* Trotter-Suzuki decomposition: Intro

Trotter-Suzuki decomposition is the simplest method for Hamiltonian simulation. The basic idea is simple. Suppose $H = A + B$. For short time,

$$
\begin{aligned}
e^{-iHt} &\approx I - iHt \\
&= I - iAt - iBt \\
&\approx (I - iAt)(I - iBt) \\
&\approx e^{-iAt} e^{-iBt},
\end{aligned}
$$

with the error becoming small as $t \to 0$.

> * A useful fact
> $\|UA\| = \|AU\| = \|A\|$ for any unitary U. In fact, $\|UA\|_p = \|AU\|_p = \|A\|_p$.

Now let's bound $\| e^{-iHt} - e^{-iAt} e^{-iBt} \|$.

$$
\begin{aligned}
\| e^{-iHt} - e^{-iAt} e^{-iBt} \| &= \| e^{-iHt} (I - e^{iHt} e^{-iAt} e^{-iBt}) \| \\
&= \| I - e^{iHt} e^{-iAt} e^{-iBt} \| \\
&= \left\| -\int_0^t \frac{d}{dt'} e^{iHt'} e^{-iAt'} e^{-iBt'} \, dt' \right\| \\
&\leq \int_0^t \left\| \frac{d}{dt'} e^{iHt'} e^{-iAt'} e^{-iBt'} \right\| dt' \\
&= \int_0^t \| e^{iHt'} (B e^{-iAt'} - e^{-iAt'} B) e^{-iBt'} \| \, dt' \\
&= \int_0^t \| [B, e^{-iAt'}] \| \, dt'
\end{aligned}
$$

$\int_0^t f'(t') \, dt'$

$$
\begin{aligned}
\| [B, e^{-iAt'}] \| &= \| e^{iAt'} B e^{-iAt'} - B \| \\
&\leq \int_0^{t'} \left\| \frac{d}{dt''} \left(e^{iAt''} B e^{-iAt''} \right) \right\| dt'' \\
&= \int_0^{t'} \| e^{iAt''} [A, B] e^{-iAt''} \| \, dt' \\
&= \int_0^{t'} \| [A, B] \| \, dt''
\end{aligned}
$$

$$= \int_0 \| [A,B] \| dt$$

$$= \| [A,B] \| t'$$

Thus, $$\| e^{-iHt} - e^{-iAt} e^{-iBt} \| \leq \int_0^t \| [A,B] \| t' dt'$$

$$= \frac{1}{2} t^2 \| [A,B] \|$$

ex) $H = \underbrace{\left(\sum_{i=1}^{n-1} Z_i Z_{i+1} \right)}_{A} + \underbrace{\left(\sum_{i=1}^{n} X_i \right)}_{B}$

* Multi-term case

Let $H = H_1 + \cdots + H_N$

$$\| e^{-iHt} - e^{-iH_1 t} e^{-i(H_2 + \cdots H_N)t} \| \leq \frac{1}{2} t^2 \| [H_1, H_2 + \cdots + H_N] \|$$

$$\| e^{-i(H_2 + \cdots + H_N)t} - e^{-iH_2 t} e^{-i(H_3 + \cdots + H_N)t} \| \leq \frac{1}{2} t^2 \| [H_2, H_3 + \cdots + H_N] \|$$

$$\| e^{-iH_1 t} e^{-i(H_2 + \cdots + H_N)t} - e^{-iH_1 t} e^{-iH_2 t} e^{-i(H_3 + \cdots + H_N)t} \| \leq$$

Thus,
$$\| e^{-iHt} - e^{-iH_1 t} e^{-iH_2 t} \cdots e^{-iH_N t} \| \leq \frac{1}{2} t^2 \sum_{j>2} \sum_{i=1}^{N-1} \| [H_i, H_j] \|$$

ex) $H = \sum_{klmn} h_{klmn} P_{klmn}$ (Not all of them commute.)

* Long-time dynamics

So far, our strategy to approximate e^{-iHt} by $e^{-iAt} e^{-iBt}$ works only for short time (t). We can extend this to long-time dynamics by breaking it into multiple time steps.

Say we want to approximate e^{-iHT}. Break it into N steps,

$$e^{-iHT} = \left(e^{-iH\frac{T}{N}}\right)^N$$

$$\left\| e^{-iH\frac{T}{N}} e^{-iA\frac{T}{N}} e^{-iB\frac{T}{N}} \right\| \le \frac{1}{2}\left(\frac{T}{N}\right)^2 \| [A,B] \|$$

Lemma. If $\|U-\tilde{U}\| \le \varepsilon$, $\|U^n - \tilde{U}^n\| \le \varepsilon n$. $(U, U' :$ Unitary$)$

proof. $\|U^n - \tilde{U}^n\| = \| U(U^{n-1} - \tilde{U}^{n-1}) + (U-\tilde{U})\tilde{U}^{n-1} \|$

$$\begin{aligned}
&\le \| U(U^{n-1} - \tilde{U}^{n-1}) \| + \| (U-\tilde{U})\tilde{U}^{n-1} \| \\
&= \| U^{n-1} - \tilde{U}^{n-1} \| + \| U - \tilde{U} \| \\
&\le \| U^{n-1} - \tilde{U}^{n-1} \| + \varepsilon
\end{aligned}$$

$\therefore \|U^n - \tilde{U}^n\| \le \varepsilon n.$ ■

Thus, $\left\| e^{-iHT} - \left(e^{-iA\frac{T}{N}} e^{-iB\frac{T}{N}}\right)^N \right\| \le \frac{1}{2}\left(\frac{T}{N}\right)^2 N \, \|[A,B]\|$

$$= \frac{T^2}{2N} \|[A,B]\|.$$

So, by taking $N = O\left(\frac{T^2 \|[A,B]\|}{\varepsilon}\right)$, we can ensure ε error

Similarly, for $H = H_1 + \dots + H_M$, we can take

$$N = O\left(\frac{T^2 \sum_{j>2} \sum_{i=1}^{N} \| [H_i, H_j] \|}{\varepsilon} \right)$$

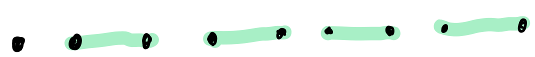
✱ Example: 1D Ising model

$$H = \underbrace{\sum_{i=1}^{n-1} Z_i Z_{i+1}}_{A} + \underbrace{\sum_{i=1}^{n} g X_i}_{B}$$

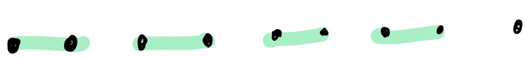
Goal: Want to approximate e^{-iHT} using one- and two-qubit gates.

Notice that e^{-iAt} and e^{-iBt} are both "simple."

$$A = \sum_{i \in \text{even}}^{n-1} Z_i Z_{i+1} + \sum_{i \in \text{odd}}^{n-1} Z_i Z_{i+1}$$



: even



: odd

Thus, $e^{-iAt} = \left(\prod_{i \in \text{even}} e^{-i Z_i Z_{i+1} t} \right) \left(\prod_{i \in \text{odd}} e^{-i Z_i Z_{i+1} t} \right)$

In particular, individual $e^{-i Z_i Z_{i+1} t}$ is a two-qubit gate.

$$e^{-iBt} = \prod_{i=1}^{n} e^{-i g X_i t}$$

single qubit.

Thus, $e^{-iAt} e^{-iBt}$ can be broken down into 3 layers of single- and two-qubit gates. The # of gates used is $O(n)$.

$$\left(e^{-iA\frac{T}{N}} e^{-iB\frac{T}{N}}\right)^N = \underbrace{\left(e^{-iA\frac{T}{N}} e^{-iB\frac{T}{N}}\right) \cdots \left(e^{-iA\frac{T}{N}} e^{-iB\frac{T}{N}}\right)}_{N}$$

Recall $N = O\left(\frac{T^2\|[A,B]\|}{\varepsilon}\right)$. Thus, the # of gates used is $O(Nn) = O\left(\frac{T^2 n \|[A,B]\|}{\varepsilon}\right)$

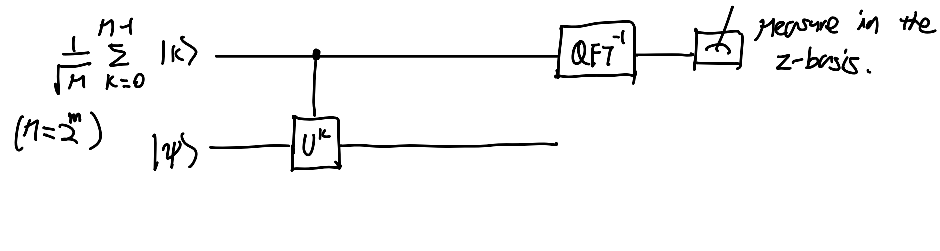
$$\begin{aligned}
\|[A,B]\| &= \left\| \lambda \left[\sum_{i=1}^{n-1} Z_i Z_{i+1}, \sum_{j=1}^{n} X_j \right] \right\| \\
&= \left\| \lambda \sum_{i=1}^{n-1} \left[Z_i Z_{i+1}, \sum_{j=1}^{n} X_j \right] \right\| \\
&= \left\| \lambda \sum_{i=1}^{n-1} \left[Z_i Z_{i+1}, X_i + X_{i+1} \right] \right\| \\
&\le |\lambda| \sum_{i=1}^{n-1} \left\| \left[Z_i Z_{i+1}, X_i + X_{i+1} \right] \right\| \\
&= O(|\lambda| n)
\end{aligned}$$

* Note that $\|[A,B]\| \le 2\|A\|\,\|B\|$ gives $O(|\lambda| n^2)$, which is worse.

So, using the simplest Trotter-Suzuki decomposition, we get the gate complexity of $O\left(\frac{T^2 n^2}{\varepsilon}|\lambda|\right) = O\left(\frac{T^2 n^2}{\varepsilon}\right)$ if $|\lambda| = O(1)$.

Now let's think about applying QPE to our decomposition.

QPE



We want $U = e^{-i\lambda H/\|H\|}$, but in practice we will have $\tilde{U}$ such that $\|U-\tilde{U}\| \le \varepsilon$. In Assignment 2, you will see that this translates into $O(\varepsilon)$ error in the eigenphase.

Question: Suppose we want to estimate the eigenvalue of H up to a precision δ, what kind of gate complexity do we need?

1. Let's first translate this precision δ to the precision of the eigenphase. We learned that we should choose $U = e^{-i\lambda H/\|H\|}$ to ensure that the eigenvalue of $\frac{\lambda H}{\|H\|}$ lies in $[0, \lambda]$. We will set the precision of the QPE to be ε_{QPE}.

2. The cost of QPE is $O\left(\frac{1}{\varepsilon_{QPE}} \mathrm{Cost}(U)\right)$.

3. What is $\mathrm{Cost}(U)$? $U = e^{-i\lambda H/\|H\|}$ means $T = \frac{\lambda}{\|H\|}$.
   Thus, $\mathrm{Cost}(U) = O\left(\frac{n^2}{\varepsilon} \frac{1}{\|H\|^2}\right) = O\left(\frac{1}{\varepsilon}\right)$
   unitary approximation error.

4. QPE cost is thus $O\left(\frac{1}{\varepsilon_{QPE}} \frac{1}{\varepsilon}\right)$. In the assignment, we will see that the eigenphase error is $\varepsilon_{QPE} + \varepsilon$, which should be bounded by $O(\delta/\|H\|)$. Thus, we see $O\left(\frac{n^2}{\delta^2}\right)$