

4. Quantum Phase Estimation

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Quantum Phase Estimation

- Quantum Phase Estimation (QPE) is one of the most widely used subroutines in quantum algorithms.
- Setup: We have a unitary \underline{U} and its eigenstate $\underline{|n\rangle}$, with an eigenvalue $e^{i\theta_n}$.
- QPE is an algorithm to measure θ_n .
- QPE serves two purposes in Quantum Simulation.
 - Estimating ground state energy.
 - Ground state preparation

$$U|n\rangle = e^{i\theta_n}|n\rangle$$

How QPE works

- There are two ingredients.
 1. Phase kick-back
 2. Quantum Fourier Transform

Phase kickback

- Simplest case: Suppose we have an ability to compute a function $f(x) \in \{0,1\}$. We wish to implement a unitary transformation:

$$\underline{|x\rangle \rightarrow (-1)^{f(x)} |x\rangle .}$$

- How would we do this?

$$|x\rangle|y\rangle \xrightarrow{\sim} |x\rangle|y \oplus f(x)\rangle$$

↓
addition mod 2.

$$|x\rangle \frac{|0\rangle - |1\rangle}{\sqrt{2}} \rightarrow |x\rangle \frac{|f(x)\rangle - |1 \oplus f(x)\rangle}{\sqrt{2}} = \begin{cases} f(x)=0 : |x\rangle \frac{|0\rangle - |1\rangle}{\sqrt{2}} \\ f(x)=1 : |x\rangle \frac{|1\rangle - |0\rangle}{\sqrt{2}} = -|x\rangle \frac{|0\rangle - |1\rangle}{\sqrt{2}} \end{cases}$$

$$\sum_x \alpha_x |x\rangle \frac{|0\rangle - |1\rangle}{\sqrt{2}} \rightarrow \sum_x \alpha_x (-1)^{f(x)} |x\rangle \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

Phase kickback

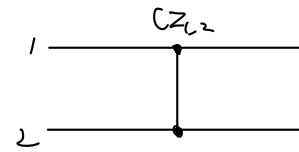
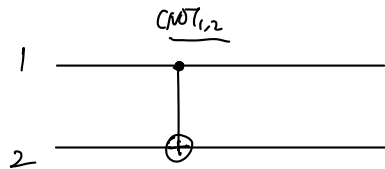
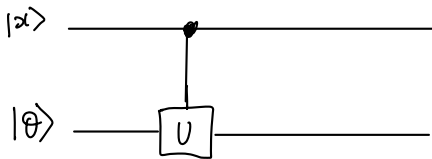
- More general case: Suppose we have an ability to implement a unitary U . We wish to implement

$$\underline{|x\rangle \rightarrow e^{i\theta x} |x\rangle},$$

where $e^{i\theta}$ is one of the eigenstates of U .

- How would we do this?

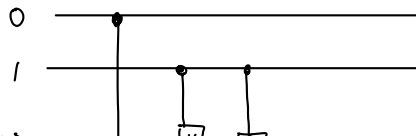
$$U|\theta\rangle = e^{i\theta} |\theta\rangle$$



$$\begin{aligned} |0\rangle|\theta\rangle &\rightarrow |0\rangle|\theta\rangle \\ |1\rangle|\theta\rangle &\rightarrow |1\rangle|\theta\rangle e^{i\theta} \end{aligned}$$

$$|x\rangle|\theta\rangle \rightarrow |x\rangle|\theta\rangle e^{i\theta x}$$

$$\begin{aligned} 0 &= 00 \\ 1 &= 01 \\ 2 &= 10 \\ 3 &= 11 \end{aligned}$$



$$|x\rangle|\theta\rangle = |x\rangle|\theta\rangle e^{i\theta x}$$

Phase kickback, in superposition

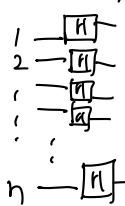
- Instead of beginning with $|x\rangle$, suppose we begin in the $\sum_{x=0}^{2^n-1} \frac{1}{2^{n/2}} |x\rangle$.
- After applying the phase kickback operation, we get a “momentum eigenstate.”

$$\sum_{x=0}^{2^n-1} \frac{1}{2^{n/2}} |x\rangle \xrightarrow{\text{Phase kickback}} \sum_{x=0}^{2^n-1} \frac{1}{2^{n/2}} e^{i\theta x} |x\rangle$$

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{i k x} |x\rangle dx$$

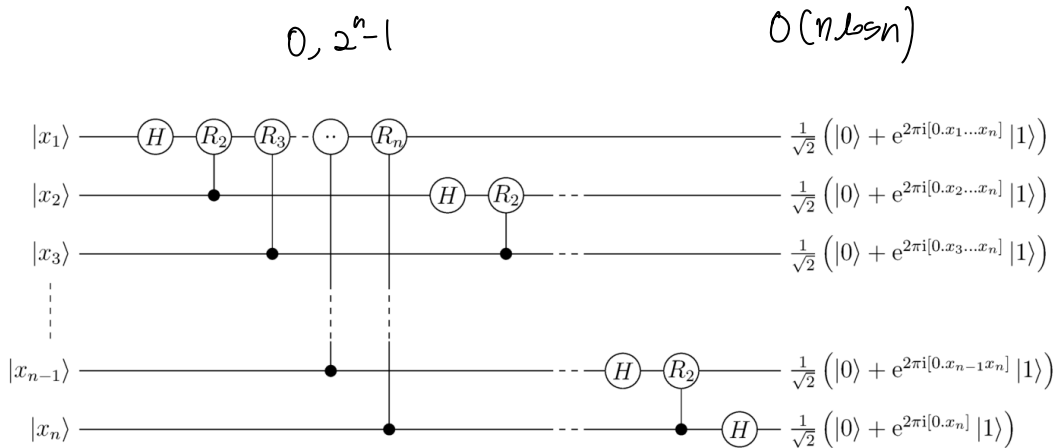
$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$H |0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$



Quantum Fourier Transform

- Quantum Fourier Transform can be performed using $O(n^2)$ one- and two-qubit gates.



Quantum Phase Estimation in a Nutshell

- In the infinite-precision limit, QPE performs a non-destructive measurement in the eigenbasis of U .
- Procedure: Phase kickback in uniform superposition $\xrightarrow{\text{Inverse}}$ QFT.
- Often the cost of QFT is subleading compared to the implementation of U .
- The dominant cost is $\sim 2^n$ times the cost of implementing controlled- U .
- Precision $\approx 1/2^n$.

$$\begin{aligned}
 \frac{1}{\sqrt{2^n}} \sum_x e^{i\theta x} |x\rangle &\xrightarrow{\text{QFT}^{-1}} \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} e^{i\theta x} \sum_{k=0}^{2^n-1} \frac{1}{\sqrt{2^n}} e^{-\frac{2\pi i k x}{2^n}} |k\rangle \\
 &= \frac{1}{2^n} \sum_{k=0}^{2^n-1} \sum_{x=0}^{2^n-1} e^{i x \left(\theta - \frac{2\pi k}{2^n} \right)} |k\rangle
 \end{aligned}$$

$\theta \approx \frac{2\pi k}{2^n}$

$k \approx \frac{2^n \theta}{2\pi}$

$\sim \frac{2\pi}{2^n} = \epsilon \approx \frac{1}{N}$

$2^n = N$

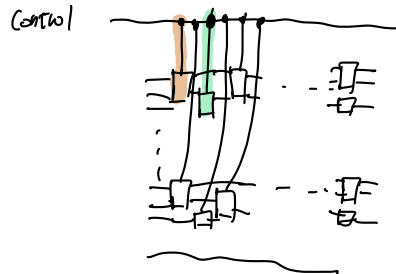
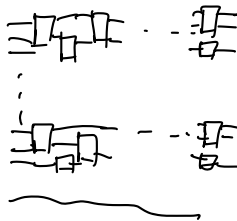
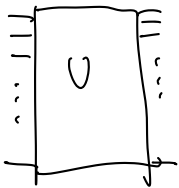
Controlled- U

- The cost of implementing controlled- U is comparable to the cost of implementing U .

1) "Momentum eigenstate": Controlled- U

2) QFT⁻¹

$$U = e^{-iHt}$$



$$\mathcal{O}(\text{Implementing } U) = \mathcal{O}(\text{Implementing controlled-}U)$$

Applications

$|n\rangle$

- We already established that e^{-iHt} can be implemented efficiently.
- Thus, e^{-iHt} can be also implemented efficiently.
- Therefore, we can compute the energy of H in time $O(1/\epsilon)$, where ϵ is the precision.
 - This is better than the naive approach of $O(1/\epsilon^2)$.
 - This can lead to a huge difference in quantum chemistry applications.
 - And, there are added benefits. (Next slide)

$$H = \sum_a h_a$$

$$\langle \psi | h_a | \psi \rangle$$

Eigenstate assumption

- We assumed that we have access to an eigenstate.
- But didn't we already say that preparing an eigenstate (e.g., ground state) is hard in general?
- More realistically, the initial state will be generally of the following form:

$$|\psi\rangle = \sqrt{1 - p_n} |n\rangle + \sqrt{p_n} |n_\perp\rangle.$$

$$|\psi\rangle = \alpha|\phi\rangle + \beta|1\rangle + \gamma|2\rangle$$

$$e^{i\theta_0} e^{i\theta_1} e^{i\theta_2}$$

$\theta_0 = \theta_1 \quad \theta_1 \neq \theta_2$

Prob $|\alpha|^2$: Measure $e^{i\theta_0}$ $|2\rangle$
 $|\alpha|^2$: $e^{i\theta_0}$ $\frac{\alpha|\phi\rangle + \beta|1\rangle}{|\alpha|^2 + |\beta|^2}$

QPE, applied to non-eigenstate

- Suppose we begin with the following state:

$$|\psi\rangle = \sum_n \alpha_n |n\rangle. \quad U = e^{-iHt}$$

- If we apply QPE (in the infinite precision limit), we will measure $|n\rangle$ with probability $|\alpha_n|^2$.
- Repeating this many times, you can get a histogram of eigenstates, each labeled by different phases. E_0, E_1, E_2, \dots
- To prepare an eigenstate corresponding to the phase $e^{i\theta_n}$, repeat QPE until you measure θ_n . If you succeed, halt.

But we rarely even know $\theta_n \dots$

- Sometimes we do, e.g., models for which we know the ground state is exactly zero. In that case, we simply repeat measuring θ_n until we get $\theta_n = 0$.
- More generally, we don't know the exact ground state energy. In that case, we simply repeat the measurement many times and pick the smallest θ_n . This will be our "guess" for the ground state energy.
- If the overlap with the true ground state is α , the probability we fail to get the correct ground state energy after m repetition is $(1 - |\alpha|^2)^m$.

$$\alpha = \frac{1}{\sqrt{5}}$$

$$m \gg 100$$



Application: Ground state preparation

1. Repeat QPE many times to get a good guess on the ground state energy.
 2. Repeat QPE many times until you measure your guess of the ground state energy.
 3. Done.
-
- Obviously, this works well only if we can create some state with nonzero overlap with the ground state.

Summary

$$\langle \psi | X_i | \psi \rangle = 0$$

$$\begin{cases} \Pr[X_i = +1] = \frac{1}{2} \\ \Pr[X_i = -1] = \frac{1}{2} \end{cases}$$

$$\frac{N_+ - N_-}{N} \approx \quad N_+ + N_- = N$$

$$\text{Deviation} \sim \frac{1}{\sqrt{N}} \lesssim \epsilon \quad N \geq \frac{1}{\epsilon^2}$$

- QPE is very useful for
 - ❖ energy estimation
 - ❖ ground state preparation
- QPE cost $\approx \frac{1}{\epsilon}$ times Hamiltonian simulation cost for a unit time.

$$H = \sum_{i=1}^N \alpha_i P_i$$

$$H' = \frac{\sum_{i=1}^N \alpha_i P_i + \sum_{i=1}^N |\alpha_i| I}{2 \sum_{i=1}^N |\alpha_i|}$$