e^{-iHt}

Lecture 3: Hamiltonian Simulation Algorithms (Pt. 1)

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Motivation

Interacting quantum many-body systems are difficult to solve unless there is a special structure underlying the problem, e.g., large symmetry group, commutation of the local terms in the Hamiltonian formulation, etc.

Wish list

1. Algorithm for preparing the ground state
2. Algorithm for preparing a thermal state
3. Dynamics

Ground State

$H = \sum_i J_i S_i \rightarrow Z_1 Z_2 Z_3 \quad Z_4 Z_5, Z_5 Z_6, \ldots$ (J_i: ± 1)

There is a good reason to believe that no efficient method for preparing ground state of an arbitrary Hamiltonian (even if the Hamiltonian is local) exists.

Basic Argument

1. One can reduce any problem in NP to the problem of checking whether the ground state energy of a spin glass with coupling ± 1 is 0 or not.
2. If there is an efficient quantum algorithm for preparing the ground state, one can compute the energy efficiently by measuring individual terms in the Hamiltonian.
3. In particular, we can check if the ground state energy is 0 or not efficiently.
4. Despite many attempts, there does not seem to be an efficient quantum (and of course, classical) algorithm that can solve problems in NP.
   - Only this argument is not rigorous.
5. Therefore, probably no quantum algorithm can find the ground state

Thermal state

For classical systems, the Metropolis algorithm is the standard algorithm approach. While there is no general rigorous guarantee on the efficiency, this works quite well in many situations. However, for quantum systems the sane approach fails to work because of the sign problem (except for special cases).

It turns out that there is a quantum version of Metropolois algorithm [Temme et al. (2009)]. Again, there is no guarantee on the efficiency, but under plausible assumptions on the density of states and eigenstate thermalization hypothesis, one can expect this to work efficiently [Chen, Brandao (2021)].

Part 1. Quantum Phase Estimation

Key subroutine: Quantum Phase Estimation

In both ground state and thermal state preparation, a technique known as the Quantum Phase Estimation (QPE) is extensively used. This is the standard technique in quantum computing, which we will discuss now.

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QPE (Ideal)

Let $H = \sum_n E_n |n\rangle\langle n|$ be the eigendecomposition of a Hamiltonian H. What QPE achieves is this:

$$|n\rangle \otimes |0\rangle \xrightarrow{U} |n\rangle \otimes |E_n\rangle.$$

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$$|n\rangle \otimes |0\rangle \to |n\rangle \otimes |E_n\rangle.$$

$$H = \begin{pmatrix} 0.50001 & 0 \\ 0 & 0.7500001 \end{pmatrix}$$

$E_1' = 0.5 = 0.10$ (binary) $\quad E_2' = 0.75 = 0.11$

Issue: E_n cannot be specified with infinite precision in general. So in reality, what we are really doing is

$|E_1'\rangle = |1\rangle|0\rangle$

$|E_2'\rangle = |1\rangle|1\rangle$

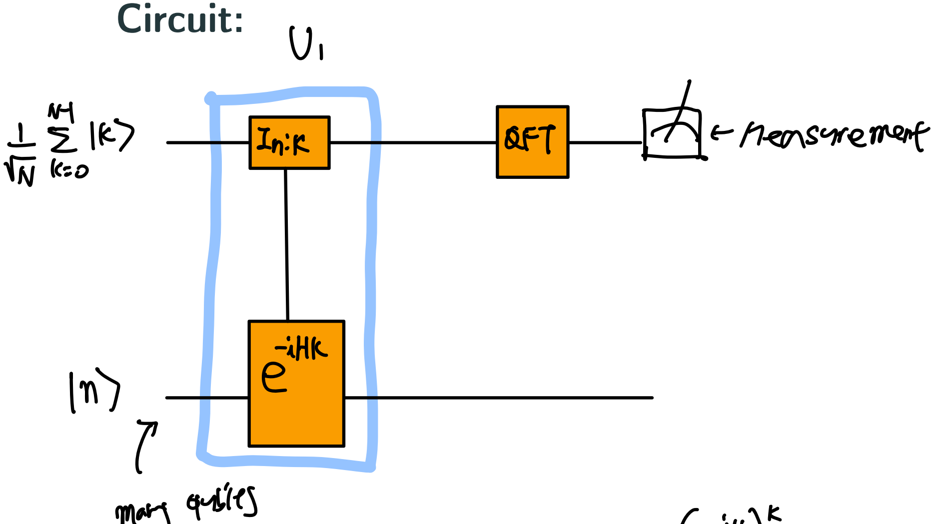
$$|n\rangle \otimes |0\rangle \to |n\rangle \otimes |E_n'\rangle,$$

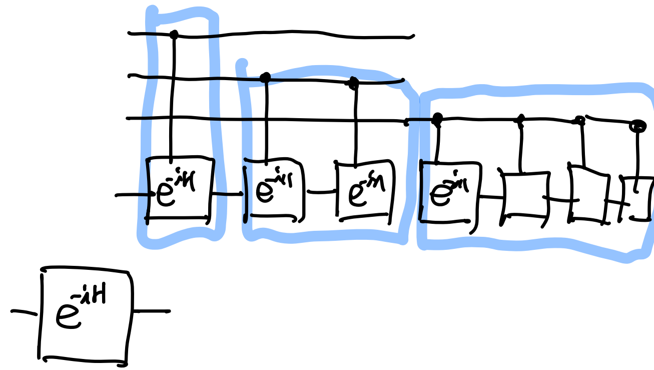
where E_n' is an approximation of E_n up to some fixed precision.

QPE can be implemented using two subroutines.

- Time evolution: e^{-iHt} for a set of values for $t \in \mathbb{R}$.
- Quantum Fourier Transform: Discrete version of the Fourier Transform.

Circuit:



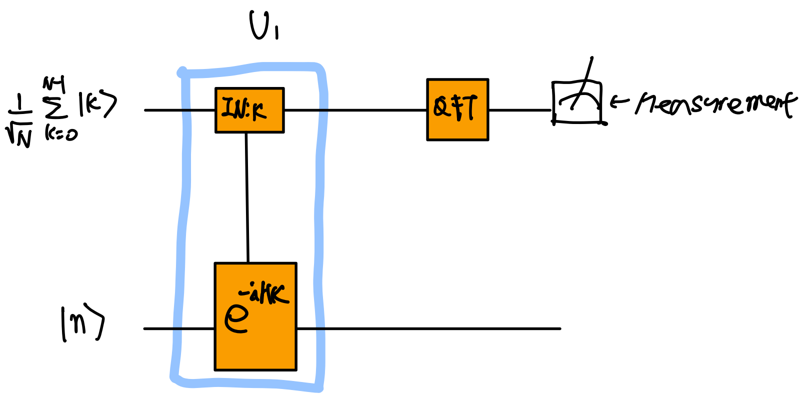


$$U_1(|k\rangle \otimes |n\rangle) = |k\rangle \otimes \left(e^{-iH}\right)^k |n\rangle$$

Quantum Fourier Transform: $|x\rangle \to \frac{1}{\sqrt{N}} \sum_{y=0}^{N-1} e^{\frac{2\pi i x}{N} y} |y\rangle$

integer

Circuit:



Analysis: $\left(\frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle\right) \otimes |n\rangle \xrightarrow{U_1} \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle \otimes e^{-iHk} |n\rangle = \left(\frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{-iE_n k} |k\rangle\right) \otimes |n\rangle$

$$\xrightarrow{QFT} \frac{1}{N} \sum_{k=0}^{N-1} \sum_{y=0}^{N-1} e^{-iE_n k} e^{\frac{2\pi i k y}{N}} |y\rangle \otimes |n\rangle$$

$$= \sum_{y=0}^{N-1} \left(\frac{\sum_{k=0}^{N-1} e^{2\pi i k \left(\frac{y}{N} - \frac{E_n}{2\pi}\right)}}{N} \right) |y\rangle \otimes |n\rangle \qquad \approx \delta\left(\frac{y}{N} - \frac{E_n}{2\pi}\right)$$

$$\approx \left| \frac{E_n}{2\pi} \cdot N \right\rangle \otimes |n\rangle$$

QPE as an eigenstate filter

Now suppose we begin with a superposition of the energy eigenstate. After applying QPE and measuring the energy, what do we get?

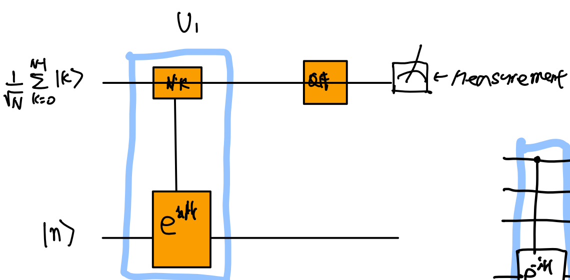
$$|0\rangle \otimes |n\rangle \xrightarrow{QPE} |E_n'\rangle \otimes |n\rangle$$

Energy eigenstate

$$|0\rangle \otimes \left(\sum_n \alpha_n |n\rangle \right) \xrightarrow{QPE} \sum_n \alpha_n |E_n'\rangle \otimes |n\rangle \rightarrow \text{Prob } |\alpha_n|^2$$

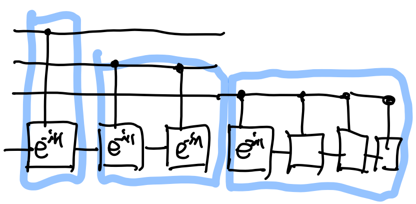
measure

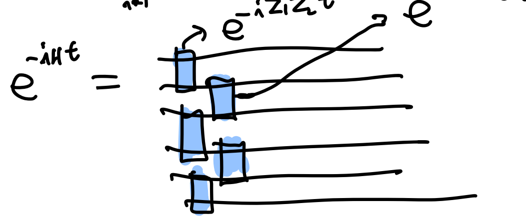
Post-measurement state will be $|n\rangle$

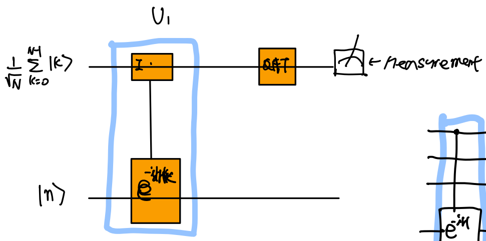


$$|\psi\rangle = \sqrt{\tfrac{1}{2}}\,|\psi_0\rangle + \sqrt{\tfrac{1}{2}}\,|\psi_e\rangle$$

$$H = \sum_{i=1}^{N} Z_i Z_{i+1}$$







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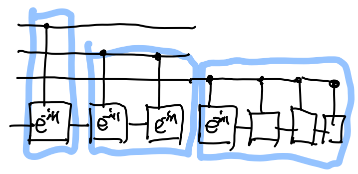

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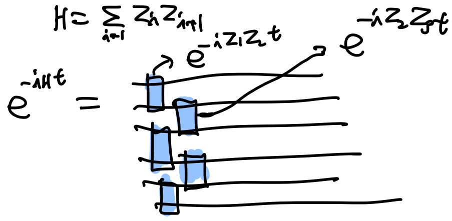
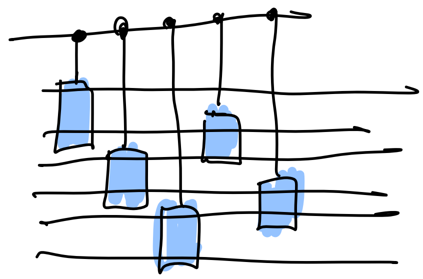
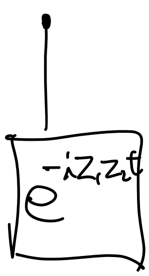
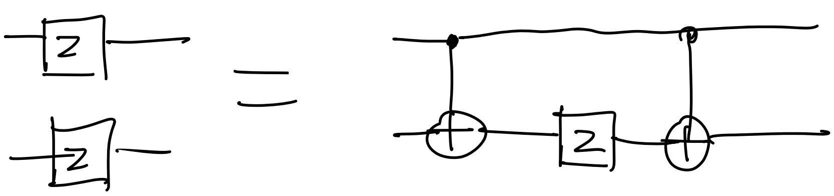


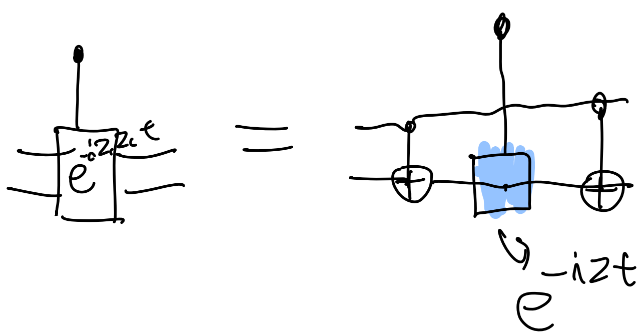
controlled version





$$Z_1 Z_2 = CX \quad Z_2 \quad CX$$





QPE: Summary

- QPE is the key subroutine in many quantum algorithms (ground state preparation, thermal state preparation, ...).
- QPE can be decomposed into controlled-time evolution and quantum Fourier transform.
  - Almost always the complexity of the time evolution dominates that of quantum Fourier transform.

$$\boxed{\text{Many algorithms} \to \text{QPE} \to \text{Time evolution}}$$

Part 2. Time evolution: Basics

Time evolution

1. Trotter-Suzuki decomposition
2. Linear Combination of Unitaries
3. Quantum Signal Processing/Qubitization/Quantum Singular Value Transformation

2010s

The goal

It is hopeless to implement e^{-iHt} with zero error. What one should aim for is to implement U such that

$$U|\psi\rangle \approx e^{-iHt}|\psi\rangle$$

for any state $|\psi\rangle$. More precisely, we will often have an error ϵ in mind that we are wishing to tolerate, in which case we want

$$\| U|\psi\rangle - e^{-iHt}|\psi\rangle \| \leq \epsilon$$

for any state $|\psi\rangle$, where $\||\phi\rangle\| = \sqrt{\langle\phi|\phi\rangle}$.

Operator norm

Clearly, this means that we want

$$\max_{|\psi\rangle} \|(U - e^{-iHt})|\psi\rangle\| \leq \epsilon$$

. For a general operator O, we can define a norm

$$\|O\| = \max_{|\psi\rangle} \|O|\psi\rangle\|.$$

This is known as the operator norm.

Construct U s.t. $\| U - e^{-iHt} \| \leq \epsilon$

Operator norm: Properties

1. Triangle inequality $\|O+O'\| \le \|O\| + \|O'\|$
2. $\|OO'\| \le \|O\|\|O'\|$
3. $\|U\| = 1$ for any unitary U.

$$\|U\| = \max_{|\psi\rangle} \| U|\psi\rangle \|$$

$$= \max_{|\psi\rangle} \sqrt{\langle\psi|U^\dagger U|\psi\rangle}$$

$$= 1$$

Suppose $\|U - e^{-iHt}\| \leq \epsilon$.

$$\underbrace{\|U^n - e^{-iHnt}\| \leq ?}$$

$$\|U^2 - e^{-2iHt}\| = \|U(U - e^{-iHt}) + Ue^{-iHt} - e^{-2iHt}\|$$

$$= \|U(U - e^{-iHt}) + (U - e^{-iHt})e^{-iHt}\|$$

Triangle

$$\leq \|U(U - e^{-iHt})\| + \|(U - e^{-iHt})e^{-iHt}\|$$

submultiplicativity

$$\leq \underset{1}{\|U\|}\,\|U - e^{-iHt}\| + \|U - e^{-iHt}\|\,\underset{1}{\|e^{-iHt}\|}$$

$\|U\| = 1$

$$= 2\|U - e^{-iHt}\|$$

$$\leq 2\epsilon$$

$$\|U^n - e^{-iHnt}\| \leq n\epsilon$$

Some exercises

Suppose $\|U - e^{-iHt}\| \leq \epsilon$.

$$|\langle\psi U^\dagger OU|\psi\rangle - \langle\psi|e^{iHt}Oe^{-iHt}|\psi\rangle| \leq ?$$

Part 3. Trotter-Suzuki decomposition

Trotter-Suzuki decomposition

Let $H = A + B$.

$$e^{-iHT} = \lim_{N\to\infty} (e^{-iAT/N} e^{-iBT/N})^N.$$

We will take N to be finite and estimate the error.

$$\lim_{N\to\infty} \quad e^{-iAT\frac{1}{N}} e^{-iBT\frac{1}{N}} \to \left(I - iA\frac{T}{N}\right)\left(I - iB\frac{T}{N}\right) + \cdots$$

$$= \left(I - i(A+B)\frac{T}{N}\right) + \cdots$$

$$\approx e^{-i(A+B)T/N}$$

Taylor Expansion

Let $H = A + B$.

$$e^{-iHT} = \lim_{N\to\infty} (e^{-iAT/N} e^{-iBT/N})^N.$$

Taking $t = T/N$ to be infinitesimally small, we can compare

$$e^{-iHt} \text{ vs. } e^{-iAt} e^{-iBt}$$

order by order.

$$I - iHt + \frac{(-iHt)^2}{2!} + \cdots \quad \text{vs.} \quad \underset{+\cdots}{(I - iAt)} \; \underset{+\cdots}{(I - iBt)}$$

Error $O(t^2)$

Evolve for time T $\rightarrow$ $t = \frac{T}{N}$

Total Error $\rightarrow$ $O\left(\left(\frac{T}{N}\right)^2 \cdot N \right) = O\left(\frac{T^2}{N}\right)$

Differential equation

The issue with the previous approach is that the bound is very lousy when A and B commute. One approach to avoid this problem is to inspect the equation.

$$\frac{d}{dt}\left(e^{iAt}e^{iBt}e^{-iHt}\right) = ?$$

$$\frac{d}{dt}\left(e^{iAt}e^{iBt}e^{-iHt}\right) = i\Big(e^{iAt}Ae^{iBt}e^{-iHt} + e^{iAt}e^{iBt}\cancel{B}e^{-iHt} - e^{iAt}e^{iBt}(A+\cancel{B})e^{-iHt}\Big)$$

$$= i\left(e^{iAt}\left(Ae^{iBt} - e^{iBt}A\right)e^{-iHt}\right)$$

$$\left\| e^{iAt}e^{iBt}e^{-iHt} - I \right\| = \left\| \int_0^t \frac{d}{dt'}\left(e^{iAt'}e^{iBt'}e^{-iHt'}\right) dt' \right\|$$

$$\|e^{iAt}\| \le 1 \qquad \|e^{-iHt}\| \le 1$$

$$\le \int_0^t \left\| \frac{d}{dt'}\left(e^{iAt'}e^{iBt'}e^{-iHt'}\right) \right\| dt'$$

$$\le \int_0^t \left\| Ae^{iBt'} - e^{iBt'}A \right\| dt'$$

$$= \int_0^t \left\| e^{-iBt'}Ae^{iBt'} - A \right\| dt' = \int_0^t \int_0^{t'} \left\| e^{-iBt''}[A,B]e^{iBt''} \right\| dt'' dt'$$

$$\le \frac{1}{2}t^2 \left\| [A,B] \right\|$$

Trotter-Suzuki decomposition

Thus, we have concluded that the Trotter-Suzuki decomposition yields an error of $O(\|[A,B]\|t^2)$. For approximating e^{-iHT}, the error then becomes:

$$O(\|[A,B]\|T^2/N),$$

which we can systematically reduce by choosing large N.

Case study: Transverse field Ising model

$$H = \sum_{i=1}^{n} \lambda Z_i Z_{i+1} + X_i$$

$$\| [Z_1 Z_2, X_1] \| = \| 2 Y_1 Z_2 \| = 2$$

$A = \sum_i \lambda Z_i Z_{i+1}$ $\quad$ $B = \sum_i X_i$

$$\epsilon = O\left(T^2 \|[A,B]\| / N\right)$$

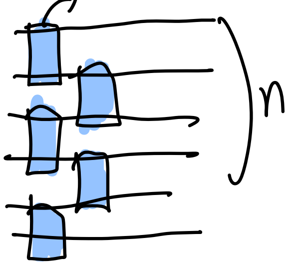
$$e^{-iHT} \to \left(e^{-iA\frac{T}{N}} e^{-iB\frac{T}{N}}\right)^{\frac{N}{T}}$$

Single Trotter step

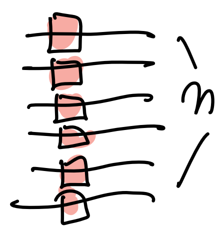
$O(n)$ gates

Total # of Trotter steps

$e^{-i\lambda Z_1 Z_2 \frac{T}{N}}$

$e^{-iA\frac{T}{N}} =$ 

$O(n)$

$e^{-iB\frac{T}{N}} =$ 

$O(n)$

Gate complexity $= O(Nn)$

$$O\left(\frac{T^2 n^3}{\epsilon}\right)$$

$$\|[A,B]\| = \|AB - BA\| \le \cancel{\#}\, (\|AB\| + \|BA\|)$$
$$\le 2\|A\|\,\|B\|$$
$$\le O(n^2)$$

$$\to \quad N = O\left(\frac{T^2 n^2}{\epsilon}\right)$$

Higher order Trotter-Suzuki

We can consider decompositions that cancel higher order terms of the Taylor expansion, e.g.,

$e^{-iBt} e^{-iAt}$

$$e^{-iHt} \text{ vs. } e^{-i\frac{A}{2}t} e^{-iBt} e^{-i\frac{A}{2}t}.$$

These higher order decompositions yield higher order suppression in terms of N.

* Useful reference: arXiv:1912.08854

Summary

Trotter-Suzuki decomposition:

- Pro: Very simple and intuitive. Works well in practice, too.
- Con: Scaling in inverse error is polynomial. This is not optimal.

Next lecture: Post-Trotter methods