

# Continuous time quantum algorithms

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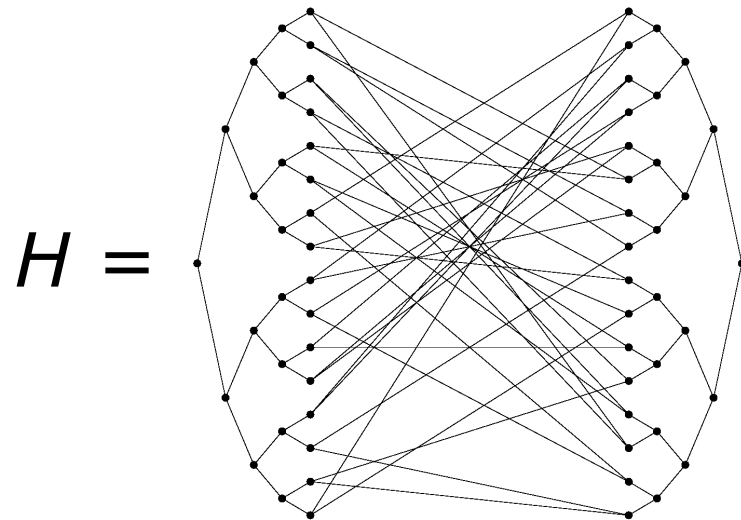
# Review

Quantum systems evolve according to the Schrödinger equation  $i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$

Such systems can be efficiently simulated by a universal quantum computer when  $H$  has an appropriate form.

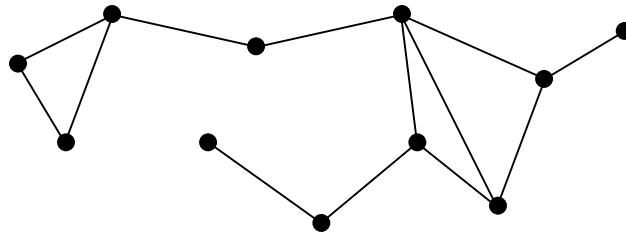
Maybe these dynamics can be used to do interesting computations.

# I. Quantum walk



# Graphs and matrices

Undirected graph  $G$  with no self loops



**Adjacency matrix:**  $A_{jk} = \begin{cases} 1 & (j, k) \in G \\ 0 & \text{otherwise} \end{cases}$

**Laplacian:**  $L = A - D$  [ $D$  diagonal,  $D_{jj} = \text{deg}(j)$ ]

$-L$  is positive semidefinite

$$L(\sum_j |j\rangle) = 0$$

All other eigenvalues are positive (if  $G$  is connected)

# Random walk

Random walks/Markov chains are used in many classical algorithms.

## Discrete time random walk

At each step, equal probability of jumping to each connected vertex

$$p_a(t + 1) = \sum_{b:(a,b) \in G} \frac{p_b(t)}{\deg(b)}$$

## Continuous time random walk

Probability per unit time  $\gamma$  of jumping to each connected vertex

$$\begin{aligned} \frac{dp_a(t)}{dt} &= \sum_{b:(a,b) \in G} \gamma p_b(t) - \gamma \deg(a) p_a(t) \\ &= \sum_b L_{ab} p_b(t) \end{aligned}$$

# Quantum walk

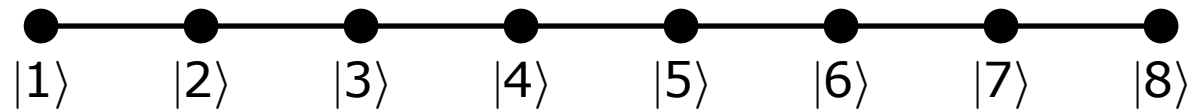
How to define a quantum analogue of a random walk on an  $N$ -vertex graph  $G$ ?

## Proposal:

- Basis state  $|a\rangle$  for each vertex  $a$
- At each step, move to all adjacent sites with equal amplitude

**This does not work!**

## Example:



$$|4\rangle \rightarrow \frac{1}{\sqrt{2}}(|3\rangle + |5\rangle)$$

$$|6\rangle \rightarrow \frac{1}{\sqrt{2}}(|5\rangle + |7\rangle)$$

Walk cannot be unitary.

# Quantum walk

## Two alternatives:

### 1. Introduce extra variables

State space: Directed edges  $|a,b\rangle$



$$|j, L\rangle \rightarrow \frac{1}{\sqrt{2}}(|j-1, L\rangle + |j-1, R\rangle)$$
$$|j, R\rangle \rightarrow \frac{1}{\sqrt{2}}(|j+1, L\rangle - |j+1, R\rangle)$$

### 2. Continuous time

## Random walk

### State space

$N$  vertices  $j=1, \dots, N$

$p_j$  = probability of being at vertex  $j$

### Differential equation

$$\frac{dp_j}{dt} = \gamma \sum_k L_{jk} p_k$$

### Generator

$\gamma L$ ,  $L$  = Laplacian of  $G$

### Probability conservation

$$\sum_j L_{jk} = 0 \Rightarrow \frac{d}{dt} \sum_j p_j = 0$$

## Quantum walk

$N$  basis states  $|1\rangle, \dots, |N\rangle$

$q_j = \langle j|\psi\rangle$  = amplitude to be at vertex  $j$

$$i \frac{dq_j}{dt} = \sum_k H_{jk} q_k$$

Can choose  $H = -\gamma L$   
(or  $\gamma A$ , etc.)

$$H = H^\dagger \Rightarrow \frac{d}{dt} \sum_j |q_j|^2 = 0$$



# Walk on a line

## Infinite line:



$$i \frac{d}{dt} q_x = q_{x-1} + q_{x+1}$$

Eigenstates of A:  $\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{ipx}$ ,  $-\pi \leq p \leq \pi$

Eigenvalues:  $E_p = 2 \cos p$

Amplitude to go from  $x$  to  $y$ :

$$\begin{aligned} \langle y|e^{-iAt}|x\rangle &= \frac{1}{2\pi} \int_{-\pi}^{\pi} dp e^{ip(y-x) - 2it \cos p} \\ &= (-i)^{y-x} J_{y-x}(2t) \end{aligned}$$

Big for  $y-x \sim 2t$   
Small for  $y-x \gg 2t$

⇒ Walk propagates with speed 2: in time  $t$ , walk moves a distance  $2t$ .

(Classical random walk: in time  $t$ , walk moves a distance  $\propto \sqrt{t}$ .)

# Mixing times

How long does it take for the walk to spread out over the entire graph?

**Classical random walk:**  $p$  approaches a limiting distribution as  $t \rightarrow \infty$

$$\begin{aligned} e^{Lt} &= \sum_j e^{-E_j t} |\phi_j\rangle\langle\phi_j| & E_0 &= 0 & |\phi_0\rangle &= \frac{1}{\sqrt{N}} \sum_a |a\rangle \\ &\rightarrow |\phi_0\rangle\langle\phi_0| & E_j &> 0 & \text{for } j > 0 \\ &= \frac{1}{N} \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \cdots & \vdots \\ 1 & \cdots & 1 \end{pmatrix} \\ p_a^\infty &= \frac{1}{N} \end{aligned}$$

Mixing time:  $T \propto 1/E_1$

# Mixing times

**Quantum walk:** no limiting distribution — dynamics are unitary!

But consider:

$$\begin{aligned}
 q_{ab} &= \frac{1}{T} \int_0^T dt |\langle a | e^{-iHt} | b \rangle|^2 \\
 &= \frac{1}{T} \int_0^T dt \left| \sum_{j,k} \langle a | \phi_j \rangle \langle \phi_j | e^{-iHt} | \phi_k \rangle \langle \phi_k | b \rangle \right|^2 \\
 &= \frac{1}{T} \int_0^T dt \left| \sum_j e^{-iE_j t} \langle a | \phi_j \rangle \langle \phi_j | b \rangle \right|^2 \\
 &= \frac{1}{T} \int_0^T dt \sum_{j,k} e^{-i(E_j - E_k)t} \langle a | \phi_j \rangle \langle \phi_j | b \rangle \langle b | \phi_k \rangle \langle \phi_k | a \rangle
 \end{aligned}$$

for  $T \gg \min_{\substack{j,k \\ E_j \neq E_k}} \frac{1}{|E_j - E_k|}$  :

$$\begin{aligned}
 q_{ab}^\infty &= \sum_{j,k} \delta_{E_j, E_k} \langle a | \phi_j \rangle \langle \phi_j | b \rangle \langle b | \phi_k \rangle \langle \phi_k | a \rangle \\
 &= \sum_j |\langle a | \phi_j \rangle \langle \phi_j | b \rangle|^2
 \end{aligned}$$

no degeneracy:

# Hitting times

How long does it take for the walk to reach a particular vertex?

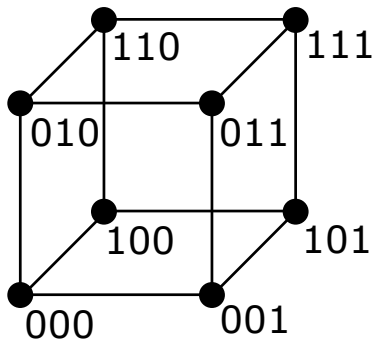
More precisely, we say the hitting time of the walk from  $a$  to  $b$  is polynomial in  $n$  if for some  $t = \text{poly}(n)$  there is a probability  $1/\text{poly}(n)$  of being at  $b$ , starting from  $a$ .

# Hitting times: quantum vs. classical

**Theorem:** Let  $G_n$  be a family of graphs with designated ENTRANCE and EXIT vertices. Suppose the hitting time of the classical random walk from ENTRANCE to EXIT is polynomial in  $n$ . Then the hitting time of the quantum walk from ENTRANCE to EXIT is also polynomial in  $n$  (for a closely related graph).

Proof idea: Analytically continue the classical walk,  $t \rightarrow i t$ .

# Hypercube



$$A = \sum_{j=1}^n \sigma_x^{(j)}$$

$$\begin{aligned} e^{-iAt} &= e^{-i\sigma_x^{(1)}t} \otimes e^{-i\sigma_x^{(2)}t} \dots \otimes e^{-i\sigma_x^{(n)}t} \\ &= \begin{pmatrix} \cos t & i \sin t \\ i \sin t & \cos t \end{pmatrix}^{\otimes n} \end{aligned}$$

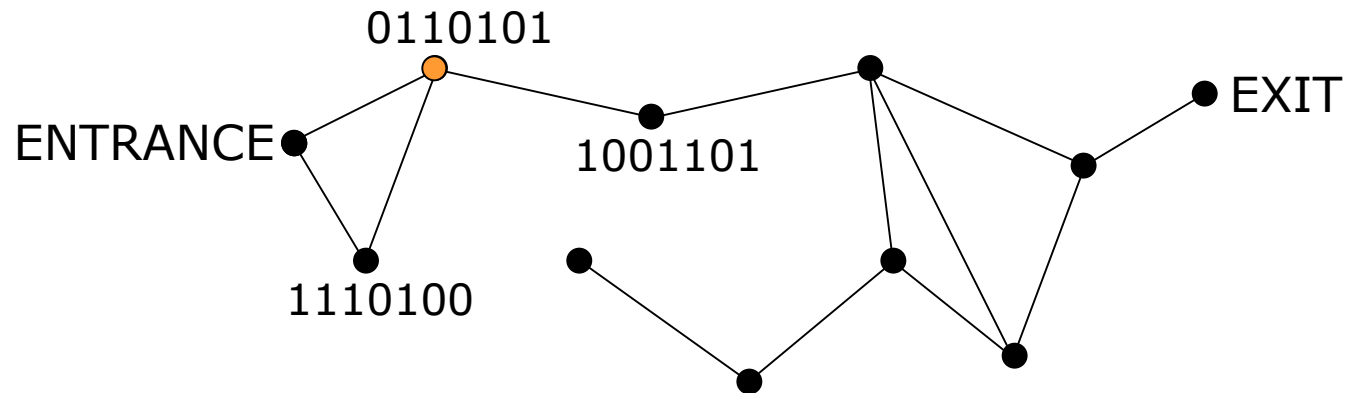
Let  $|\psi(0)\rangle = |00\dots 0\rangle$ ; then  $|\psi(t)\rangle = e^{-iAt} |00\dots 0\rangle$ .

Probability of reaching opposite corner in time  $t$ :

$$|\langle \psi(t) | 11\dots 1 \rangle|^2 = (\sin t)^{2n}$$

Classical hitting time is exponential in  $n$ !

# Black box graph traversal problem



Names of vertices: random  $2n$ -bit strings ( $n = \lceil \log N \rceil$ )

Name of ENTRANCE is known

Oracle outputs the names of adjacent vertices

$v_c(a) = c$ th neighbor of  $a$

## Examples:

$$v_1(\text{ENTRANCE}) = 0110101$$

$$v_2(\text{ENTRANCE}) = 1110100$$

$$v_3(\text{ENTRANCE}) = 1111111$$

$$v_4(\text{ENTRANCE}) = 1111111$$

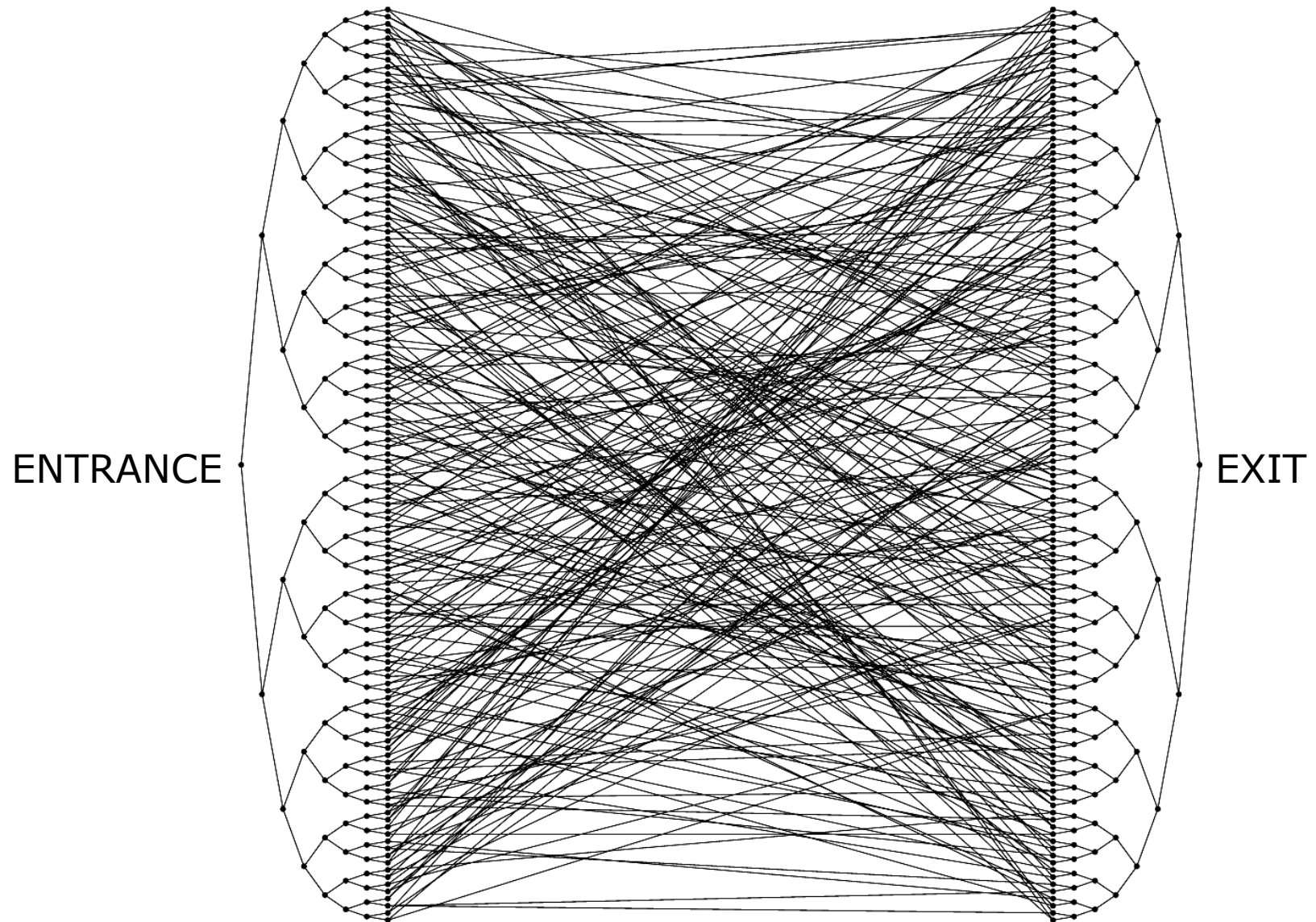
$$v_1(0110101) = 1001101$$

$$v_2(0110101) = \text{ENTRANCE}$$

$$v_3(0110101) = 1110100$$

$$v_4(0110101) = 1111111$$

# Exponential speedup





# Reduction of the quantum walk

## Column subspace

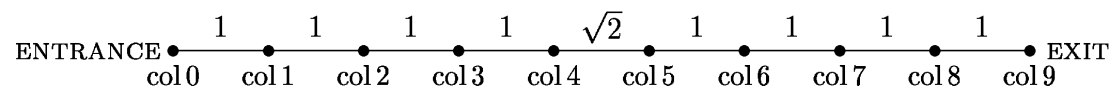
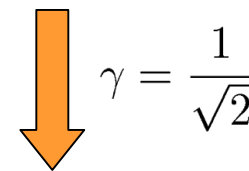
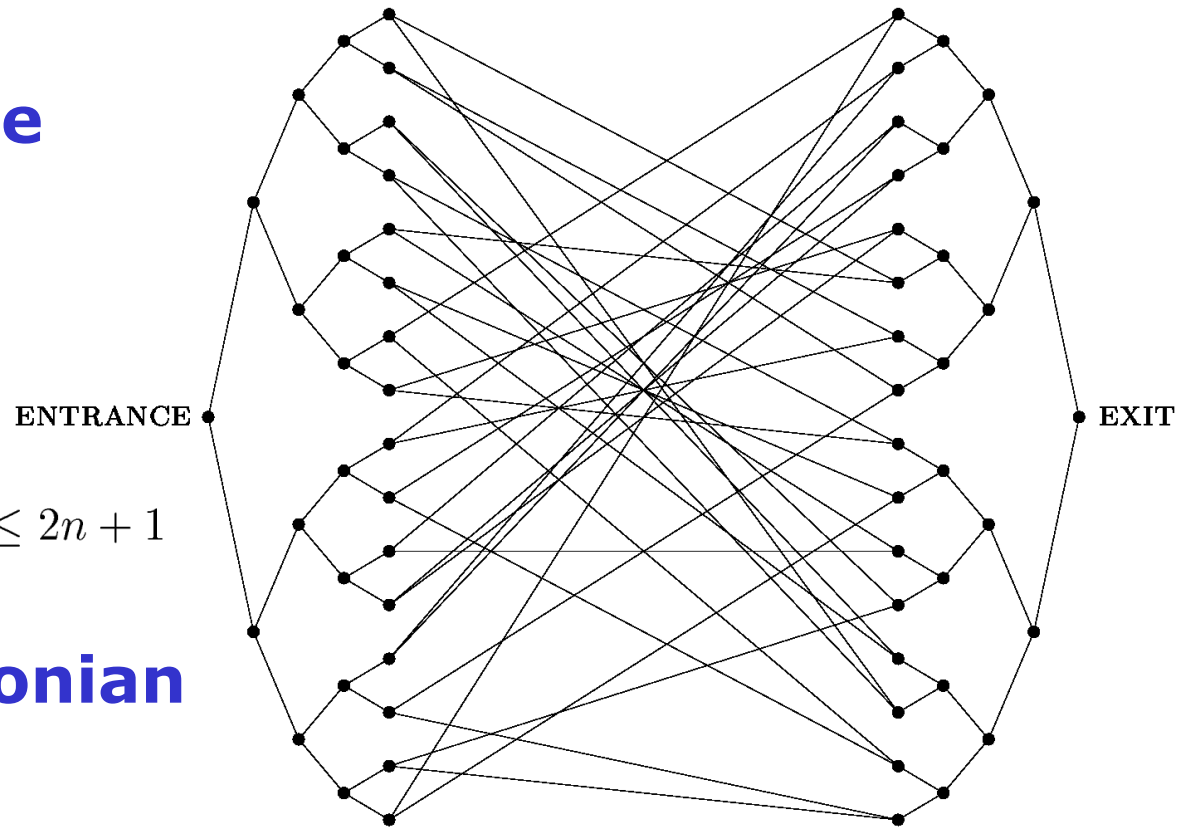
$$|\text{col } j\rangle = \frac{1}{\sqrt{N_j}} \sum_{a \in \text{column } j} |a\rangle$$

where

$$N_j = \begin{cases} 2^j & 0 \leq j \leq n \\ 2^{2n+1-j} & n+1 \leq j \leq 2n+1 \end{cases}$$

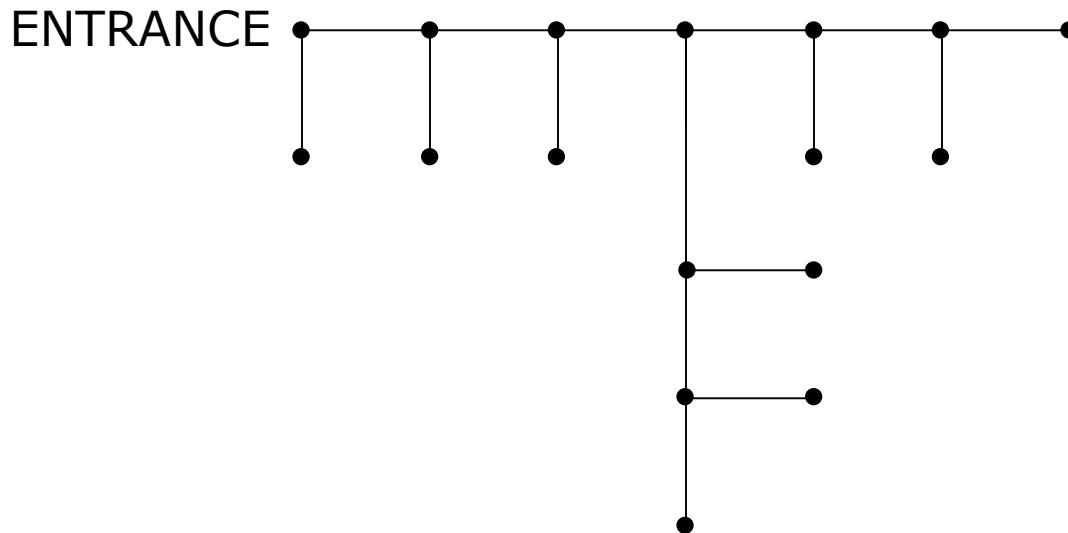
## Reduced Hamiltonian

$$\begin{aligned} &\langle \text{col } j | H | \text{col}(j+1) \rangle \\ &= \begin{cases} \sqrt{2}\gamma & 0 \leq j \leq n-1, \\ & n+1 \leq j \leq 2n \\ 2\gamma & j = n \end{cases} \end{aligned}$$

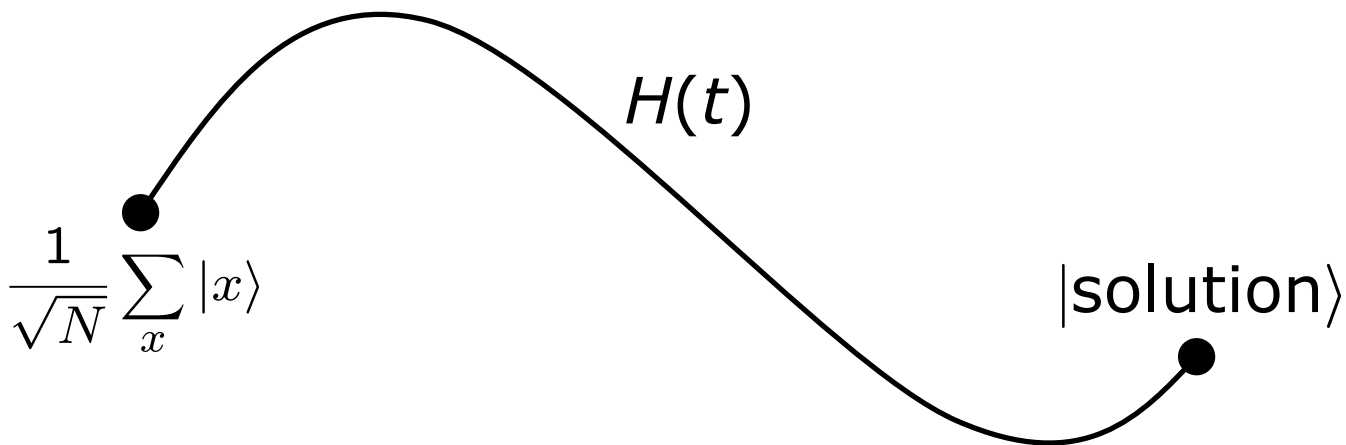


# Classical lower bound

**Theorem:** Any classical algorithm that makes at most  $2^{n/6}$  queries to the oracle finds the EXIT with probability at most  $4 \cdot 2^{-n/6}$ .



## II. Quantum computation by adiabatic evolution



# Computation and ground states

Encode the solution of a computational problem in the ground state of a Hamiltonian.

**Example:**  $k$ -SAT

$\exists x_1, \dots, x_n \in \{0, 1\}$ :

$$(x_1 \vee x_3 \vee \neg x_{11}) \wedge \dots \wedge (\neg x_{23} \vee x_{42} \vee \neg x_{17}) = 1$$

Let  $h_C = 0$  if clause  $C$  is satisfied

$h_C = 1$  if clause  $C$  is not satisfied

Minimize  $h = \sum_C h_C$

Equivalently, find the ground state of

$$H = \sum_x h(x) |x\rangle\langle x|$$

**Notation:** Eigenstates of  $H$ :  $H |\phi_j\rangle = E_j |\phi_j\rangle$

$$E_0 \leq E_1 \leq \dots \leq E_N$$

# The adiabatic theorem

## Rough version:

Let  $H(t)$  be slowly varying.

Let  $|\psi(0)\rangle = |E_j(0)\rangle$ .

Then  $|\psi(T)\rangle \approx |E_j(T)\rangle$ .

## More precisely:

Let  $\tilde{H}(s)$  be a smooth function of  $s \in [0, 1]$ .

Let  $H(t) = \tilde{H}(t/T)$

Let  $|\psi(0)\rangle = |E_0(0)\rangle$ .

Then  $|\psi(T)\rangle \approx |E_0(T)\rangle$  so long as

$$T \gg \frac{\Gamma(s)}{[E_1(s) - E_0(s)]^2} \quad \text{where}$$

$$\Gamma^2(s) = \langle \phi_0(s) | \left( \frac{dH}{ds} \right)^2 | \phi_0(s) \rangle - \langle \phi_0(s) | \frac{dH}{ds} | \phi_0(s) \rangle^2$$

# Adiabatic quantum computation

Let  $\tilde{H}(0)=H_B$  be a Hamiltonian whose ground state is easy to prepare.

**Example:**  $H_B = -\sum_j \sigma_x^{(j)}$ , ground state  $\frac{1}{2^{n/2}} \sum_{z=0}^{2^n-1} |z\rangle$

Let  $\tilde{H}(1)=H_P$  be a Hamiltonian whose ground state encodes the solution to the problem.

**Example:**  $H_P = \sum_z h(z) |z\rangle\langle z|$  to minimize  $h(z)$

Let  $\tilde{H}(s)$  interpolate from  $H_B$  to  $H_P$ .

**Example:**  $\tilde{H}(s) = (1-s) H_B + s H_P$

Start in  $|E_0(0)\rangle$ , evolve for time  $T$ , and measure.

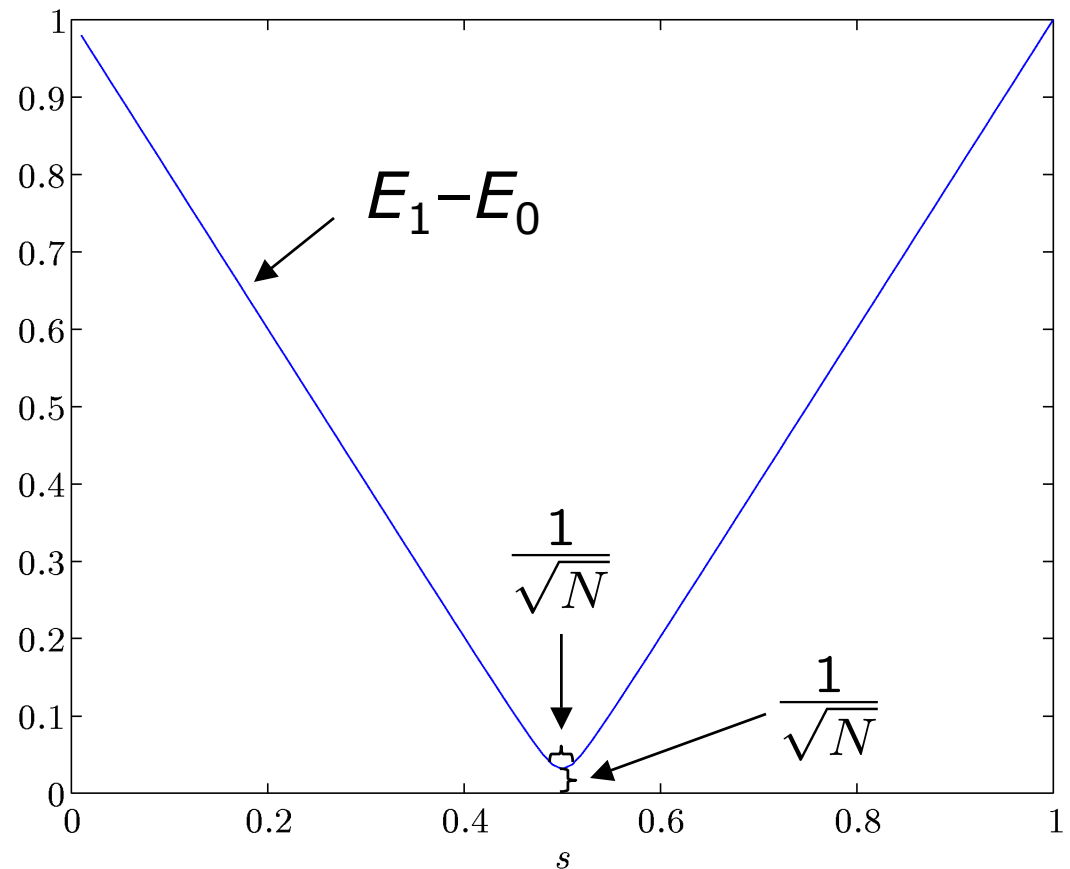
# Adiabatic Grover search

Minimize function  $h(z) = \begin{cases} 0 & z = w \\ 1 & z \neq w \end{cases}$

$$H_P = -|w\rangle\langle w|$$

$$H_B = -|s\rangle\langle s|$$

$$|s\rangle = \frac{1}{\sqrt{N}} \sum_x |x\rangle$$



# Adiabatic Grover search

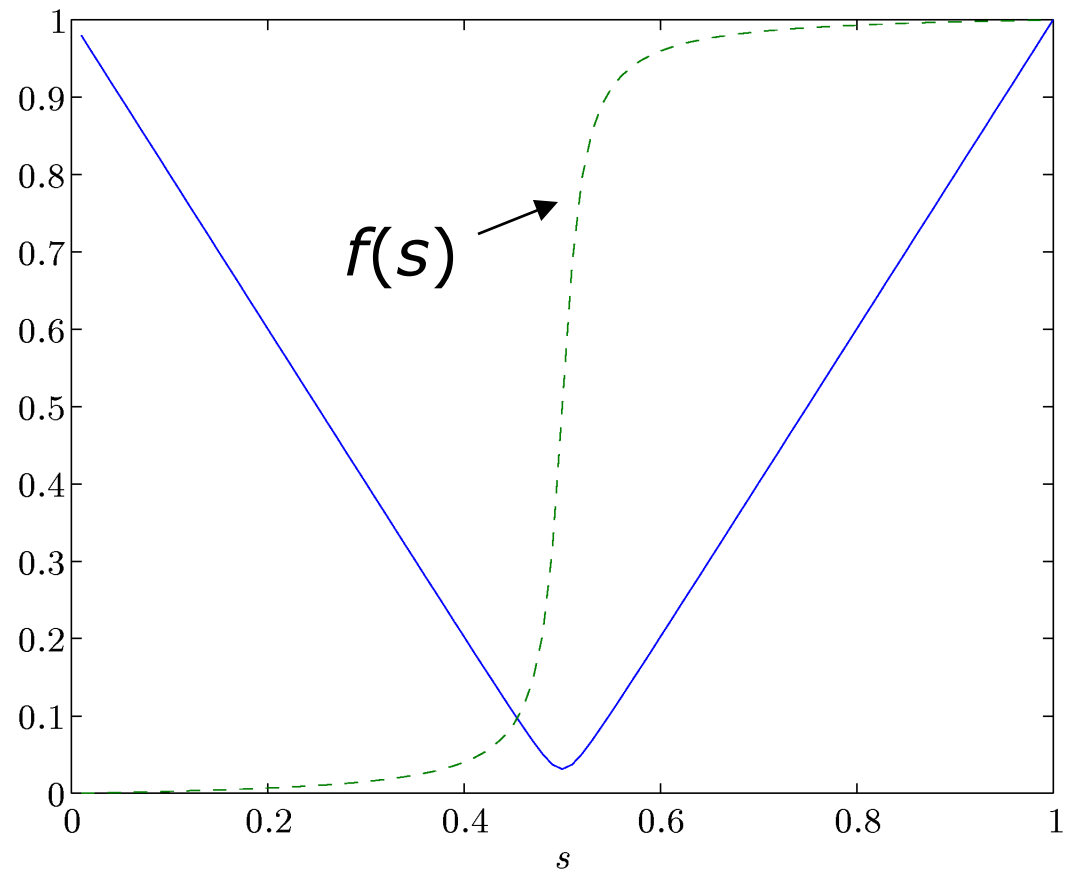
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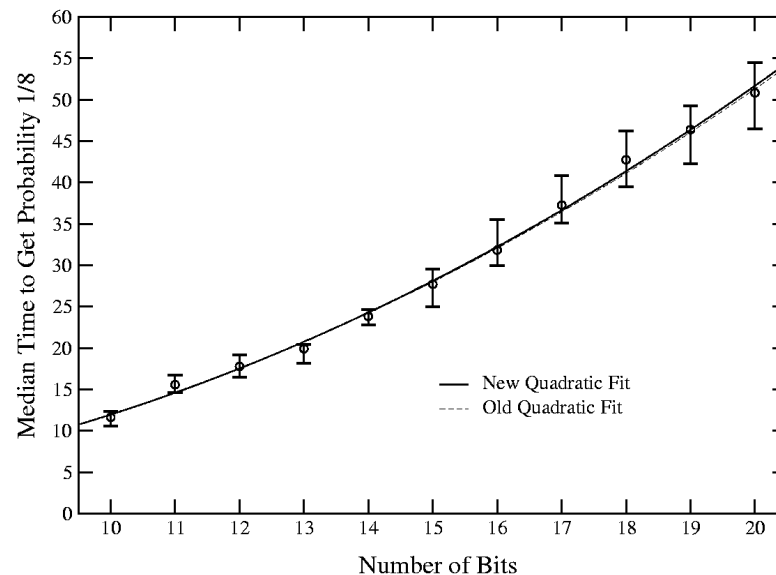
$$\tilde{H}(s) = [1-f(s)] H_B + f(s) H_P$$





# Hard problems

How well does the adiabatic algorithm work on hard problems?



**Note:** We could learn a lot more if we had even a small quantum computer (say 30 qubits)!

# Adiabatic computation is universal

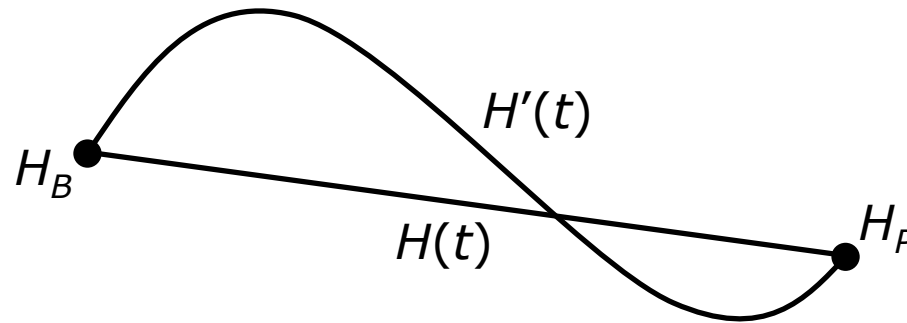
**Theorem:** The output of any quantum circuit (acting on the  $|0\rangle$  state) can be efficiently simulated by an adiabatic quantum computation with linear interpolation  $\tilde{H}(s) = (1-s) H_B + s H_P$  where  $H_B$  and  $H_P$  are sums of Hermitian operators acting on a constant number of qubits.

**Proof:** Based on Feynman's proof that any (quantum) computation can be performed by time-independent Hamiltonian evolution.

Also related to the proof that LOCAL HAMILTONIAN is QMA-Complete (Kitaev).

# Adiabatic computation is robust

**Robustness to control error:** Computation depends on going smoothly from  $H_B$  to  $H_P$ , not on the particular path between them.



**Robustness to thermal noise:** Computation depends on (and is protected by) a gap  $E_1 - E_0$ . If  $k_B T \ll 1/(E_1 - E_0)$  then thermal transitions are suppressed.

# Summary

Many kinds of Hamiltonian evolution can be efficiently simulated by universal quantum computers.

This allows us to simulate quantum physics much more efficiently than is possible using classical computers.

Hamiltonian evolution can also be used to build quantum algorithms.

- Quantum walks
- Adiabatic quantum computation
- ...

# References

## Continuous time quantum walks

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