Hamiltonian simulation w/ Trotterization

- ~~Efficient~~ Simulation of physics & chemistry is one of the critical applications of q. computing

- Recall the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

where $\hbar$ is the reduced Planck constant & H is the Hamiltonian (Hermitian energy operator) & we assume it is time independent

In many settings $H = \sum_{j=1}^{r} H_j$

where each H_j acts locally on one or two particles.

Rewriting as

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -iH/\hbar\, |\psi(t)\rangle$$

Solution is given by

$$|\psi(t)\rangle = e^{-iHt/\hbar}\, |\psi(0)\rangle$$

where $|\psi(0)\rangle$ is some initial state

b/c $\frac{\partial}{\partial t}|\psi(t)\rangle =$

$$\frac{\partial}{\partial t} e^{-iHt/\hbar}\, |\psi(0)\rangle$$

$$= -iH/\hbar\, e^{-iHt/\hbar}\, |\psi(0)\rangle$$

$$= -iH/\hbar\, |\psi(t)\rangle$$

So to simulate a physical system, we should simulate the unitary $e^{-iHt/\hbar}$ acting on a state $|\psi(0)\rangle$

Set $\hbar = 1$.

So then we should simulate

$$e^{-iHt}$$

As mentioned above, for many physical systems of interest,

$$H = \sum_{j=1}^{r} H_j \, ,$$ so then

we need to simulate

$$e^{-i \sum_{j=1}^{r} H_j t}$$

If $[H_j, H_k] = 0 \quad \forall j, k$

then we have

$$e^{-i \sum_{j=1}^{r} H_j t} = \prod_{j=1}^{r} e^{-iH_j t}$$

& so we can just simulate them one after another

Example Ising model

$$H_I = \sum_{j=1}^{r} \sigma_j^z \otimes \sigma_{j+1}^z$$

acts on jth qubit

acts on $j+1$ qubit

$$\Rightarrow e^{-iH_I t} = \prod_{j=1}^{r} \underbrace{e^{-i\sigma_j^z \otimes \sigma_{j+1}^z t}}$$

each of these is a 2-qubit rotation unitary

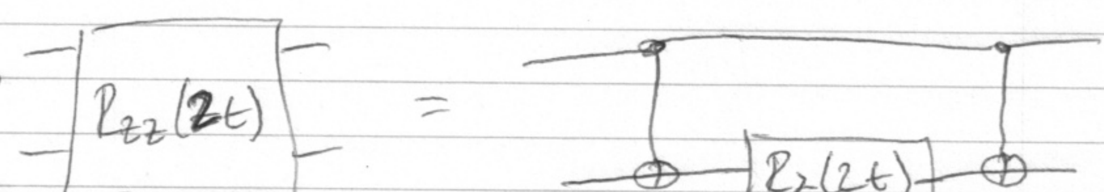
Using the fact that

$$\text{CNOT}(I \otimes Z)\,\text{CNOT} = Z \otimes Z,$$

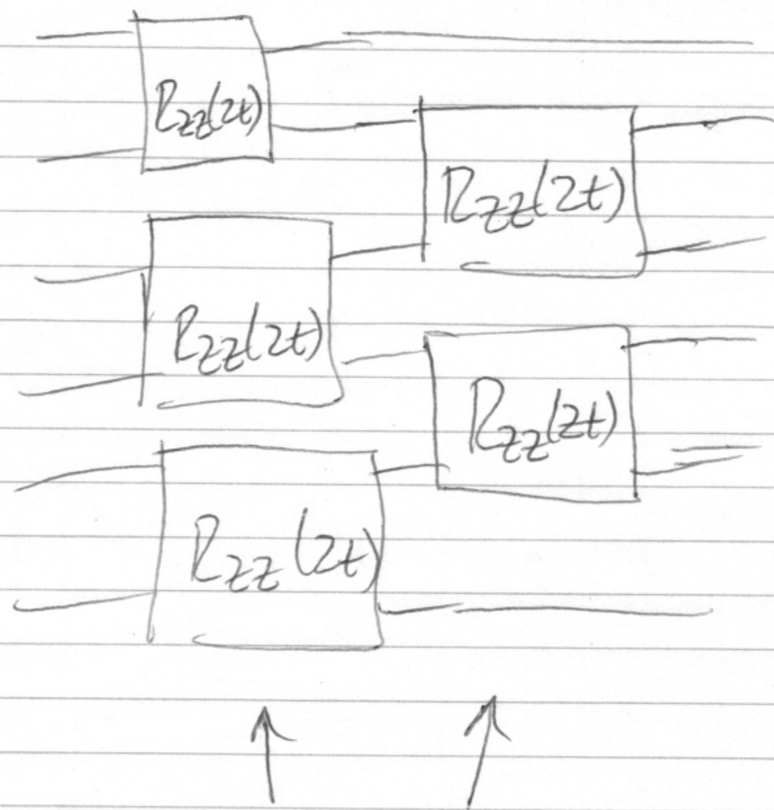
it follows that

$$e^{-iZ\otimes Z t} = \text{CNOT}(I \otimes e^{-iZt})\,\text{CNOT}$$

$\Rightarrow$



then we can realize $e^{-iH_I t}$ as



can parallelize for shorter depth

Most Hamiltonians of interest in q. physics have non-commuting terms. If $[A,B] \neq 0$, then $e^{A+B} \neq e^{A} e^{B}$.

So what to do in this case?

Use idea called trotterization

The following bound holds:

$$\left\| \exp\left(-it \sum_{j=1}^{r} H_j\right) - \left[\exp\left(\frac{-it}{\ell} H_r\right) \cdots \exp\left(\frac{-it H_1}{\ell}\right)\right]^{\ell} \right\|_{\infty} \leq O\left(\frac{(rt)^2}{\ell}\right)$$

This has a profound implication:

To simulate any Hamiltonian that is a sum of local terms, we can simulate each individual one for a small time $\frac{t}{\ell}$ then repeat the process ℓ times

Now consider example of transverse field Ising model

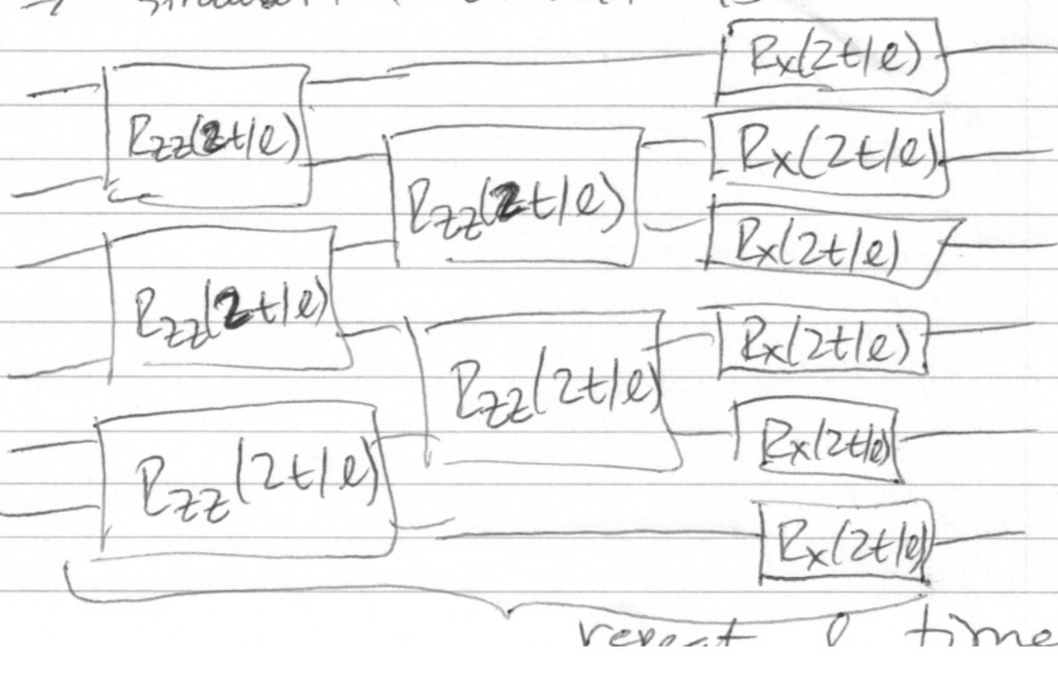
$$H_{TFIM} = \underbrace{\sum_{j=1}^{r} \sigma_j^z \otimes \sigma_{j+1}^z}_{\substack{\text{all these}\\ \text{terms}\\ \text{commute}}} + \underbrace{\sum_{j=1}^{r} \sigma_j^x}_{\substack{\text{all these}\\ \text{terms}\\ \text{commute}}}$$

but the cross terms don't

Apply Trotterization, we conclude that

$$e^{-iH_{TFIM}t} \approx \left(e^{-\frac{it}{l}\sum_{j=1}^{r} \sigma_j^z \otimes \sigma_{j+1}^z} \; e^{-\frac{it}{l}\sum_{j=1}^{r} \sigma_j^x} \right)^l$$

$\Rightarrow$ simulation circuit is



repeat l times

How to prove the error bound above?

Consider simple case of

$$e^{A+B} \approx \left(e^{A/\ell} e^{B/\ell}\right)^{\ell}$$

i.e. two operators

First consider that

$$e^{(A+B)/\ell} = I + \frac{A+B}{\ell} + \overbrace{\cancel{\frac{1}{2}\frac{(A+B)^2}{\ell^2} + O\left(\frac{1}{\ell^3}\right)}}^{O(1/\ell^2)}$$

then

$$e^{A/\ell} e^{B/\ell} = \left[I + \frac{A}{\ell} + O\left(\frac{1}{\ell^2}\right)\right]\left[I + \frac{B}{\ell} + O\left(\frac{1}{\ell^2}\right)\right]$$

$$= I + \frac{A}{\ell} + \frac{B}{\ell} + O\left(\frac{1}{\ell^2}\right)$$

$$\Rightarrow \quad e^{(A+B)/\ell} - e^{A/\ell} e^{B/\ell} = O\left(\frac{1}{\ell^2}\right)$$

$$\Rightarrow \quad \left\| e^{(A+B)/\ell} - e^{A/\ell} e^{B/\ell} \right\|_{\infty} \leq O\left(\frac{1}{\ell^2}\right)$$

Now consider that

$$C^l - D^l = \sum_{m=0}^{l-1} C^m [C - D] D^{l-m-1}$$

e.g., for $l=3$, this amounts to

$$C^3 - D^3 = [C-D]D^2 + C[C-D]D + C^2[C-D]$$

$$\Rightarrow \|C^l - D^l\| = \left\|\sum_{m=0}^{l-1} C^m [C-D] D^{l-m-1}\right\|$$

$$\leq \sum_{m=0}^{l-1} \|C\|^m \|C-D\| \|D\|^{l-m-1}$$

using triangle inequality & submultiplicativity of norm

$$= \|C-D\| \sum_{m=0}^{l-1} \|C\|^m \|D\|^{l-m-1}$$

plug in $C = e^{(A+B)/l}$

$D = e^{A/l} e^{B/l}$

to get

$$\left\| \left[e^{(A+B)/l} \right]^l - \left(e^{A/l} e^{B/l} \right)^l \right\|$$

$$\leq \left\| e^{(A+B)/l} - e^{A/l} e^{B/l} \right\| \cdot \sum_{m=0}^{l-1} \left\| e^{(A+B)/l} \right\|^m \left\| e^{A/l} e^{B/l} \right\|^{l-m-1}$$

consider that

$$\| e^X \| = \left\| \sum_{k=0}^{\infty} \frac{X^k}{k!} \right\| \leq \sum_{k=0}^{\infty} \frac{1}{k!} \|X\|^k$$

$$= \exp(\|X\|)$$

$$\Rightarrow \left\| e^{(A+B)/l} \right\|^m \left\| e^{A/l} e^{B/l} \right\|^{l-m-1}$$

$$\leq \exp\left(\|A+B\|/l \right)^m \exp\left(\|A\|/l + \|B\|/l \right)^{l-m-1}$$

$$\leq \exp\left(\frac{\|A\|+\|B\|}{l}\right)^m \exp\left(\frac{\|A\|+\|B\|}{l}\right)^{l-m-1}$$

$$= \exp\left(\|A\|+\|B\|\right)\frac{l-1}{l}$$

$$\leq \exp\left(\|A\|+\|B\|\right)$$

$\Rightarrow$

$$\left\|e^{A+B} - \left(e^{A/l} e^{B/l}\right)^l\right\|$$

$$\leq O\left(\frac{1}{l^2}\right)\cdot\sum_{m=0}^{l-1} \exp\left(\|A\|+\|B\|\right)$$

$$= O\left(\frac{1}{l^2}\right)\cdot l \cdot \exp\left(\|A\|+\|B\|\right)$$

$$= O\left(\frac{1}{l}\right)\cdot \exp\left(\|A\|+\|B\|\right)$$

to include time t substitute $A = H_1 t$ $B = H_2 t$ earlier & this gives bound

$$\left\|e^{-i(H_1+H_2)t} - \left(e^{-iH_1t/l} e^{-iH_2t/l}\right)^l\right\|$$

$$\leq O\left(\frac{t^2}{l}\right) \exp\left(\left(\|H_1\|+\|H_2\|\right)t\right)$$

We can use higher-order trotter formulas for improvements in error. For example, the 2nd order would be

$$\left\| \exp\left(-it\sum_{j=1}^{r} H_j\right) - \left[\exp\left(\frac{-itH_1}{2\ell}\right)\cdots\exp\left(\frac{-itH_r}{2\ell}\right)\exp\left(\frac{-itH_r}{2\ell}\right)\cdots \exp\left(\frac{-itH_1}{2\ell}\right)\right]^{\ell} \right\| = O\left(\frac{r^3t^3}{\ell^2}\right)$$

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consider analysis for $r=2$ again

then $$e^{(A+B)/\ell} = I + \frac{A+B}{\ell} + \frac{(A+B)^2}{2\ell^2} + O\left(\frac{1}{\ell^3}\right)$$

while

$$e^{A/2\ell}e^{B/2\ell}e^{B/2\ell}e^{A/2\ell} = e^{A/2\ell}e^{B/\ell}e^{A/2\ell}$$

$$= \left[I + \frac{A}{2\ell} + \frac{A^2}{8\ell^2} + O\left(\frac{1}{\ell^3}\right)\right]\left[I + \frac{B}{\ell} + \frac{B^2}{2\ell^2} + O\left(\frac{1}{\ell^3}\right)\right]$$
$$\times\left[I + \frac{A}{2\ell} + \frac{A^2}{8\ell^2} + O\left(\frac{1}{\ell^3}\right)\right]$$

$$= \left[I + \frac{A}{2\ell} + \frac{A^2}{8\ell^2} + \frac{B}{\ell} + \frac{AB}{2\ell^2} + \frac{B^2}{2\ell^2} + O\left(\frac{1}{\ell^3}\right)\right]$$

$$\times \left[I + \frac{A}{2\ell} + \frac{A^2}{8\ell^2} + O\left(\frac{1}{\ell^3}\right)\right]$$

$$= I + \frac{A}{2\ell} + \frac{A^2}{8\ell^2} + \frac{B}{\ell} + \frac{AB}{2\ell^2} + \frac{B^2}{2\ell^2}$$

$$+ \frac{A}{2\ell} + \frac{A^2}{4\ell^2} + \frac{BA}{2\ell^2} + \frac{A^2}{8\ell^2} + O\left(\frac{1}{\ell^3}\right)$$

$$= I + \frac{A+B}{\ell} + \frac{(A+B)^2}{2\ell^2} + O\left(\frac{1}{\ell^3}\right)$$

$$\Rightarrow \left\| e^{(A+B)/\ell} - \left(e^{A/2\ell} e^{B/\ell} e^{A/2\ell}\right) \right\|$$

$$= O\left(\frac{1}{\ell^3}\right)$$

Using same bound as before implies

$$\left\| e^{A+B} - \left(e^{A/2\ell} e^{B/\ell} e^{A/2\ell}\right)^\ell \right\|$$

$$\leq \left\| e^{(A+B)/\ell} - e^{A/2\ell} e^{B/\ell} e^{A/2\ell} \right\| \cdot \ell \cdot$$

$\exp(\|A\| + \|B\|)$

$$= \mathcal{O}\left(\frac{1}{\ell^3}\right) \ell \cdot \exp(\|A\|+\|B\|)$$

$$= \mathcal{O}\left(\frac{1}{\ell^2}\right) \exp(\|A\|+\|B\|)$$