Efficient Quantum Algorithms for Simulating Sparse Hamiltonians

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Sparse Hamiltonians

Given: Hamiltonian H (that's d-sparse), initial state $|\psi\rangle$, time t, accuracy ε

Goal: construct the state $e^{-iHt}|\psi\rangle$ within precision ε

$$H = \begin{bmatrix} 0 & 0 & 0 & \alpha_{14} & 0 & \alpha_{16} & 0 & \alpha_{18} \\ 0 & \alpha_{22} & 0 & 0 & 0 & 0 & \alpha_{27} & \alpha_{28} \\ 0 & 0 & \alpha_{33} & 0 & \alpha_{35} & \alpha_{36} & 0 & 0 \\ \alpha_{41} & 0 & 0 & 0 & \alpha_{45} & 0 & \alpha_{47} & 0 \\ 0 & 0 & \alpha_{53} & \alpha_{54} & 0 & 0 & \alpha_{57} & 0 \\ \alpha_{61} & 0 & \alpha_{63} & 0 & 0 & 0 & 0 & \alpha_{68} \\ 0 & \alpha_{72} & 0 & \alpha_{74} & \alpha_{75} & 0 & 0 & 0 \\ \alpha_{81} & \alpha_{82} & 0 & 0 & 0 & \alpha_{86} & 0 & 0 \end{bmatrix}$$

Can specify $|\psi\rangle$ by an efficient quantum circuit that generates it

Can add a final measurement (specified as a quantum circuit)

With these modifications, inputs and outputs become ***classical***

Specifications of *H*

Decomposition into a sum of local Hamiltonians

$H = H_1 + H_2 + \cdots + H_m$, where each H_j is local, or otherwise of a form that is easily simulatable *a priori*

In this setting, operation $e^{-iH_j s}$, for any s, can be considered as a basic operation

Sparse specification [Aharonov, Ta-Shma ’03]

Mechanism for determining local relationships among states

Roughly speaking, for every basis state $|x\rangle$, the infinitesmal transitions can be determined

More about this later ...

Trotter formula I

$$e^{-i(H_1+H_2+\cdots+H_m)\delta}$$

$$=\left(e^{-iH_1\delta}e^{-iH_2\delta}\cdots e^{-iH_m\delta}\right)+O\left(\delta^2\right)$$

(δ small)

$$e^{-i(H_1+H_2+\cdots+H_m)t}$$

$$=\left(e^{-iH_1(t/r)}e^{-iH_2(t/r)}\cdots e^{-iH_m(t/r)}\right)^r+O\left(r(t/r)^2\right)$$

$$=\left(e^{-iH_1(t/r)}e^{-iH_2(t/r)}\cdots e^{-iH_m(t/r)}\right)^r+O\left(t^2/r\right)$$

Sufficient to set $r \geq t^2/\varepsilon$, which leads to a sequence of $O\left((m/\varepsilon)t^2\right)$ basic operations (of the form $e^{-iH_j s}$)

Trotter formula II

$$e^{-i(H_1+H_2+\cdots+H_m)\delta}$$

$$= \left(e^{-iH_1\delta/2}\cdots e^{-iH_m\delta/2}\right)\left(e^{-iH_m\delta/2}\cdots e^{-iH_1\delta/2}\right)+O\left(\delta^3\right)$$

$$e^{-i(H_1+H_2+\cdots+H_m)t}$$

$$= \left(\left(e^{-iH_1t/2r}\cdots e^{-iH_mt/2r}\right)\left(e^{-iH_mt/2r}\cdots e^{-iH_1t/2r}\right)\right)^r + O\left(r(t/r)^3\right)$$

$$= \left(\left(e^{-iH_1t/2r}\cdots e^{-iH_mt/2r}\right)\left(e^{-iH_mt/2r}\cdots e^{-iH_1t/2r}\right)\right)^r + O\left(t^3/r^2\right)$$

Sufficient to set $r^2 \geq t^3/\varepsilon$, which leads to a sequence of $O\left(\left(2m/\sqrt{\varepsilon}\right)t^{3/2}\right)$ basic operations (of the form e^{-iH_js})

Suzuki formula

$$e^{-i(H_1+H_2+\cdots+H_m)\delta} =$$

($\lambda_1, \ldots, \lambda_N$ carefully chosen)

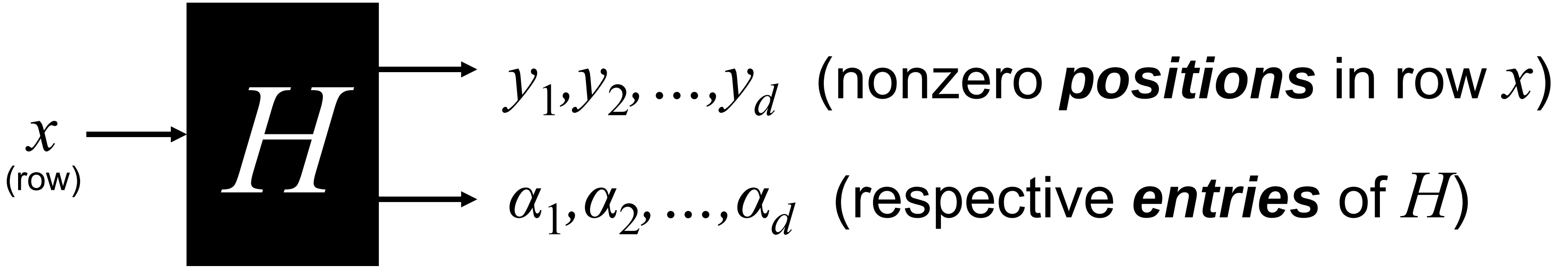
$$\left.\begin{aligned} &\left(e^{-iH_1\delta\lambda_1}\cdots e^{-iH_m\delta\lambda_1}\right)\left(e^{-iH_m\delta\lambda_1}\cdots e^{-iH_1\delta\lambda_1}\right)\\ \times&\left(e^{-iH_1\delta\lambda_2}\cdots e^{-iH_m\delta\lambda_2}\right)\left(e^{-iH_m\delta\lambda_2}\cdots e^{-iH_1\delta\lambda_2}\right)\\ &\ \vdots\\ \times&\left(e^{-iH_1\delta\lambda_N}\cdots e^{-iH_m\delta\lambda_N}\right)\left(e^{-iH_m\delta\lambda_N}\cdots e^{-iH_1\delta\lambda_N}\right)+\overset{\boxed{(5^k m\delta)^{2k+1}}\ \downarrow}{O\left(\delta^{2k+1}\right)} \end{aligned}\right\} 5^{k-1}\text{ clusters}$$

Slicing into intervals of length *t*/*r* and repeating *r* times yields an accumulated error of $O((5^k mt)^{2k+1}/r^{2k})$

This leads to $O\left(\frac{5^{2k}m}{\varepsilon^{1/2k}}\,(mt)^{1+1/2k}\right)$ basic operations

Generic black-box sparse representation

Essentially, we're given a mechanism that, for any given column of H, computes the positions and values of all non-zero entries

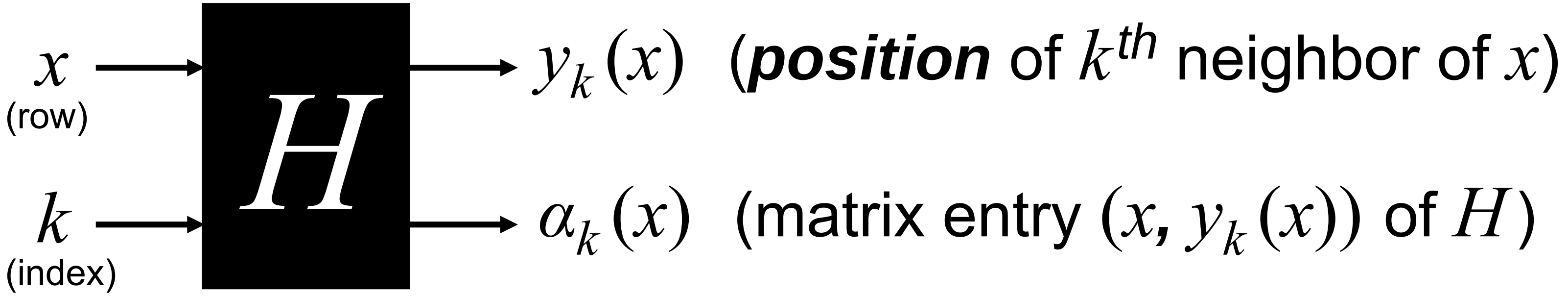


x (row) $\rightarrow$ H

$\rightarrow y_1, y_2, \ldots, y_d$ (nonzero ***positions*** in row x)

$\rightarrow \alpha_1, \alpha_2, \ldots, \alpha_d$ (respective ***entries*** of H)

Alternatively:



x (row) $\rightarrow$ H

k (index) $\rightarrow$ H

$\rightarrow y_k(x)$ (***position*** of k^{th} neighbor of x)

$\rightarrow \alpha_k(x)$ (matrix entry $(x, y_k(x))$ of H)

[Aharonov, Ta-Shma '03]

Simulations of sparse Hamiltonians

Let H be a d-sparse Hamiltonian (assume $\|H\| = O(1)$) acting on n qubits

Simulation costs for e^{-iHt} within precision ε:

- ***polynomial*** with respect to $t, n, d,\ 1/\varepsilon$ [Aharonov & Ta-Shma ’03]
- growth rate is $t^{3/2}$ and n^9 (later improved to n^2 [Childs ’03])

Question: how efficient can the scaling of the simulation be?

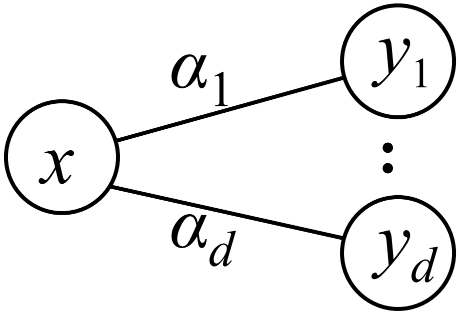
We will show: $O\left(\log^*(n)\, 5^{2k} d^{4+1/2k}\, t^{1+1/2k} / \varepsilon^{1/2k}\right)$ for all k

Smaller than $O(t^{1+\delta})$ for all $\delta > 0$ (optimizing setting of k)

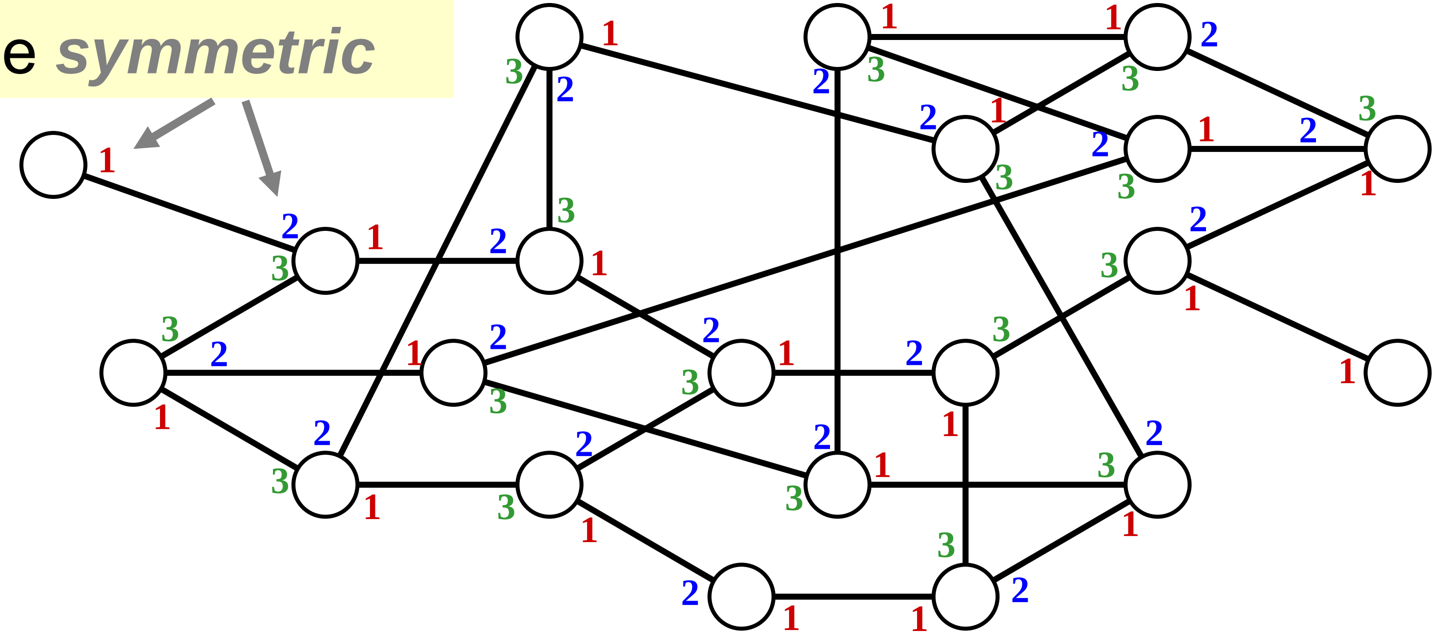
... but larger than $O\left(t\,(\log t)^q\right)$ for all $q > 0$

Graph associated with *H*

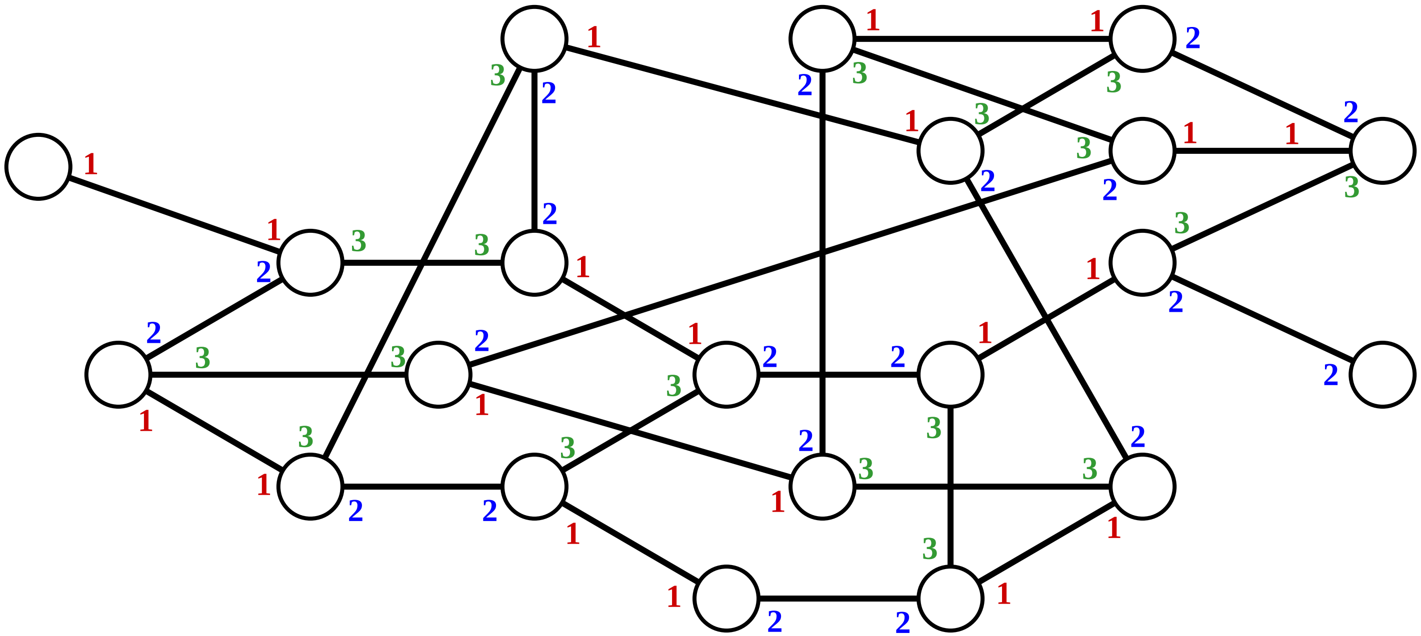
Connect x to $y_k(x)$ with an edge of weight $\alpha_k(x)$



Note: the label structure may not be *symmetric*

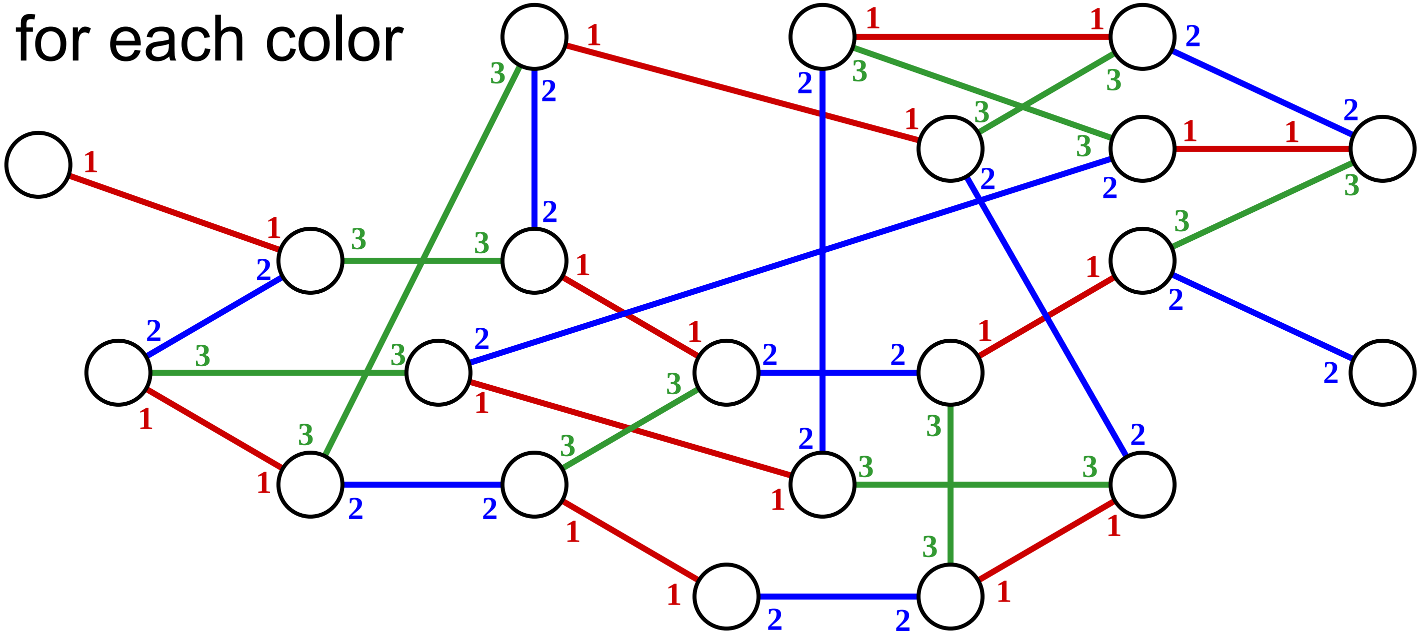


Symmetrically labeled graphs



Symmetrically labeled graphs

Matching for each color



Symmetrically labeled Hamiltonians can be decomposed into sums of simple Hamiltonians, $H_1 + H_2 + \cdots + H_m$, one for each "color", as follows ...

Simulation in symmetric case

[Childs, C, Deotto, Farhi, Gutmann, Spielman ’03]

Fact: for any Hermitian H and unitary U, $e^{-iUHU^{-1}s} = Ue^{-iHs}U^{-1}$

For each fixed label k (color), consider the mapping:

$$\begin{array}{rl}
|x\rangle|0\rangle|0\rangle \mapsto |x\rangle|y_k(x)\rangle|\alpha_k(x)\rangle & \text{query (unitary)} \\
\begin{array}{r}\mapsto \alpha_k(x)|x\rangle|y_k(x)\rangle|\alpha_k(x)\rangle \\ \mapsto \alpha_k(x)|y_k(x)\rangle|x\rangle|\alpha_k(x)\rangle\end{array} & \left.\begin{array}{l}\text{amplitude in front}\\ \text{swap}\end{array}\right\} H \\
\mapsto \alpha_k(x)|y_k(x)\rangle|0\rangle|0\rangle & \text{query (its own inverse)}
\end{array}$$

This mapping corresponds to the matching Hamiltonian H_k

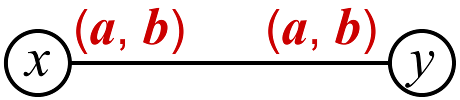
Note: $H_k = UHU^{-1}$, and e^{-iHs} is straightforward to compute

Therefore: each $e^{-iH_k s}$ is straightforward to compute

Non-symmetric case

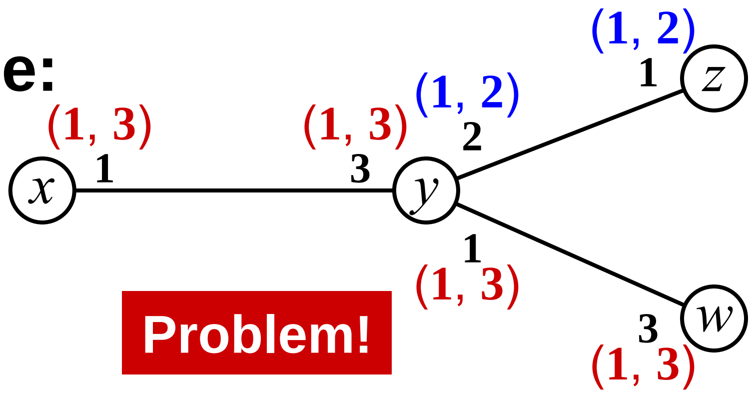
Given a non-symmetric Hamiltonian, it is possible to modify its labeling so as to be symmetric (with an overhead cost)

with $x < y$



We now have d^2 labels instead of d labels, but a ***symmetric*** labeling

Example:

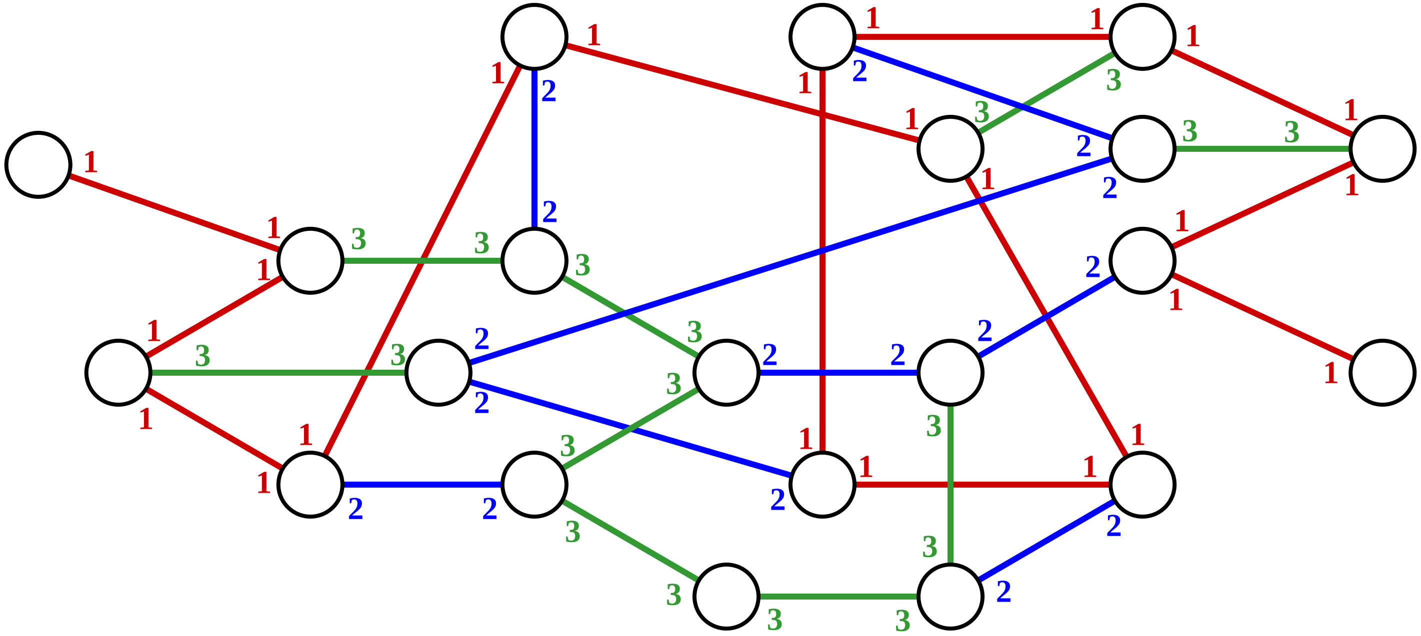


with $z < y$

with $y < w$

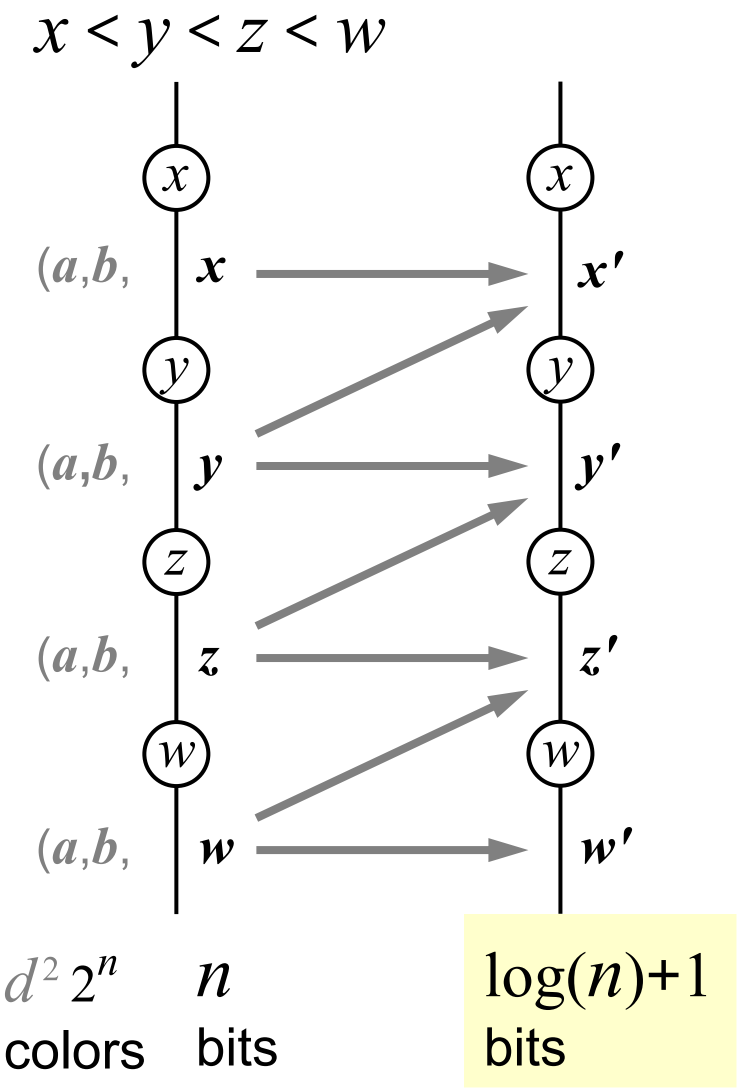
Problem!

Graph with monochromatic paths



To break up the paths, we increase the number of colors a bit ...

Breaking up the paths I



$d^2 2^n$ colors

n bits

$\log(n)+1$ bits

"Deterministic coin-tossing"
[Cole & Vishkin '86]

$y' \leftarrow (i, y_i)$, where $i = \min\{j : y_j \neq z_j\}$

010

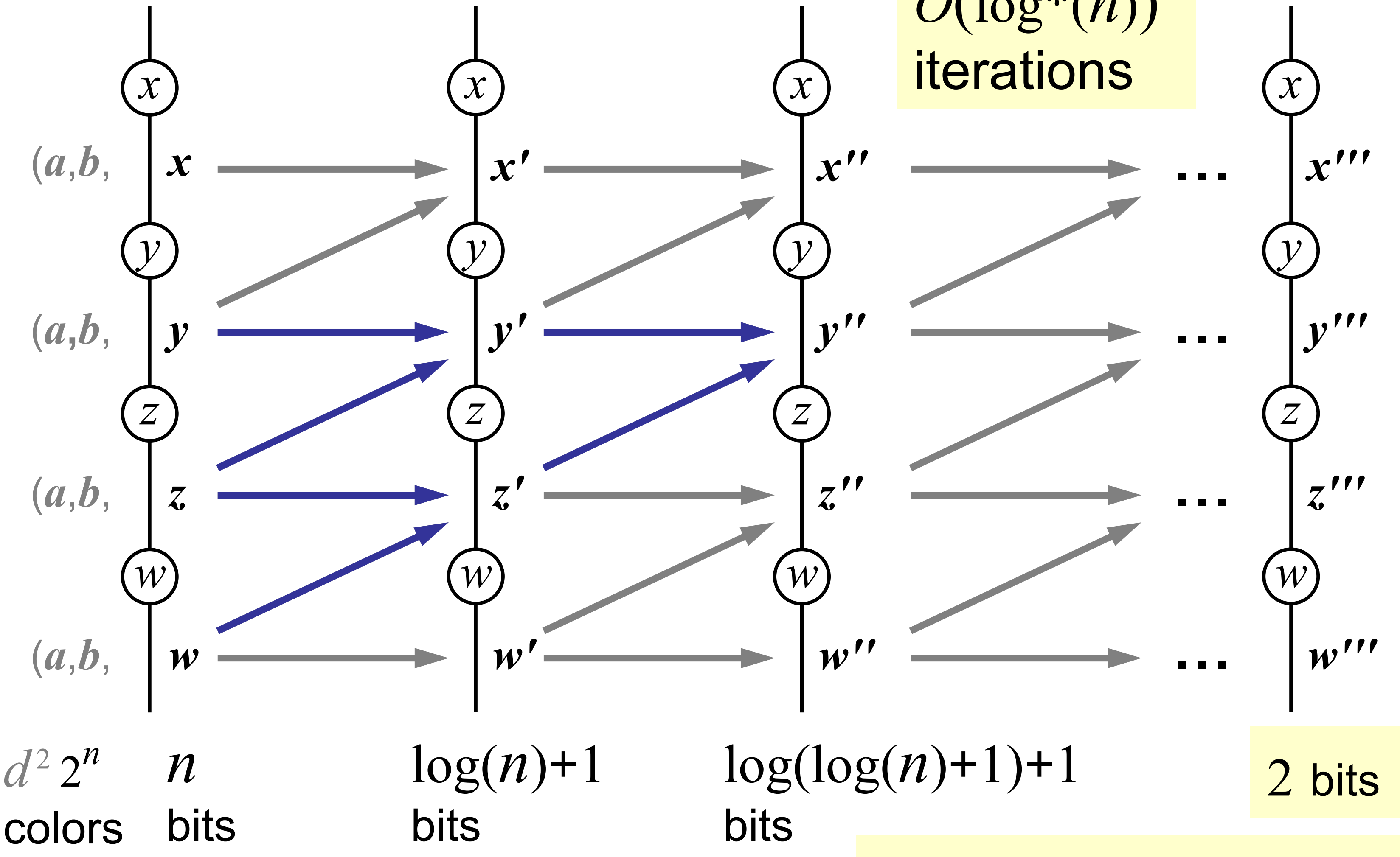
Example: y = 01100101

z = 01001101

Then y' = (010,1)

Note: still a valid coloring!
$x' \neq y'$ & $y' \neq z'$ & $z' \neq w'$

Breaking up the paths II



$O(\log^*(n))$ iterations

2 bits

Just 5 iterations for $n \le 10^{10^{37}}$

Cost of making labels symmetric

Summary:

Starting with a given Hamiltonian specification of H with d labels, we obtain a new specification of H with $3d^2$ ***symmetric*** labels, where each query in the new specification costs $O(\log^* n)$ queries to the original specification

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This completes the

$$O\left(\log^*(n)\, 5^{2k} d^{4+1/2k}\, t^{1+1/2k} / \varepsilon^{1/2k}\right)$$

algorithm for simulating sparse Hamiltonians

Lower bound

Theorem: given a general black-box for H acting on n qubits, the number of queries required to produce an approximation of the state $e^{-iHt}|00...0\rangle$ is $\Omega(t)$ (for $t \leq 2^n$)

Proof idea: by a reduction from existing lower bounds on the query complexity of the parity function $X_1 \oplus X_2 \oplus \cdots \oplus X_N$
[Beals, Buhrman, C, Mosca, de Wolf ’98][Farhi, Goldstone, Gutmann, Sipser ’98]

THE END