1 Efficient simulation of commutators

H_1, H_2 are Hamiltonians of two n-qubit systems.

(a) Prove $e^{-[H_1,H_2]t} = \lim_{m\to\infty} \left(e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}}\right)^m$

Proof.

$$A(m) := \left\| \left(e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}}\right)^m - e^{-[H_1,H_2]t} \right\|$$

$$= \left\| \left(e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}}\right)^m - \left(e^{\frac{-H_1H_2t + H_2H_1t}{m}}\right)^m \right\|$$

$$\leq m \left\| e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}} - e^{-H_1H_2t/m + H_2H_1t/m} \right\|$$

$$\cdot \max\left\{ \left\| e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}} \right\|, \left\| e^{-H_1H_2t/m + H_2H_1t/m} \right\| \right\}^{m-1}$$

$e^{\pm iH_1\sqrt{t/m}}$, $e^{\pm iH_2\sqrt{t/m}}$ are unitaries

$$\Rightarrow \left\| e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}} \right\| \leq 1$$

$$\left\| e^{-H_1H_2t/m + H_2H_1t/m} \right\| \leq e^{\|-H_1H_2t/m + H_2H_1t/m\|} = e^{\frac{t}{m}\|-H_1H_2 + H_2H_1\|}$$

$$e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}} - e^{-H_1H_2t/m + H_2H_1t/m}$$

$$= \left(I - iH_1\sqrt{t/m} - \tfrac{1}{2}H_1^2 t/m + O(\|H_1\|^4 t^2/m^2)\right)\left(I - iH_2\sqrt{t/m} - \tfrac{1}{2}H_2^2 t/m + O(\|H_2\|^4 t^2/m^2)\right)$$
$$\left(I + iH_1\sqrt{t/m} - \tfrac{1}{2}H_1^2 t/m + O(\|H_1\|^4 t^2/m^2)\right)\left(I + iH_2\sqrt{t/m} - \tfrac{1}{2}H_2^2 t/m + O(\|H_2\|^4 t^2/m^2)\right)$$
$$- \left(I - H_1H_2t/m + H_2H_1t/m + O(\|H_1H_2 - H_2H_1\|^2 t^2/m^2)\right)$$

$$= I - I - iH_1\sqrt{t/m} - iH_2\sqrt{t/m} + iH_1\sqrt{t/m} + iH_2\sqrt{t/m} - \tfrac{1}{2}H_1^2 t/m - \tfrac{1}{2}H_2^2 t/m$$
$$- \tfrac{1}{2}H_1^2 t/m - \tfrac{1}{2}H_2^2 t/m - H_1H_2 t/m + H_1^2 t/m + H_1H_2 t/m + H_2H_1 t/m + H_2^2 t/m$$
$$- H_1H_2 t/m + H_1H_2 t/m - H_2H_1 t/m + O(\max\{\|H_1H_2 - H_2H_1\|^2, \|H_1\|^4, \|H_2\|^4\} t^2/m^2)$$

$$= O(\max\{\|H_1H_2 - H_2H_1\|^2, \|H_1\|^4, \|H_2\|^4\} t^2/m^2)$$

We have $A(m) \leq e^{\frac{t}{m}\|H_1H_2 - H_2H_1\|}\, O(\max\{\|H_1H_2 - H_2H_1\|^2, \|H_1\|^4, \|H_2\|^4\} t^2/m)$

Let $m \to \infty$, we are done. #

(b) H_1, H_2 can be efficiently simulated, then $i[H_1, H_2]$ is Hermitian and can be efficiently simulated.

Proof. $(i[H_1, H_2])^\dagger = (iH_1H_2 - iH_2H_1)^\dagger = -iH_1H_2 + iH_2H_1 = i[H_1, H_2]$

So $i[H_1, H_2]$ is Hermitian

We also have $A(m) = \| e^{-[H_1, H_2]t} - (e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}})^m \|$

$\leq e^{\frac{t}{m}\|H_1H_2 - H_2H_1\|} O(\max\{\|H_1\|^4, \|H_2\|^4, \|H_1H_2 - H_2H_1\|^2\} \frac{t^2}{m})$

To have $A(m) \leq \varepsilon$, it sufficies to let

$m = O(\frac{1}{\varepsilon} t^2 \max\{\|H_1\|^4, \|H_2\|^4, \|H_1\|^2\|H_2\|^2\}) + O(t\|H_1H_2 - H_2H_1\| \frac{1}{\log 2})$

And each $e^{-iH_1\sqrt{t/m}} e^{-iH_2\sqrt{t/m}} e^{iH_1\sqrt{t/m}} e^{iH_2\sqrt{t/m}}$ can be i plemented in $\mathrm{poly}(n, t, \frac{1}{\varepsilon})$

As $\|H_1\| = \mathrm{poly}(n)$, $\|H_2\| = \mathrm{poly}(n)$, $m = \mathrm{poly}(n, t, \frac{1}{\varepsilon})$

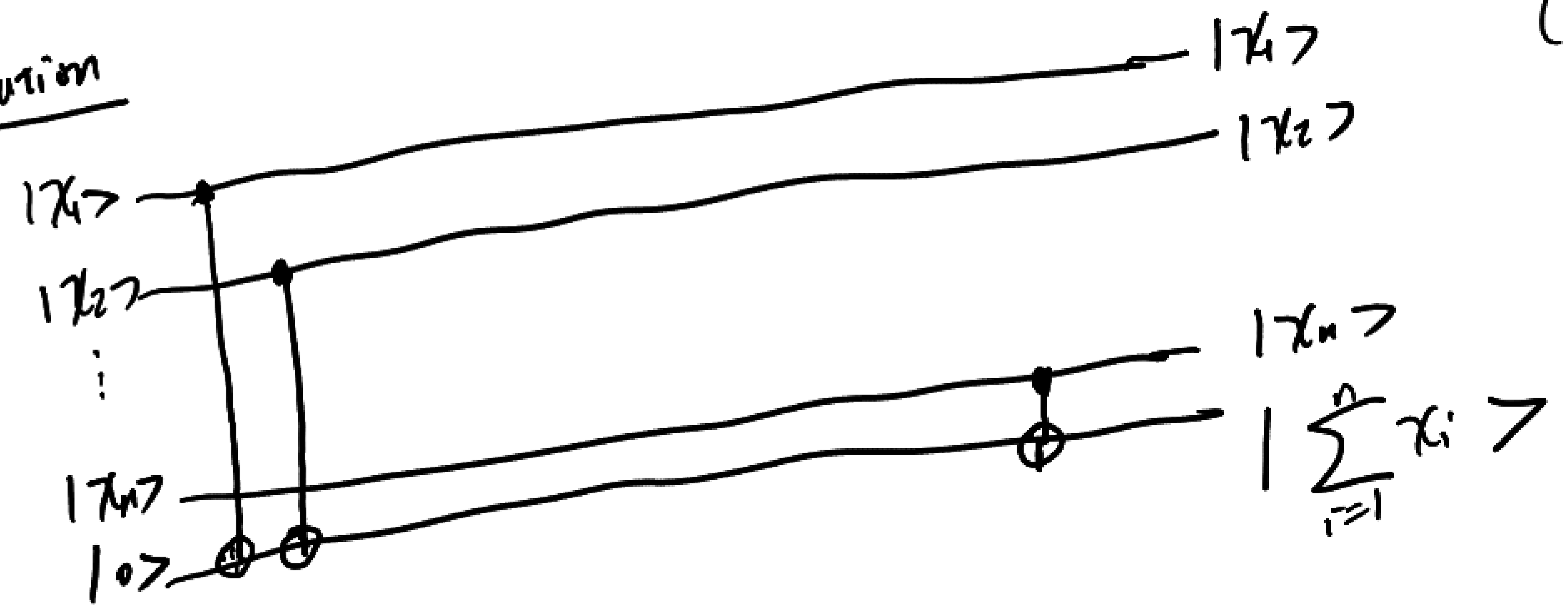
So total cost is $\mathrm{poly}(n, t, \frac{1}{\varepsilon})$ to achieve error $\leq \varepsilon$. #

2 Simulation of Pauli Hamiltonians

(a) Design circuit for $|x\rangle|0\rangle \rightarrow |x\rangle|\sum_{i=1}^{n} x_i \bmod 2\rangle$, $\forall x \in \{0,1\}^n$ with $O(n)$ 1-qubit and 2-qubit gates

(where $\oplus$ is CNOT gate)

Solution



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(b) $P = Z \otimes \cdots \otimes Z$ what is $P|x\rangle$ where $|x\rangle$ is a basis?

Solution.

$$P|x_1 \cdots x_n\rangle = Z|x_1\rangle \otimes \cdots \otimes Z|x_n\rangle = (-1)^{\sum_{i=1}^{n} x_i}|x_1 \cdots x_n\rangle$$

where $x_i = 0$ or 1, because $\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$. #

(c) $U = e^{-iPt}$ what is $U|x\rangle$ where $|x\rangle$ is a basis?

Solution.

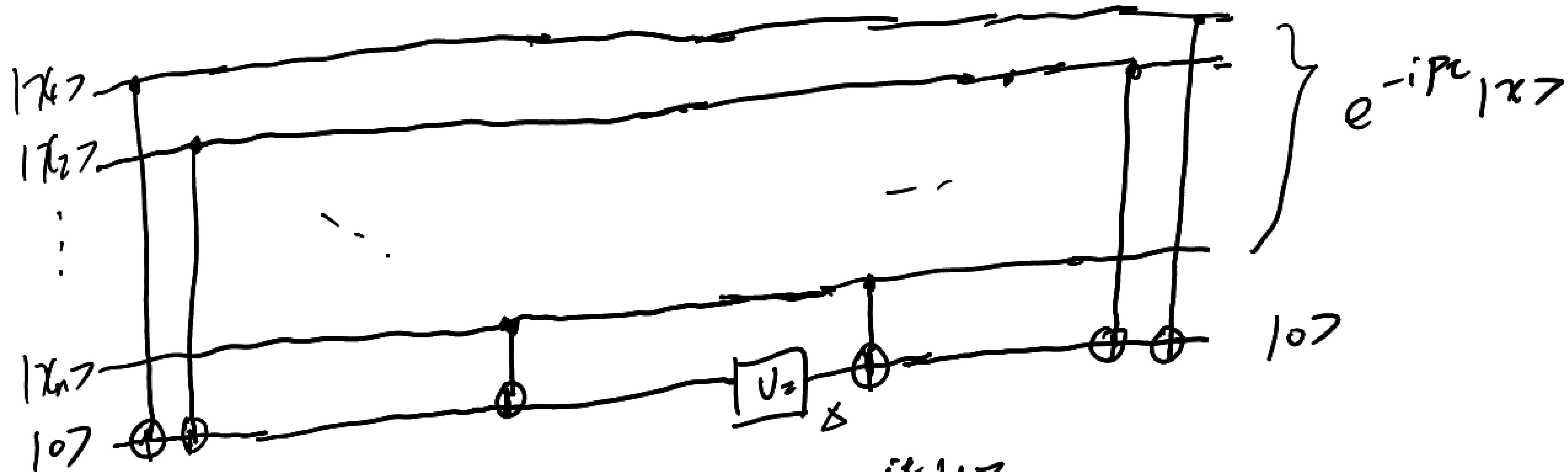
$$U|x_1 \cdots x_n\rangle = e^{-iPt}|x_1 \cdots x_n\rangle = \sum_{k=0}^{\infty} \frac{(-i)^k t^k}{k!} P^k |x_1 \cdots x_n\rangle$$

$$= \sum_{k=0}^{\infty} \frac{(-i)^k t^k}{k!} (-1)^{k \sum_{i=1}^{n} x_i} |x_1 \cdots x_n\rangle = \sum_{k=0}^{\infty} \frac{(-it(-1)^{\sum_{i=1}^{n} x_i})^k}{k!} |x_1 \cdots x_n\rangle$$

$$= e^{-it(-1)^{\sum_{i=1}^{n} x_i}} |x_1 \cdots x_n\rangle$$, where $x_i = 0$ or 1. #

(d) Implement U with $O(n)$ 1-qubit gates and 2-qubit gates with $|0\rangle$ as auxillary gate.

Solution.



where $U_z|0\rangle = e^{-it}|0\rangle$, $U_z|1\rangle = e^{it}|1\rangle$.

Correctness:

At point Δ, we get $\begin{cases} e^{-it}|x\rangle|0\rangle & \text{if } \sum x_i = 0 \\ e^{it}|x\rangle|1\rangle & \text{if } \sum x_i = 1 \end{cases}$

Finally, we get $\begin{cases} e^{-it}|x\rangle|0+\sum x_i\rangle = e^{-it}|x\rangle|0\rangle & \text{if } \sum x_i = 0 \\ e^{it}|x\rangle|1+\sum x_i\rangle = e^{it}|x\rangle|0\rangle & \text{if } \sum x_i = 1 \end{cases}$

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3 Estimating ground state energy

Given n-qubit $|\psi\rangle$ with $|\langle\psi|\psi_{min}\rangle|^2 \geq 0.7$ $H = \sum_i a_i U_i$, U_i acts on 2-qubit systems. Output λ_{min} with precision of $\lfloor 2\log_2 n \rfloor$ bits with poly(n) gates with probability $\geq \frac{2}{3}$.

<u>Solution</u>. WLOG, $Spec(H) = \{\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{2^n}\}$, $0 \leq \lambda_i < 1$.

$$H = \sum_{i=1}^{2^n} \lambda_i |\lambda_i\rangle\langle\lambda_i|$$

$$e^{-iHt} = \sum_{j=1}^{2^n} e^{-i\lambda_j t} |\lambda_j\rangle\langle\lambda_j|$$

$$= e^{-i\lambda_1 t}|\lambda_1\rangle\langle\lambda_1| + \sum_{j>1} e^{-i\lambda_j t}|\lambda_j\rangle\langle\lambda_j|$$

Since $|\langle\psi|\lambda_1\rangle|^2 \geq 0.7$

Expand $|\psi\rangle = b_1|\lambda_1\rangle + \sum_{j>1} b_j|\lambda_j\rangle$ We have $|b_1|^2 \geq 0.7$, $b_j \in \mathbb{C}$, $j>1$

$e^{-iHt}|\psi\rangle = b_1 e^{-i\lambda_1 t}|\lambda_1\rangle + \sum_{j>1} c_j|\lambda_j\rangle$, $c_j \in \mathbb{C}$.

We know H is sparse, can be efficiently simulated

Let $\|U - e^{-iH}\| \leq \varepsilon$ in poly$(n, \frac{1}{\varepsilon})$

Choose ε small enough s.t. $U|\psi\rangle = b_1' e^{-i\lambda_1 t}|\lambda_1\rangle + \sum_{j>1} c_j'|\lambda_j\rangle$

with $\|b_1'\|^2 \geq \frac{2}{3}$. ($\varepsilon \geq \|U|\psi\rangle - e^{-iHt}|\psi\rangle\| \geq \|b_1' - b_1\|$, take $\varepsilon = 0.01$ sufficies)

Algorithm.

Step 1. Prepare U.

Step 2. Apply phase estimation with precision $\lfloor 2\log_2 n \rfloor$ on $|\psi\rangle$ and U

Read output.

By linearity, after phase estimation we reach

$$b_1'|ps(1)\rangle|\psi\rangle + \sum_{j\geq 2} c_j'|ps(j)\rangle|\psi\rangle$$

where $|ps(j)\rangle$ is $\lfloor 2\log_2 n \rfloor$ bit value of jth eigenvector

Measurement yields success probability $\|b_1'\|^2 \geq \frac{2}{3}$.

Total cost is poly(n).

4 Testing graph properties

(a) Left part has $2^{2n+1}-1$ vertices

right part has $2^{n+2}-2$ vertices

$$p = \frac{2^{2n+1}-1}{2^{2n+1}+2^{n+2}-2} = 1 - O(2^{-n})$$

(b) Algorithm.

Step 1. random choose a vertex

Step 2. Do random walk until reach s or a leaf.

Step 3. If reaches a leaf, reach from level 0 to level 1.

For $k=1, \dots 2n-1$ do:

Determine which one of two edges is towards s

by walking k steps and see whether reaches a leaf.

Reach from level k to level k+1.

End for

Analysis: Step 1 has high probability of reaching the left side;

Step 2 can be seen as random walk on $\mathbb{Z} \cap [1, 2^n]$

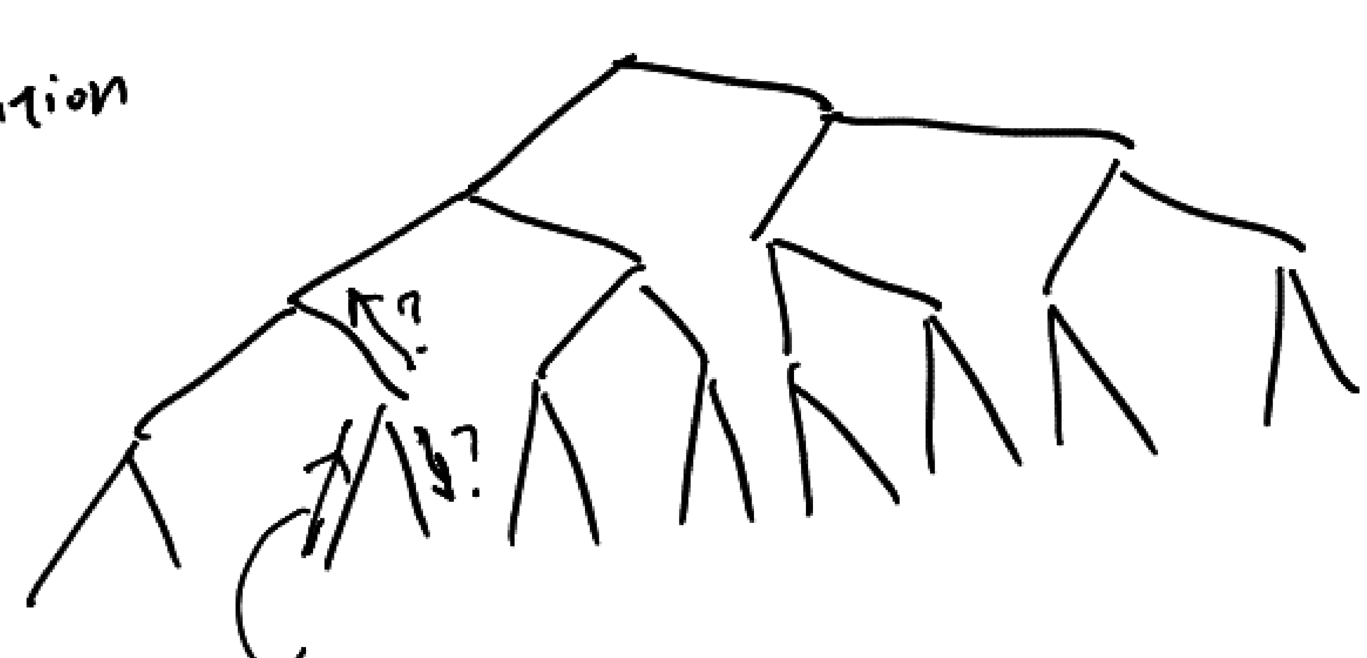
Expected hitting time of 0 (or 2n) is $O(n)$ as well known in theory of Stochastic Process.

Step 3. Worst case $O(1+2+\dots+2n) = O(n^2)$ time

Conclusion

$O(n^2)$ with high probability.

Step 3 illustration

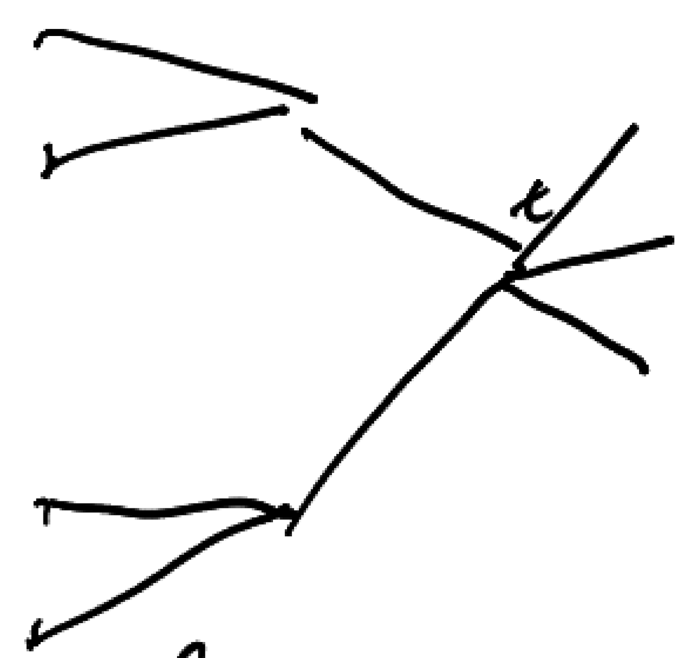


Determine which ? is correct. Searching a complete binary tree from root to leaf takes $O(\text{depth})$ time

(c)

Consider G_n be adding 3 edges to t in above graph.

$$G_n \text{ has } 2^{\Theta(n)} \text{ edges}$$



G_n

Why classical algorithm must take $2^{\Omega(n)}$ queries:

All vertexes being equal, there is high probability to fall in the left part of graph. By to travel to t from some left graph vertex v must travel $v \to s$ and $s \to t$ (as each step only knows local information)

But $s \to t$ is equivalent to the s-t connectivity problem and needs at least $2^{\Omega(n)}$ queries.

Why quantum algorithm works in poly(n):

Step 1 Pick a random vertex

Step 2 Use (b) to reach s in $O(n^2)$ queries

Step 3 For the 3 other vertex of s, use $O(3 \cdot 2n) = O(n)$ queries to determine whether it points left or right.

(random walk without going back to previous vertex. reach a leaf exactly in $2n$ steps without reaching t or s if and only if points left)

Step 4. Delete two edges in s pointing left

Use continuous quantum walk to reach t in poly(n) queries

Total poly(n) queries with high probability. #