# Hamiltonian simulation

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# Overviews

- The Schrödinger equation
- How is Hamiltonian simulation used
- Product formulas
- Linear combination of unitaries
- Relationship to quantum walks and quantum signal processing

# Physics background

# Some math that you should know

Differential equation

$$\frac{dx(t)}{dt} = k \cdot x(t), \quad k \in \mathbb{R} \tag{1}$$

$$\int \frac{dx}{x} = \int k\,dt$$

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solution $x(t) = e^{kt}x(0)$

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Eigenvectors and eigenvalues

matrix

$$A\vec{v} = a\vec{v} \tag{2}$$

It is always possible to find eigenvectors $\vec{v}$ that for a complete, orthonormal set.

# Evolution of a physical system

The Schrödinger equation

doesn't depend
on time

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \tag{3}$$

Take $\hbar = 1$. $H$ is the Hamiltonian, an operator corresponding to the total energy of a system.

Decomposition into eigenvectors and eigenvalues

$$H \left|\phi_j(t)\right\rangle = E_j \left|\phi_j(t)\right\rangle \tag{4}$$

The eigenvalues of of the Hamiltonians correspond allowed energy levels.

# Frame Title

During this lectures I will be interchangeably using

eigenvectors = eigenstates

eigenvalues = eigenenergies

# Time evolution - special case

What is the solution of the Schrödinger equation if the state is an eigenvector of $H$?

eigenstate

$$i\hbar \frac{d}{dt} |\phi_j(t)\rangle = \underbrace{H |\phi_j(t)\rangle}_{E_j |\phi_j(t)\rangle} \tag{5}$$

$$e^{-iE_j t}$$

# Time evolution - special case

What is the solution of the Schrödinger equation if the state is an eigenvector of $H$?

$$i\hbar\frac{d}{dt}\left|\phi_j(t)\right\rangle = \boxed{H\left|\phi_j(t)\right\rangle} \tag{5}$$

Eigenvectors will be only gaining a phase

$$i\hbar\frac{d}{dt}\left|\phi_j(t)\right\rangle = \boxed{E_j\left|\phi_j(t)\right\rangle} \tag{6}$$

$$\left|\phi_j(T)\right\rangle = e^{-iE_jT}\left|\phi_j(0))\right\rangle \tag{7}$$

# Time evolution

What is the solution of the Schrödinger equation for an arbitrary state?

$$i\hbar \frac{d}{dt} \left|\overset{\psi}{\cancel{\psi}}(t)\right\rangle = H \left|\overset{\psi}{\cancel{\psi}}(t)\right\rangle \tag{8}$$

Formally $\boxed{|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle.}$

$P^2 = \mathbb{1}$

$\rightarrow 2^n \times 2^n$ cos

# Decomposition into eigenvectors

Look for a solution that is a linear combination of eigenvectors

$$|\psi(t)\rangle = \sum_j a_j \underbrace{e^{-iE_jt}\,|\Phi_j\rangle}_{} \tag{9}$$

This solution satisfies the Schrödinger equation.

How do we find $a_j$-s?

$\langle\Phi_j|$

$$\langle\Phi_j \qquad |\psi(0)\rangle = \sum_j a_j\,|\Phi_j\rangle \tag{10}$$

$$\langle\Phi_j|\psi(0)\rangle = a_j\overset{=1}{\langle\Phi_j|\Phi_j\rangle} \tag{11}$$

$$a_j = \langle\Phi_j|\psi(0)\rangle \tag{12}$$

”Overlaps” of the initial state and eigenstates.

# Example: Spin in a magnetic field

scalars

Hamiltonian $H = -\mu B \sigma_X$

initial state $|\psi(0)\rangle = |0\rangle$

How will the state $|\psi(t)\rangle$ evolve?

$|+\rangle \quad |-\rangle$

$|0\rangle = \frac{1}{\sqrt{2}}\left(e^{-iEt}|+\rangle + e^{+iEt}|-\rangle\right)$

$E = -\mu B$

$e^{-Ht} = i\sin(\quad) X + \cos(\quad) \mathbb{1}$

$\downarrow$

$X^2$

# Hamiltonian simulation

# Why is computing time evolution hard?

# Why is computing time evolution hard?

A Hamiltonian on $n$ particles is a $2^n \times 2^n$ matrix. Using eigen-decomposition method that we described would take exponentially (in $n$) long time.

Every quantum computation can be described as an evolution of a quantum system. Thus, simulating Hamiltonian evolution is BQP-hard.

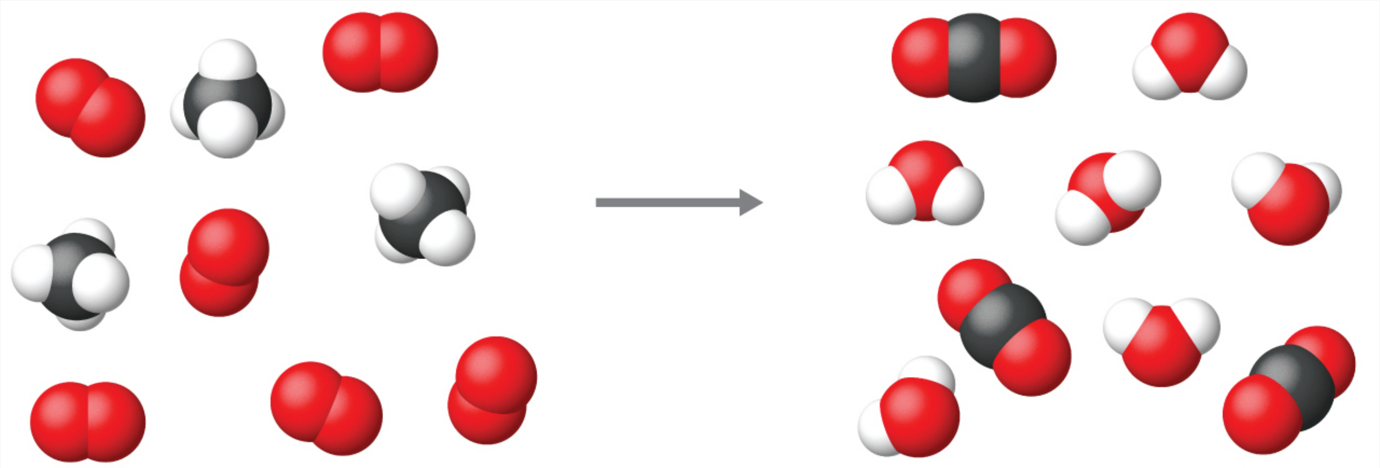
# Why is computing time evolution hard?

A Hamiltonian on $n$ particles is a $2^n \times 2^n$ matrix. Using eigen-decomposition method that we described would take exponentially (in $n$) long time. classically

Every quantum computation can be described as an evolution of a quantum system. Thus, simulating Hamiltonian evolution is **BQP**-hard.

For a range of Hamiltonians, there is an efficient quantum algorithm. The Hamiltonian evolution for these Hamiltonians is thus **BQP**-complete.

# Simulating quantum dynamics is a natural application of quantum computing

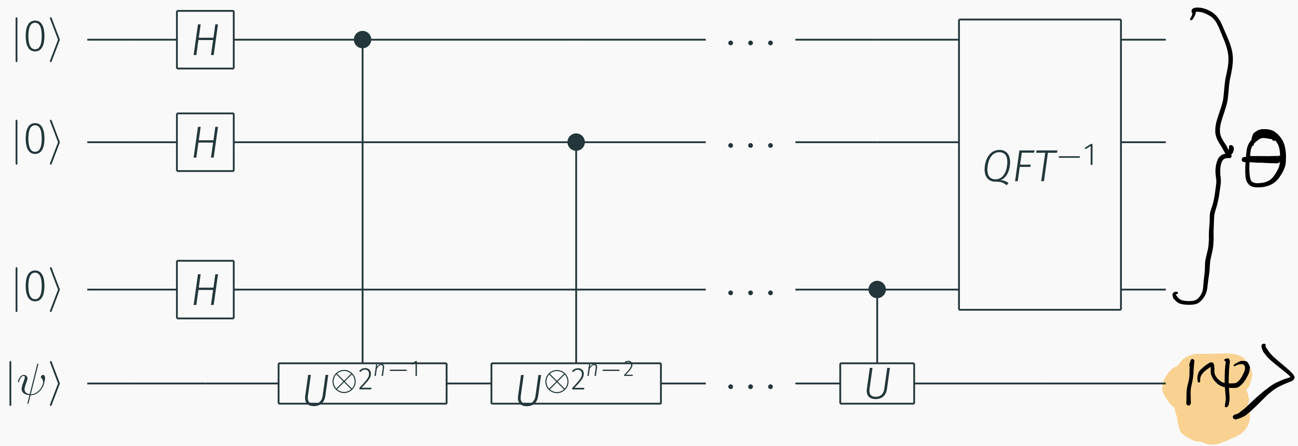


Product formulae: [Lloyd 1996, Aharonov & Ta-Shma 2003, Berry et al. 2007, Wiebe 2010, Campbell 2018, ...]

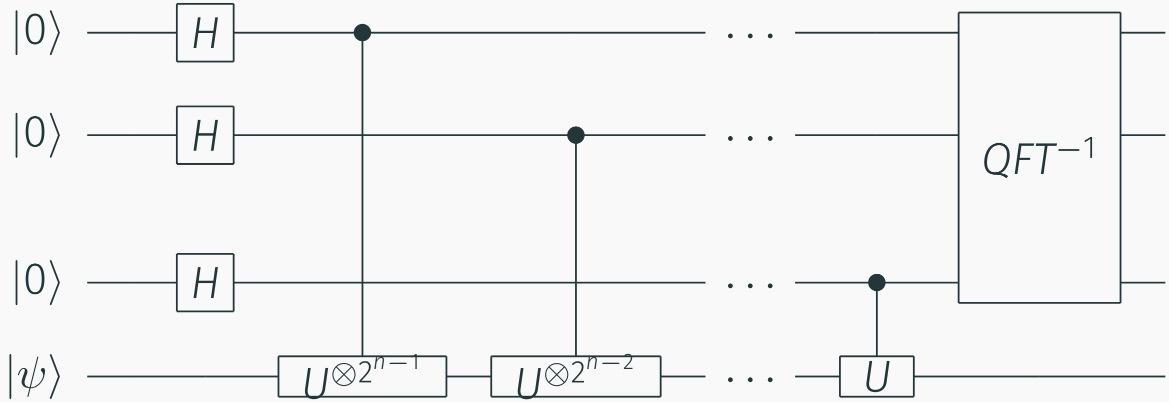
LCU: [Childs & Wiebe 2012, Berry et al. 2013, Berry et al. 2014, Berry et al. 2015, Berry et al. 2017, ...]

Other: [Childs 2010, Berry & Childs 2009, Low & Chuang 2016, Low & Chuang 2017, Low & Wiebe 2018, Gilyén 2019, ...]

# Phase estimation




What is the output if $U\left|\psi\right\rangle = e^{-i\theta}\left|\psi\right\rangle$?




$E_j$

$|g\rangle$ X

What is the output if $U|\psi\rangle \cancel{= e^{-i\theta}|\psi\rangle}$?

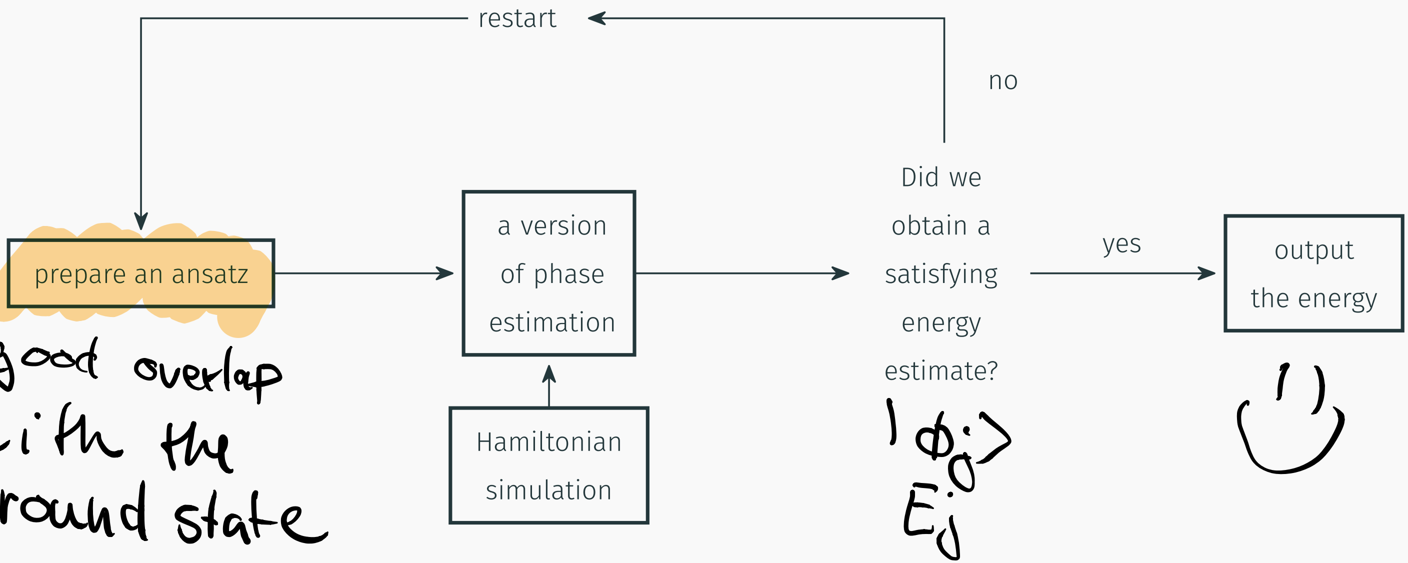
$|\psi\rangle = \cos\theta|g\rangle + \sin\theta|\dots\rangle$

Now take $U = e^{-iHt}$.

$t=1$

# Eigenenergy Estimation

Goal: compute the ground state energy of a molecule




good overlap with the ground state

$\langle \phi | g \rangle > 1/\mathrm{poly}(n)$

[Abrams, Lloyd PRL (1997), Aspuru-Guzik et al. Science (2005)]

# The Hamiltonian simulation problem

Design a (logical) circuit $U$ consisting of gates and Hamiltonian oracles that approximates the time evolution up to an error $\epsilon$ such that

$$\left\| e^{-iHt} - U \right\|_2 < \epsilon.$$

$\forall |\psi\rangle$
$\| U|\psi\rangle - e^{-iHt}|\psi\rangle \|$
$< \varepsilon$

The Hamiltonian oracle can represent

- Terms $e^{-iH_l t}$ where $H = \sum_l \alpha_l H_l$ and each $H_l$ is hermitian
- Access to matrix elements ($H$ is sparse)
- Terms $V_i$ where $H = \sum_l \alpha_l V_l$ and each $V_l$ is unitary

# Local Hamiltonians

# Infinitesimal evolution

Hamiltonian $H = A + B$. $A$ and $B$ don't commute, but:

$[A, B] \neq 0 \quad e^{A+B} \neq e^{A} e^{B}$

$\varepsilon \to 0$

$e^{A\varepsilon} e^{B\varepsilon} = e^{B\varepsilon} \cdot e^{A\varepsilon}$

$$
\begin{aligned}
\lim_{r\to\infty}\left(e^{A/r}e^{B/r}\right)^r &= \lim_{r\to\infty}\left(\left(1+\frac{A}{r}\right)\left(1+\frac{B}{r}\right)\right)^r \\
&= \lim_{r\to\infty}\left(1+\frac{A+B}{r}+\cancel{\frac{AB}{r^2}}\right)^r \\
&= \lim_{r\to\infty}\left(1+\frac{A+B}{r}\right)^r \\
&= e^{A+B}
\end{aligned}
$$

Lie-Trotter formula

## Product formulae simulation


For a finite $t/r$:

$$\left\| e^{(A+B)t/r} - \left( e^{At/r} e^{Bt/r} \right) \right\| \tag{13}$$

$$= \left\| \left( 1 + \frac{(A+B)t}{r} + \frac{((A+B)t)^2}{2r^2} + \dots \right) - \left( 1 + \frac{At}{r} + \frac{(At)^2}{2r^2} + \dots \right) \left( 1 + \frac{Bt}{r} + \frac{(Bt)^2}{2r^2} + \dots \right) \right\| \tag{14}$$

$$= \left\| \left( \cancel{1} + \cancel{\frac{(A+B)t}{r}} + \frac{((A+B)t)^2}{2r^2} + \dots \right) - \left( \cancel{1} + \cancel{\frac{(A+B)t}{r}} + \frac{(At)^2}{2r^2} + \frac{(Bt)^2}{2r^2} + \frac{ABt^2}{r^2} + \dots \right) \right\| \tag{15}$$

$$\in O\left( \frac{t^2}{r^2} \right) \tag{16}$$

$H = A + B$

$e^{iHt}$

After $r$ steps, the error is at most $O\left(\frac{t^2}{r}\right)$.

$r \cdot \frac{t^2}{r^2}$

# Product formulae simulation

For a finite $t/r$: $\left\| e^{(A+B)t} - \left(e^{At/r}e^{Bt/r}\right)^r \right\| \in \mathcal{O}\left(\frac{t^2}{r}\right)$

For a Hamiltonian $H = \sum_{j=1}^{m} H_j$, one can decompose the evolution with respect to $H$ into the evolution with respect to each $H_j$ as

$$\widetilde{U} = \left(e^{-iH_1 t/r} e^{-iH_2 t/r} \dots e^{-iH_m t/r}\right)^r + \mathcal{O}(\|H\|^2 t^2/r).$$

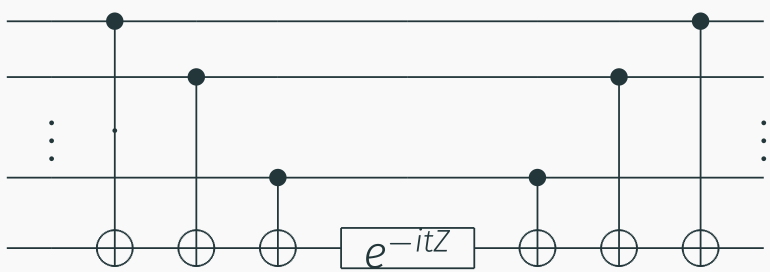
# Simulating Pauli Hamiltonians

Pauli Z

$$e^{-itZ} = e^{-it}|0\rangle\langle 0| + e^{it}|1\rangle\langle 1|$$

Tensor product of Zs

$$H = Z \otimes Z \otimes Z$$



# Other Paulis

Pauli X and Y

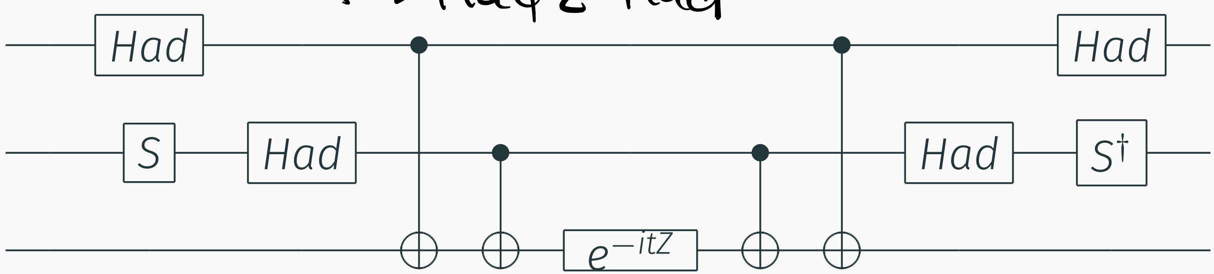
$$X = Had\; Z\; Had$$

$$Y = SHad\; Z\; Had\; S^{\dagger}$$

Same transformation for $e^{-iXt}$, $e^{-iYt}$

$$\rightarrow e^{-iZt} = \cos(t)\,\mathbb{1} - i\sin(t)\,Z$$

$X \rightarrow Had\, Z\, Had$




$X \otimes Y \otimes Z$

# Putting it all together

$Z \otimes X \otimes Y \ldots$

Hamiltonian $H = \sum_{l=1}^{L} P_l$ where $P_l$ are Paulis on at most $n$ qubits

Each $e^{-i\alpha_l P_l t}$ can be simulated with $\mathcal{O}(n)$ gates for any $\alpha_l$ and $t$.

Using the lowest order product formula we get algorithm with complexity

$$\mathcal{O}\left(L^2 t^2 n \epsilon^{-1}\right). \tag{17}$$

$O(t)$

# Trotter-Suzuki formulate

Can we find a better approximation of an exponential of a sum?

$$U_2 = \left( \prod_{j=1}^{m} e^{-iH_j \frac{t}{2r}} \prod_{j=m}^{1} e^{-iH_j \frac{t}{2r}} \right)^r \tag{18}$$

Better Scaling $t, \varepsilon$

**Exercise:**

What is the error for $H = A + B$ and

$$U_2 = \left( e^{-A\frac{t}{2r}} e^{-B\frac{t}{r}} e^{-A\frac{t}{2r}} \right)^r \tag{19}$$

$e^{-At/r} e^{-Bt/r}$

Can we find a better approximation of an exponential of a sum?

$$e^{A/2} e^{B/2} e^{C/2} e^{C/2} e^{B/2} e^{A/2}$$

$$U_2 = \left( \prod_{j=1}^{m} e^{-iH_j \frac{t}{2r}} \prod_{j=m}^{1} e^{-iH_j \frac{t}{2r}} \right)^r \tag{18}$$

Break!

Class continues at 4:40

**Exercise:**

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Error $O\left(\frac{t^3}{r^2}\right)$. For $H = \sum_{l=1}^{L} H_l$, we get $\cancel{O\left(\frac{L^{3/2} m^{3/2}}{\sqrt{\epsilon}}\right)}$.

# Sparse Hamiltonians

We can implement time evolution for $d$-sparse Hamiltonians. The Hamiltonian is given to us through oracles:

row    k-th nozero element

$$O_{loc}|r,k\rangle = |r, k \oplus l\rangle$$

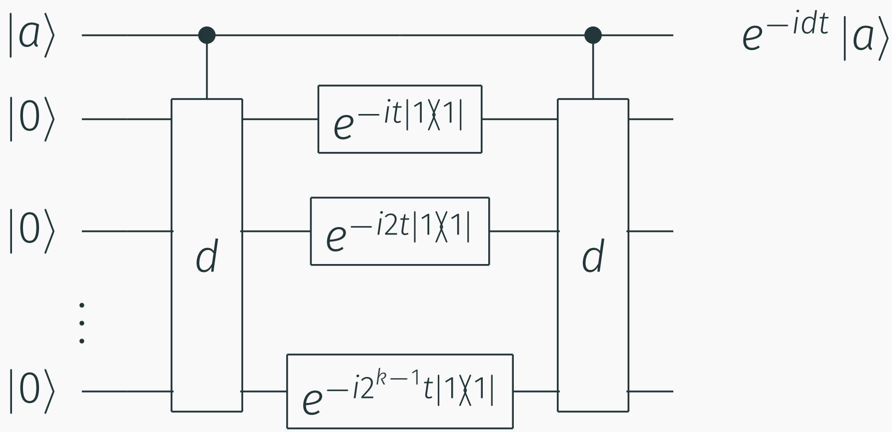
$$O_{val}\,|r,l,z\rangle = \big|r,l,z \oplus H_{r,l}\big\rangle.$$

A d-sparse Hamiltonian can be decomposed into $d^2$ 1-sparse Hamiltonians.

# Diagonal Hamiltonians

Computational states $|a\rangle$ are the eigenstates of the Hamiltonian. Let $d(a)$ be the $a$th diagonal element expressed in binary.

We have an oracle $d : |a, 0\rangle \rightarrow |a, d\rangle$.




Convince yourself that the circuit works!

# Simulating physical systems

1 particle Hamiltonian $H = \frac{p^2}{2m} + V(x)$.

Choose the computational basis as (discretized) x-eigenstates.

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How can we diagonalize the kinetic term?

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How can we diagonalize the kinetic term?

Trotterization: $\left( e^{-V(x)\frac{t}{r}} \mathrm{QFT}^{-1} e^{-i\frac{p^2 t}{2mr}} \mathrm{QFT} \dots \right)^r$

# Simulating sparse Hamiltonians

Higher-order formulae can be obtained using the recursion relation

$$S_{2k}(\delta) = [S_{2k-2}(p_k\delta)]^2 \, S_{2k-2}((1-4p_k)\delta) \, [S_{2k-2}(p_k\delta)]^2 \,, \tag{20}$$

where

$$S_2(\delta) = \prod_{j=1}^{m} e^{H_j\delta/2} \prod_{j'=m}^{1} e^{H_j'\delta/2}. \tag{21}$$

The number $N_{exp}$ of exponentials of the form $e^{-iH_jt}$ for the $k$-th order Trotterization algorithm is then bounded by

$$N_{exp} \leq \frac{2m5^{2k}(m\tau)^{1+1/2k}}{\epsilon^{1/2k}}, \tag{22}$$

for $\epsilon < 2mr^{k-1}$ and $\tau = \|H\| \, t$.

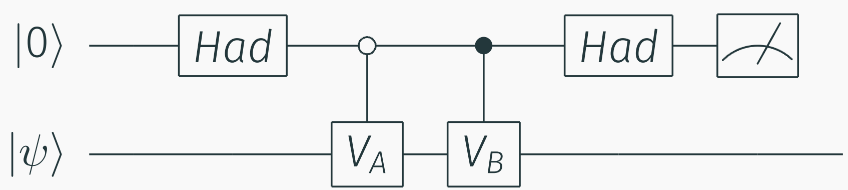
# Linear Combination of Unitaries

# Linear Combination of Unitaries (LCU)

Can we implement a sum of unitaries?

Exercise:

If we measure 0 on the first qubit, what operation do we implement on the data $|\psi\rangle$?




$\sim V_A + V_B |\psi\rangle$

# Truncated Taylor series

The Hamiltonian $H = \sum_{l=1}^{L} \alpha_l H_l$ where $\alpha_l \in \mathbb{R}$ and $H_l$s are unitaries.

The Hamiltonian evolution

$K \leftarrow \log(1/\varepsilon)/\log\log(1/\varepsilon)$

$$e^{-iHt/r} = \sum_{k=0}^{K} \frac{(-iHt/r)^k}{k!}. \tag{23}$$

Truncate at an order $K$

$\frac{\|H\|t}{r} < 1$

$$\tilde{U} = \sum_{k=0}^{K} \frac{(-it/r)^k}{k!} \sum_{l_1} \sum_{l_2} \cdots \sum_{l_k} \alpha_{l_1}\alpha_{l_2}\dots\alpha_{l_k} H_{l_1}H_{l_2}\dots H_{l_k}, \tag{24}$$

$$\tilde{U} = \sum_{j} \beta_j V_j \tag{25}$$

The evolution can be written as an LCU.

# Linear combination of unitaries

Prepare an ancillary state $B\,|0\rangle = \sum_j \beta_j\,|j\rangle$ where $s = \sum_{j=0}^{m-1} \beta_j$

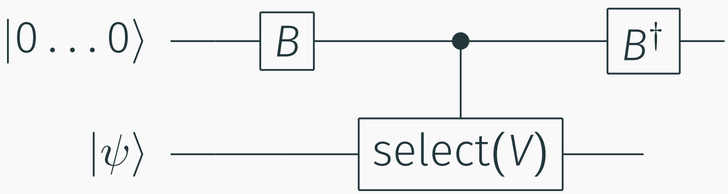
$\beta > 0$

real

Oracle select$(V)\,|j\rangle\,|\psi\rangle = |j\rangle\, V_j\,|\psi\rangle$

$\beta_j$

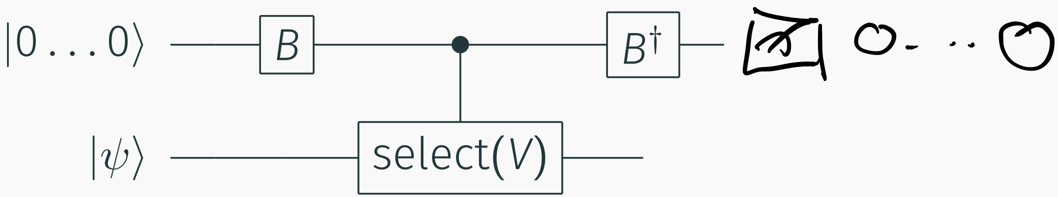
Can we implement $\sum_j V_j$?




$$W = \left(B^\dagger \otimes \mathbb{I}\right) \text{select}(V) \left(B \otimes \mathbb{I}\right). \tag{26}$$

# Prepare-select

$W$ applies the $\widetilde{U}$ if the ancilla is in the correct state (in this case it is $|0\rangle$) and prepares some garbage state if that ancilla is not zero.




$$W = \left(B^\dagger \otimes \mathbb{I}\right) \text{select}(V) \left(B \otimes \mathbb{I}\right). \tag{27}$$

Successful application

$$\left(|0\rangle\langle 0| \otimes \mathbb{I}\right) W |\psi\rangle |0 \ldots 0\rangle = \frac{1}{s} |0\rangle \widetilde{U} |\psi\rangle \tag{28}$$

What is probability of success (000 on ancilla) ?

$s = 2 \qquad p(0\ldots0| = \frac{1}{4}$

# Oblivious amplitude amplification

good

$$W|0\rangle_{\text{flag}}|\psi\rangle_{\text{data}} = \sin\theta\,|0\rangle_{\text{flag}} U|\psi\rangle_{\text{data}} + \cos\theta\,|\text{bad}\rangle\,, \tag{29}$$

where $\left(|0\rangle\langle 0|_{\text{flag}} \otimes \mathbb{I}_{\text{data}}\right)|\text{bad}\rangle = 0$.

$WRW^\dagger R$ acts as a rotation

$$\left(WRW^\dagger R\right)^k W|0\rangle|\psi\rangle = \sin\left((2k+1)\theta\right)|0\rangle U|\psi\rangle + \cos\left((2k+1)\theta\right)|\text{bad}\rangle\,, \tag{30}$$

where $R$ is the reflection around all zero in the flag register

$R = 2|0\rangle\langle 0| \otimes \mathbb{I} - \mathbb{I}$.

$R$ is not a reflection around the initial state.

prob $= \frac{1}{4}$ $\xrightarrow{\text{1. round AA}}$ 1

$(|0\rangle\langle 0| \otimes \mathbb{I})\, W\,|\psi\rangle\,|0\ldots 0\rangle = \frac{1}{s}\,|0\rangle\,\widetilde{U}\,|\psi\rangle$. If $s$ is close to 2, we can use $W$ to implement oblivious amplitude amplification.

Applying $-WRW^{\dagger}RW$ where $R = \mathbb{I} - (|0\rangle\langle 0| \otimes \mathbb{I})$ results in the state $|0\rangle\,\widetilde{U}\,|\psi\rangle$ with high accuracy.

product form. $O(\varepsilon^{m})$

Complexity is

$$\mathcal{O}\left(\tau\frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right), \tag{31}$$

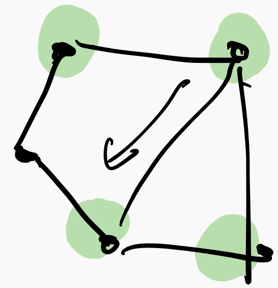
where $\tau = L\,\|H\|_{\max}\,t$ for $\sqrt{L}$-sparse matrices.

# Quantum walk and quantum signal processing

# Alternative random walk

One step of a random walk

$$\vec{p}(t+1) = A\vec{p}(t). \tag{32}$$



where $A$ is a stochastic matrix.

Continuous version

$$\frac{d}{dt}\vec{p}(t) = A\vec{p}(t) \tag{33}$$

is a diffusion process/stochastic equation. The solution is

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$$p(t) = e^{At}p(0). \tag{34}$$

# Continuous-time quantum walk

Replace $A \to -iH$.

# Continuous-time quantum walk

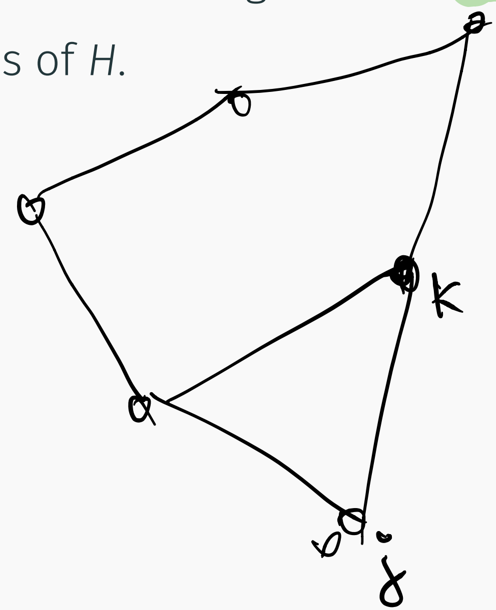
Replace $A \to -iH$.

We recover the Schrödinger equation. How do CTQW walks compare with quantum walks from the last lecture?

# Quantum walks (review)

Last week Troy defined discrete time quantum walks on a larger Hilbert space $|j, k\rangle$.

Walk operator $W$ has eigenvalues $\pm e^{\pm i \cos^{-1} E}$ where $-1 < E \leq 1$ are eigenvalues of $H$.




- W
  A adj. matrix
  Ham. sim
  $e^{-iE}$
- walk
  $e^{-i\cos^{-1}E}$

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Walk operator $W$ has eigenvalues $\pm e^{\pm i \cos^{-1} E}$ where $-1 < E < 1$ are eigenvalues of $H$.

We can use a quantum walk on the graph corresponding to the Hamiltonian for time evolution.

# Quantum walks for Hamiltonian simulation

QPE (H) → E QPE(W) $\cos^{-1}(E)$

We can use $W$ directly to compute energies using phase estimation

For evolution, we need to transform the eigenvalue spectrum

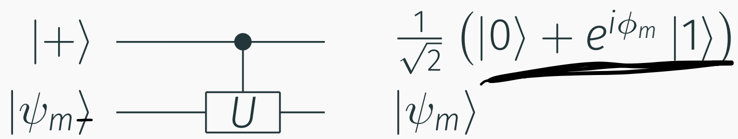
$$\pm e^{\pm i \cos^{-1} E_j t} \to e^{-iE_j t} \quad (35)$$

A "quantum signal processing" algorithm achieves the optimal complexity

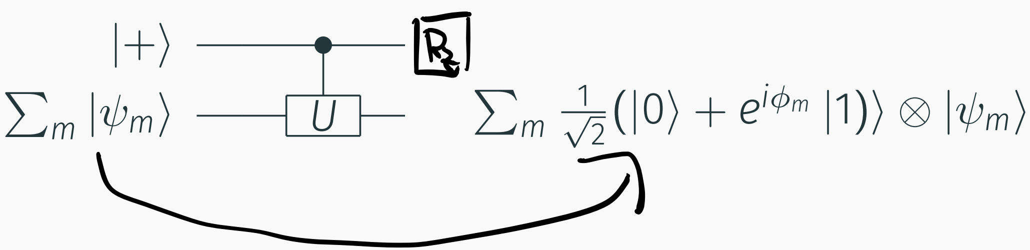
$$O\left(\tau + \frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right), \quad (36)$$

where $\tau = d\,||H||_{max}\,t$.

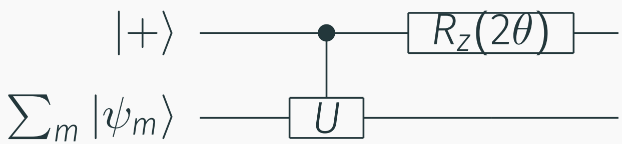
Let $\cancel{\mathcal{U}}$ $U$ be a unitary with eigenvalues $e^{i\phi_m}$ and $|\psi_m\rangle$ its eigenvector




Now take a superposition of eigenstates



# Phase kickback




$$\sum_m \frac{1}{\sqrt{2}}(|0\rangle + e^{i\theta+\phi_m}|1\rangle) \otimes |\psi_m\rangle$$

$Z$ measurement:

$e^{i\theta+\phi_m}$

0: $\sum_m |\psi_m\rangle$

1: $e^{i\theta} U \sum_m |\psi_m\rangle$

$X$ measurement (=apply Hadamard at the end)

+: $\propto \sum_m \left(1 + e^{i(\theta+\phi_m)}\right) |\psi_m\rangle$

−: $\propto \sum_m \left(1 - e^{i(\theta+\phi_m)}\right) |\psi_m\rangle$

$U|\psi\rangle$

modifying the ancilla applies a modified operation $f(U)|\psi\rangle$

# Goal

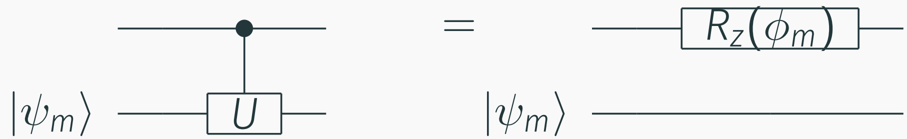
Given a unitary $U$ with eigenstates $|\psi_m\rangle$ and corresponding eigenvalues $e^{i\phi_m}$

$$U \to V = \sum_m e^{ih(\phi_m)} |\psi_m\rangle\langle\psi_m|$$

note: the spectrum of $\cancel{W}$ $U$ doesn't need to be known

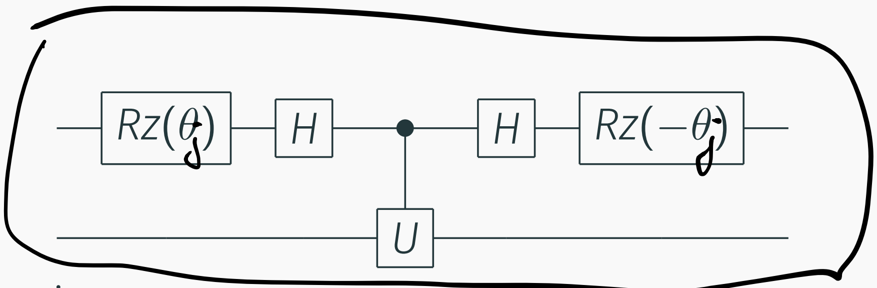
# Quantum signal processing

1. Signal transduction




2. Signal transformation

   Repeatedly apply control-~~W~~ U and rotations to modify the spectrum of ~~W~~ U




3. Signal projection

   Measure the ancilla in the X basis and post-select on + outcome

# Other resources

Q# documentation Simulating Hamiltonian dynamics

Andrew Child's PhD thesis

My PhD thesis