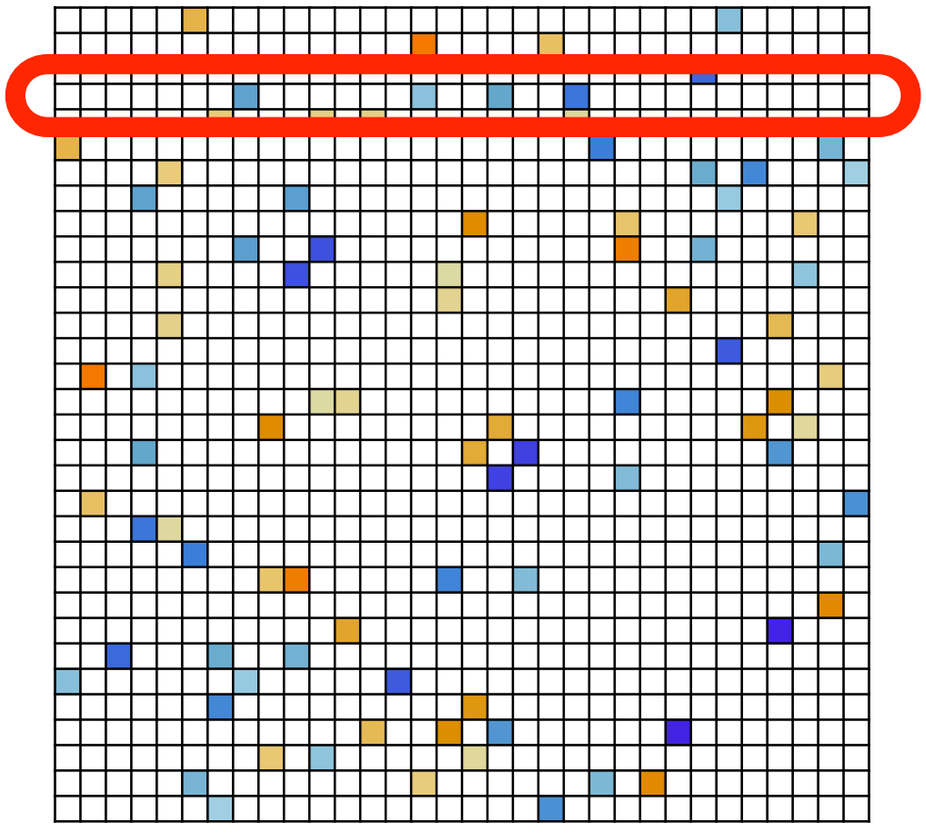
$H = \sum_{j=1}^{m} H_j$ where each $H_j$ acts on $k = O(1)$ qubits

## 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 $j$th nonzero entry and its value can be computed efficiently (or is given by a black box)

$H =$



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

# Previous simulation methods

## Product formulas

- Decompose Hamiltonian into a sum of terms that are easy to simulate
- Recombine the terms by alternating between them

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

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

$$\vdots$$

## Quantum walk

- Define an easy-to-implement unitary operation (a step of a quantum walk) whose spectrum is related to the Hamiltonian
- Use phase estimation to obtain information about the spectrum
- Introduce phases to give the desired evolution

# Complexity of previous simulation methods

Parameters: dimension $N$ sparsity $d$

evolution time $t$ allowed error $\epsilon$

[Lloyd 96]: $\mathrm{poly}(\log N)\,(\|H\|t)^2/\epsilon$ (for local Hamiltonians only)

[Aharonov, Ta-Shma 02]: $\mathrm{poly}(d, \log N)\,(\|H\|t)^{3/2}/\sqrt{\epsilon}$

[Childs 04]: $O\big((d^4 \log^4 N \|H\|t)^{1+\delta}/\epsilon^{\delta}\big)$ (for any $\delta > 0$)

[Berry, Ahokas, Cleve, Sanders 07]: $O\big((d^4 \log^* N \|H\|t)^{1+\delta}/\epsilon^{\delta}\big)$

[Childs, Kothari 11]: $O\big((d^3 \log^* N \|H\|t)^{1+\delta}/\epsilon^{\delta}\big)$

[Childs10; Berry, Childs 12]: $O(d\|H\|_{\max}t/\sqrt{\epsilon})$

**New result:** $O\big(\tau \frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\big)$ ~~$\tau := d^2\|H\|_{\max}t$~~ $\tau := d\|H\|_{\max}t$

# Improved simulation algorithms

We have 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

# 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:

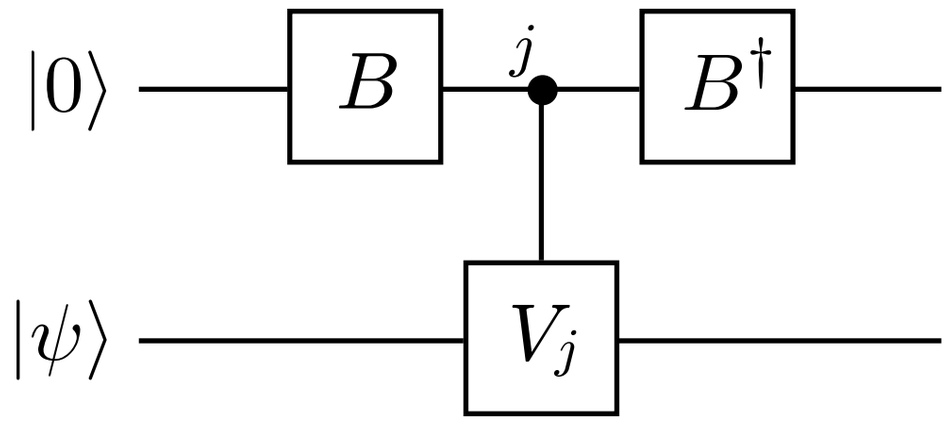
$$|0\rangle|\psi\rangle \mapsto \sin\theta|0\rangle U|\psi\rangle + \cos\theta|\Phi\rangle$$

- 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 $H_\ell$ 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

# Decomposing sparse Hamiltonians

To express $H$ as a linear combination of unitaries:

- Edge coloring: $H = \sum_{j=1}^{d^2} H_j$ where each $H_j$ is 1-sparse

  new trick: $H$ is bipartite wlog since it suffices to simulate $H \otimes \sigma_x$

  $d^2$-coloring: $\mathrm{color}(\ell, r) = (\mathrm{idx}(\ell, r), \mathrm{idx}(r, \ell))$

- Approximately decompose into terms with all nonzero entries equal

  Ex: $\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \\ 0 & 0 & 0 & 0 & 3 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$

- Remove zero blocks so that all terms are rescaled unitaries

  Ex: $\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

# 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 $\epsilon$

Higher-order formulas exist, but they only improve the power of $\epsilon$

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

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

# A discrete-time quantum walk for any $H$

Another way to simulate an $N \times N$ Hamiltonian $H$ is to implement a related discrete-time (Szegedy) quantum walk.

Expand space from $\mathbb{C}^N$ to $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$.

Walk operator is the product of two reflections:

- Swap: $S|j,k\rangle = |k,j\rangle$
- Reflect about $\mathrm{span}\{|\psi_1\rangle, \ldots, |\psi_N\rangle\}$, where

$$|\psi_j\rangle := |j\rangle \otimes \left( \frac{1}{\sqrt{\|H\|_1}} \sum_{k=1}^{N} \sqrt{H_{jk}^*}\, |k\rangle + \nu_j |N+1\rangle \right)$$

$$\|H\|_1 := \max_j \textstyle\sum_{k=1}^{N} |H_{jk}|$$

i.e., $2TT^\dagger - \mathbb{1}$ where $T|j\rangle = |\psi_j\rangle$

[Childs 10]

# Quantum walk simulation

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

Strategy: Use phase estimation to determine and correct the phase

Complexity: $O(\tau/\sqrt{\epsilon})$ $\quad \tau := d\|H\|_{\max} t$

[Childs 10], [Berry, Childs 12]

# Linear combination of quantum walk steps

Another approach: find coefficients so that

$$e^{-iH} \approx T^\dagger \sum_{k=-K}^{K} \beta_k U^k T$$

and implement this using the LCU Lemma

By a generating series for Bessel functions,

$$e^{-i\lambda t} = \sum_{k=-\infty}^{\infty} J_k(-t)\, e^{ik \arcsin \lambda}$$

Coefficients drop off rapidly for large $k$, so we can truncate the series

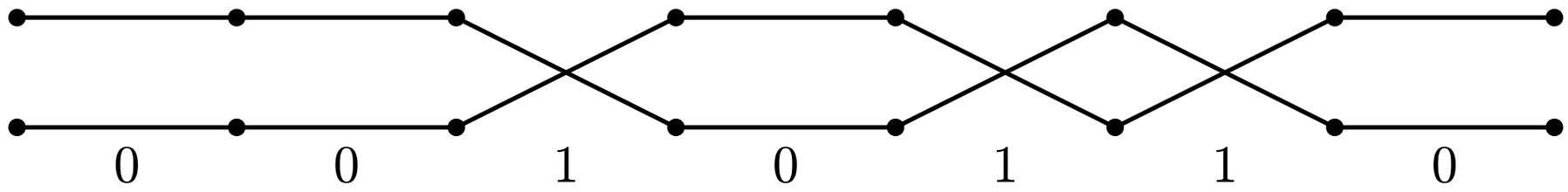
Query complexity of this approach: $O\left(\tau \frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right)$

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

# Lower bounds

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

- 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:** $\Omega(\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)})$

- 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 $\Theta(1/n!)$.

**New lower bound:** $\Omega(dt)$

- Replacing each edge with $K_{d,d}$ effectively boosts Hamiltonian by $d$.

# Query complexity of sparse Hamiltonian simulation

Quantum walk + phase estimation [BC 10]: $O\left(\frac{\tau}{\sqrt{\epsilon}}\right)$ $\tau := d\|H\|_{\max}t$

Quantum walk + LCU [BCK 15]: $O\left(\tau\frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right)$

or for $\alpha \in (0,1]$: $O\left(\tau^{1+\alpha/2} + \tau^{1-\alpha/2}\log(1/\epsilon)\right)$

Lower bound: $\Omega\left(\tau + \frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$

Notes:

- Gate complexity is only slightly larger than query complexity
- These techniques assume time-independent Hamiltonians (otherwise, use fractional queries/LCU on Dyson series [BCCKS 14])

# Outlook

## Improved simulation algorithms

- Optimal tradeoff for sparse Hamiltonian simulation
- Faster algorithms for structured problems
- Simulating open quantum systems

## Applications to simulating physics

- What is the cost in practice for simulating molecular systems?
- How do recent algorithms compare to naive methods?

## New quantum algorithms

- Improved algorithms for linear systems
- New applications of linear systems
- Other quantum algorithms from quantum simulation