Simulating Hamiltonian dynamics

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arXiv:0810.0312 (Commun. Math. Phys. 294, 581-603, 2010)
arXiv:0908.4398 (with Robin Kothari, IQC)
arXiv:0910.4157 (with Dominic Berry, IQC)
arXiv:1003.3683 (with Robin Kothari, IQC)

Hamiltonian dynamics

Schrödinger:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = H|\psi\rangle$$

When H is time-independent:

$$|\psi(t)\rangle = e^{-\mathrm{i}Ht}|\psi(0)\rangle$$

Hamiltonian simulation

Problem: Given* a Hamiltonian H, find a quantum circuit that performs the unitary operation $e^{-\mathrm{i}Ht}$ (on an unknown quantum state) with error at most ϵ (say, in trace distance).

* For an efficient simulation, H should be concisely specified.

Applications:

- Simulating physics
- Implementing continuous-time quantum algorithms (quantum walk, adiabatic optimization, ...)

Outline

1. Previous results
2. Star decompositions
3. Hamiltonians and discrete-time quantum walk
4. Faster simulation of sparse Hamiltonians
5. Limitations on simulating non-sparse Hamiltonians
6. Black-box simulation of non-sparse Hamiltonians
7. Summary and open questions

Local and sparse Hamiltonians

Local Hamiltonians [Lloyd 96]

$H = \sum_j H_j$ where each H_j acts on $O(1)$ qubits

Sparse Hamiltonians [Aharonov, Ta-Shma 03]

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

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)

Simulating a sum of terms

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

Combine individual simulations with Lie-Trotter-Suzuki formulae:

$$\left(e^{-\mathrm{i}At/n} e^{-\mathrm{i}Bt/n}\right)^n = e^{-\mathrm{i}(A+B)t} + O(t^2/n)$$

$$\left(e^{-\mathrm{i}At/2n} e^{-\mathrm{i}Bt/n} e^{-\mathrm{i}At/2n}\right)^n = e^{-\mathrm{i}(A+B)t} + O(t^3/n^2)$$

$$\vdots$$

Systematic expansions to arbitrary order are known [Suzuki 92]

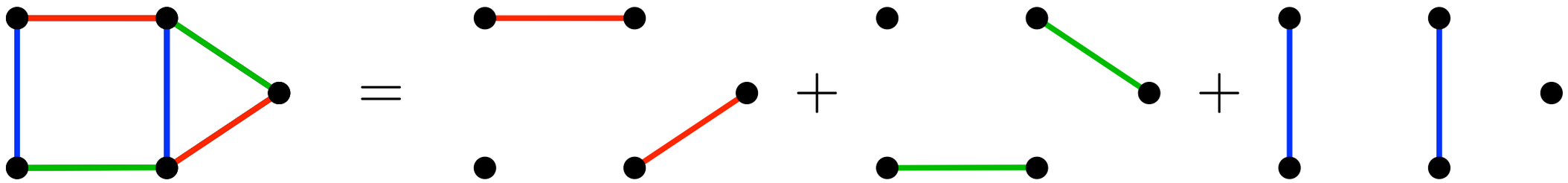
Using the kth order expansion, the number of exponentials required for an approximation with error at most ϵ is at most

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

[Berry, Ahokas, Cleve, Sanders 07]

Sparse Hamiltonians and coloring

Strategy [AMC, Cleve, Deotto, Farhi, Gutmann, Spielman 03; Aharonov, Ta-Shma 03]: 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 [Linial 87], so this gives efficient simulations.

(Efficient means $\mathrm{poly}(\|Ht\|, d, \log N, 1/\epsilon)$.)

Simulating sparse Hamiltonians

Previous best simulation [Berry, Ahokas, Cleve, Sanders 07]:

H is $N \times N$, with at most d nonzero entries per row
simulate for time t with error at most ϵ
kth order Suzuki expansion

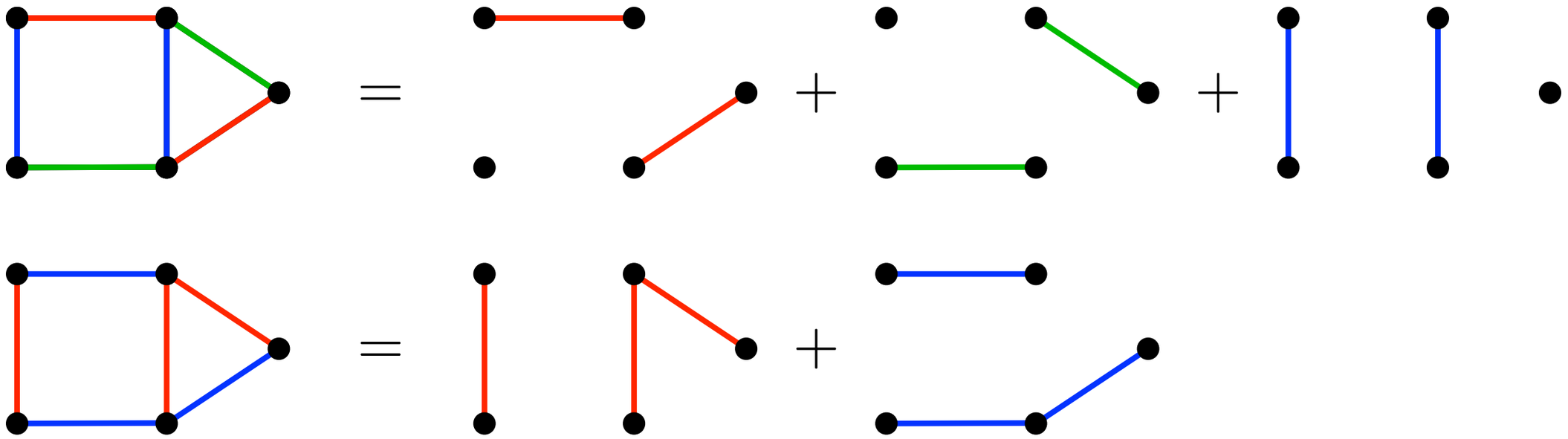
$$O\left(5^{2k} d^4 (\log^* N) \|Ht\| \left(\frac{d^2 \|Ht\|}{\epsilon}\right)^{1/2k}\right) \text{ queries}$$

Can we improve on this?

- Faster simulation of sparse Hamiltonians
- Ability to handle non-sparse Hamiltonians

With k large, this is nearly linear in t. Sub-linear simulation is impossible ("no fast-forwarding theorem" [BACS 07]).

Star decompositions



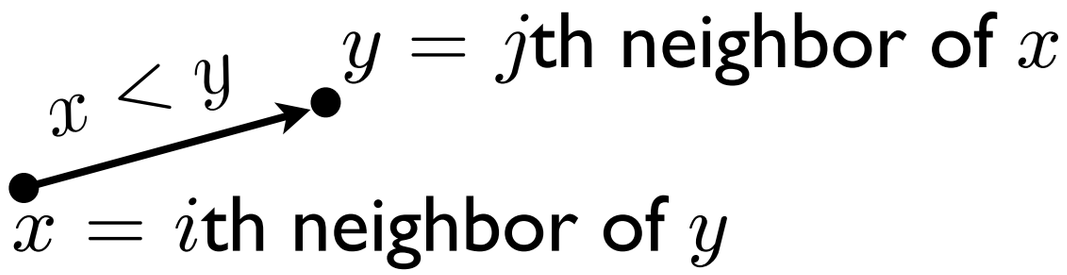
Strategy: Color the edges so that each color forms a "galaxy" (every connected component is a star graph). Simulate each galaxy by brute force and recombine.

Tradeoff vs. edge coloring:
- Decomposition has fewer terms
- Each term is harder to simulate (2nd neighbors)

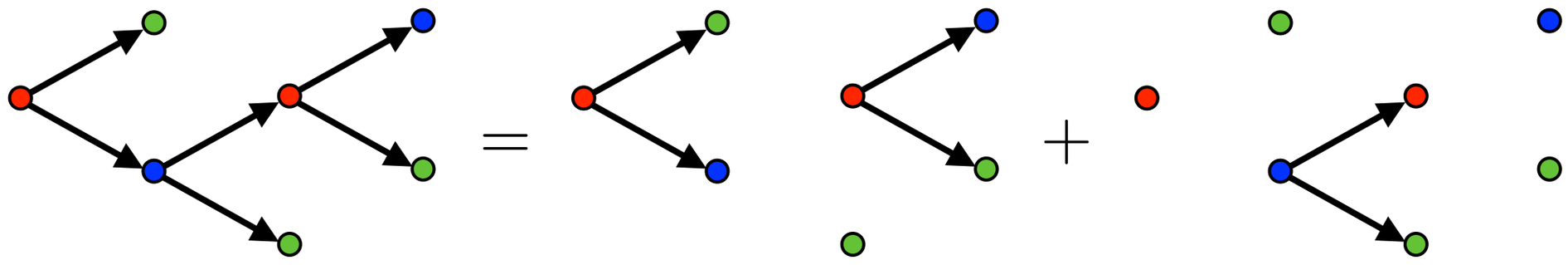
[AMC, Kothari arXiv:1003.3683]

Locally constructing a star decomposition

Color the edges using black box indices, such that edges of each color form a forest [Paneconesi, Rizzi 01]



Color the vertices of each forest to break them into galaxies; with "deterministic coin tossing" [Cole, Vishkin 86; Goldberg, Plotkin, Shannon 88] the number of colors per forest is at most 6



Total query complexity: $O\left(5^{2k} d^2 (d + \log^* N) \|Ht\| \left(\frac{d\|Ht\|}{\epsilon}\right)^{1/2k}\right)$

[AMC, Kothari arXiv:1003.3683]

Hamiltonian simulation by quantum walk

Another way to simulate a Hamiltonian H is to implement a related discrete-time (Szegedy) quantum walk.

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

Alternately swap the two registers and reflect about $\mathrm{span}\{|\psi_1\rangle, \ldots, |\psi_N\rangle\}$, where

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

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

Using phase estimation, $O(\|Ht\|_1/\epsilon)$ steps of this walk suffice to simulate H for time t with error at most ϵ (in trace distance).

[AMC arXiv:0810.0312, Commun. Math. Phys. 294, 581-603, 2010]

Faster simulation of sparse Hamiltonians

Perform quantum walk steps by brute force (query all d neighbors):

$$O(d\|Ht\|_1/\epsilon) \leq O(d^{3/2}\|Ht\|/\epsilon)$$

This is exactly linear in t; also scales better in d, but worse in ϵ.

Even better alternative: using only two queries, prepare

$$|\psi'_j\rangle := |j\rangle \otimes \frac{1}{\sqrt{d}} \sum_{k=1}^{N} \left(\sqrt{\frac{H^*_{jk}}{\max(H)}} |k,0\rangle + \sqrt{1 - \frac{|H_{jk}|}{\max(H)}} |k,1\rangle \right)$$

Overall simulation:

$$O\left(\frac{\|Ht\|}{\sqrt{\epsilon}} + d\max(Ht)\right) \leq O\left(\|Ht\|(\tfrac{1}{\sqrt{\epsilon}} + d)\right)$$

[AMC, Berry arXiv:0910.4157]

Non-sparse Hamiltonians: $\|H\|$ vs. $\|H\|_1$

Number of quantum walk steps to simulate H: $O(\|Ht\|_1/\epsilon)$

If H is d-sparse, $\|H\| \leq \|H\|_1 \leq \sqrt{d}\|H\|$.

In general, if H is $N \times N$, the best possible bounds are

$$\|H\| \leq \|H\|_1 \leq \sqrt{N}\|H\|$$

so this simulation can be exponentially worse than $\mathrm{poly}(\|Ht\|)$

Can we do better?

Potential applications:
- approximately computing exponential sums
- breaking pseudorandom generators from strongly regular graphs

[AMC arXiv:0810.0312, Commun. Math. Phys. 294, 581-603, 2010]

Limitation on simulating non-sparse H

Problem: Given a random $s \in \{-1, +1\}^M$ with $\sum_i s_i = \pm\sqrt{M \log M}$, determine which is the case.

By an adversary lower bound, $\Omega(\sqrt{M/\log M})$ quantum queries are needed to solve this problem.

We can solve the problem by simulating a symmetric circulant matrix H with first row $0, s_1, \ldots, s_M, s_M, \ldots, s_1$ for time $O(1/\sqrt{M \log M})$.

Since $\|H\|$ is tightly concentrated around $O(\sqrt{M \log M})$, a simulation in time $\mathrm{poly}(\|Ht\|)$ would violate the above lower bound.

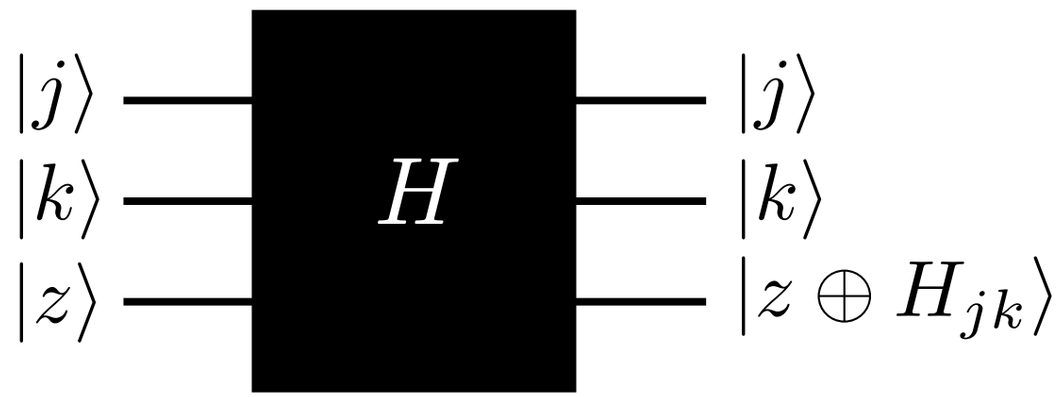
(Note $\|H\|_1 = 2M$.)

[AMC, Kothari arXiv:0908.4398v2]

Black-box Hamiltonians

Generic non-sparse Hamiltonians are hard to simulate.

Black-box description of a non-sparse Hamiltonian:

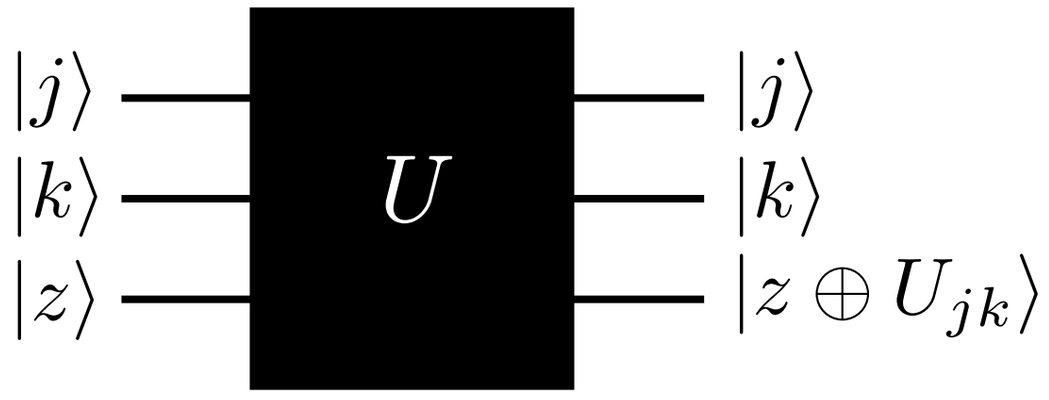


Various simulations are possible, with tradeoffs in the scaling with respect to N and different measures of the size of H.

[AMC, Berry arXiv:0910.4157]

Black-box unitaries

Related problem: the matrix elements of a unitary transformation U are provided by a black box; we want to perform U.



What we know: To implement U with bounded error,

$\Omega(\sqrt{N})$ queries are necessary

$O(N^{2/3}(\log\log N)^{4/3})$ queries are sufficient

[AMC, Berry arXiv:0910.4157]

Summary

Sparse Hamiltonians: best known simulations have query complexity

$$O\left(5^{2k}d^2(d+\log^* N)\|Ht\|\left(\frac{d\|Ht\|}{\epsilon}\right)^{1/2k}\right) \text{ or } O\left(\|Ht\|(\frac{1}{\sqrt{\epsilon}}+d)\right)$$

star decompositions — discrete-time quantum walk

Non-sparse Hamiltonians:

- can simulate in $O(\|Ht\|_1/\epsilon)$ steps of a discrete-time quantum walk
- generic simulations in $\mathrm{poly}(\|Ht\|)$ steps are impossible

Open questions

- Tradeoff of error scaling vs. other scaling
- Optimality of error scaling
- Simulating time-dependent Hamiltonians [Wiebe, Berry, Høyer, Sanders 10]
- Improved simulation of specific non-sparse Hamiltonians
- Query complexity of black-box unitaries