CPEN 400Q Lecture 20
Hamiltonian simulation: error and resources in practice

Wednesday 20 March 2024

Announcements

- Assignment 3 due tonight at 23:59 (last technical assignment, except for two more hands-on)
- One more literacy assignment
- Quiz 9 Monday
- Monday's class: hands-on with variational eigensolver

Last time

We had two main questions:

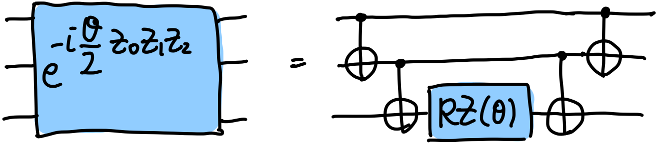
1. How do we construct circuits for interaction terms like

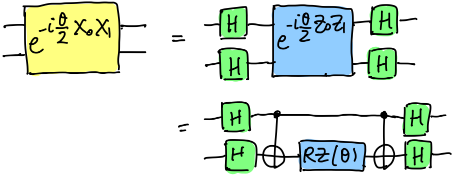
$$\hat{H} = -\alpha Z_0 Z_1$$

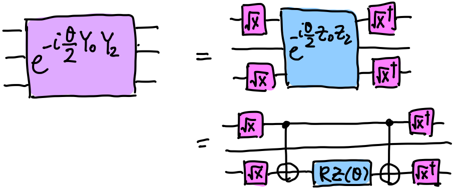
2. How do we construct circuits where a qubit is acted on in more than one term?

$$\hat{H} = -\alpha Z_0 - \beta X_0$$

We answered the first one:

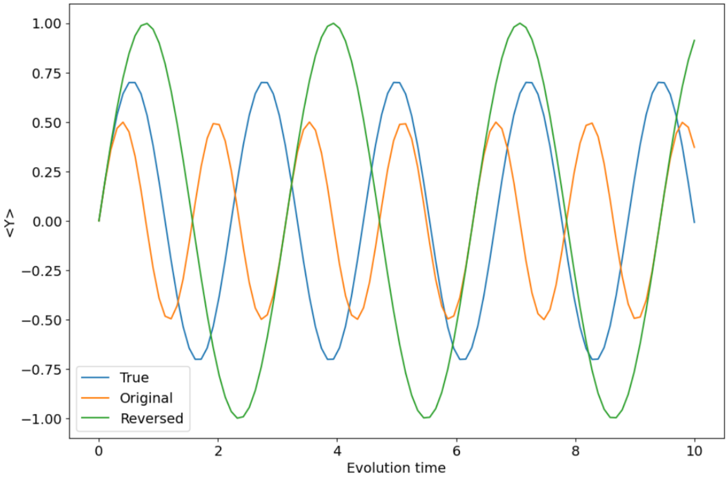






Last time

We saw an example that highlighted challenges of the second...



Learning outcomes

- perform Hamiltonian simulation with Trotterization
- describe pitfalls and consequences encountered in Trotterizing Hamiltonians with many interaction terms
- use QPE to estimate the ground state energy of a Hamiltonian, and quantify the resources required to do so

Dealing with sums of Pauli terms

More generally, simulation of something like

$$e^{-i\alpha P - i\beta Q}$$

depends on whether the Paulis *commute*.

Dealing with sums of Pauli terms

Exercise: evaluate the commutation relations for X, Y, Z.

- $[X, Y] =$
- $[Y, Z] =$
- $[Z, X] =$
- $[Y, X] =$
- $[Z, Y] =$
- $[X, Z] =$

Dealing with sums of Pauli terms

Exercise: Do $X_0 Y_1 X_2$ and $Z_0 X_1 X_2$ commute?

Dealing with sums of Pauli terms

Exercise: Do $Z_0 Y_1 X_3$ and $Z_0 X_1 Z_2$ commute?

Trick: check number of non-identity qubits on which they differ.

X	I	Z	Z	X	Y	X
X	Y	Y	X	I	Z	X
✓	✓	✗	✗	✓	✗	✓

✗ = 3 ⇒ DO NOT COMMUTE

(odd)

X	I	Z	Z	X	Y	X
Y	Y	Y	X	I	Z	X
✗	✓	✗	✗	✓	✗	✓

#✗ = 4 ⇒ COMMUTE

(even)

(Under the hood: binary symplectic representation of Pauli terms, and symplectic inner products.)

Dealing with sums of Pauli terms

When Paulis commute,

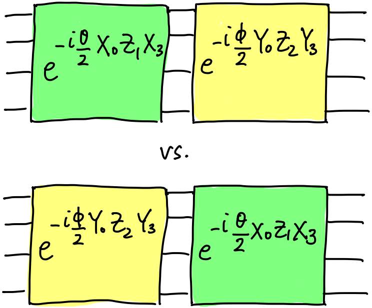
- We can split the exponential of the sum into a product of exponentials
$$e^{-i\alpha P - i\beta Q} = e^{-i\alpha P} e^{-i\beta Q}$$
- We can evolve the terms individually in any order

$$e^{-i\alpha P - i\beta Q} = e^{-i\alpha P} e^{-i\beta Q} = e^{-i\beta Q} e^{-i\alpha P}$$

Dealing with sums of Pauli terms

Example:

$$H = \frac{\theta}{2} X_0 Z_1 X_3 + \frac{\phi}{2} Y_0 Z_2 Y_3$$



Either works!

Dealing with sums of Pauli terms

First, check that order doesn't matter. If $[A, B] = 0$,

$$\begin{aligned}
Ae^B &= A(I + B + \frac{1}{2!}B^2 + \frac{1}{3!}B^3 + \cdots) \\
&= A + AB + \frac{1}{2!}AB^2 + \frac{1}{3!}AB^3 + \cdots \\
&= A + BA + \frac{1}{2!}B^2A + \frac{1}{3!}B^3A + \cdots \\
&= e^B A
\end{aligned}$$

Since e^A is sum of powers of A,

$$e^A e^B = e^B e^A$$

Dealing with sums of Pauli terms

To show relationship with e^{A+B}:

$$\begin{aligned} e^A e^B &= (I + A + \frac{1}{2!}A^2 + \frac{1}{3!}A^3 + \cdots)(I + B + \frac{1}{2!}B^2 + \frac{1}{3!}B^3 + \cdots) \\ &= (I + B + \frac{1}{2!}B^2 + \frac{1}{3!}B^3 + \cdots) + A(I + B + \frac{1}{2!}B^2 + \frac{1}{3!}B^3 + \cdots) \\ &+ \frac{1}{2!}A^2(I + B + \frac{1}{2!}B^2 + \frac{1}{3!}B^3 + \cdots) + ... \end{aligned}$$

$$\begin{aligned} e^{A+B} &= I + (A+B) + \frac{1}{2!}(A+B)^2 + \frac{1}{3!}(A+B)^3 + \cdots \\ &= I + (A+B) + \frac{1}{2!}(A^2 + BA + AB + B^2) + \\ &+ \frac{1}{3!}(A^3 + ABA + A^2B + AB^2 + BA^2 + B^2A + BAB + B^3) + \cdots \end{aligned}$$

To show relationship with e^{A+B}:

$$
\begin{aligned}
e^{A+B} &= I + (A+B) + \frac{1}{2!}(A^2 + BA + AB + B^2) + \\
&+ \frac{1}{3!}(A^3 + ABA + A^2B + AB^2 + BA^2 + B^2A + BAB + B^3) + \cdots
\end{aligned}
$$

$$
\begin{aligned}
e^{A+B} &= I + (A+B) + \frac{1}{2!}(A^2 + 2AB + B^2) + \frac{1}{3!}(A^3 + 3A^2B + 3AB^2 + B^3) \\
&= I + A + B + \frac{1}{2!}A^2 + AB + \frac{1}{2!}B^2 + \frac{1}{3!}A^3 + \frac{1}{2}A^2B + \frac{1}{2}AB^2 + \frac{1}{3!}B^3 + \\
&= (I + B + \frac{1}{2!}B^2 + \frac{1}{3!}B^3 + \cdots) + A(I + B + \frac{1}{2!}B^2 + \frac{1}{3!}B^3 + \cdots) \\
&= e^A e^B
\end{aligned}
$$

Summary:

$$e^{A+B} = e^A e^B$$

only if $[A, B] = 0$.

In general, there are extra terms. This is summarized by the **Baker-Campbell-Hausdorff** formula and related Zassenhaus formula:

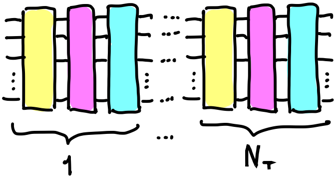
$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]} e^{\frac{1}{6}(2[B,[A,B]]+[A,[A,B]])} \ldots$$

Trotterization

When Paulis don't commute, we can approximate evolution by Trotterizing:

$$\hat{H} = \alpha P_1 + \beta P_2 + \gamma P_3$$

$$e^{-i\hat{H}} \approx \left(e^{-i\frac{\alpha P_1}{N_T}} \, e^{-i\frac{\beta P_2}{N_T}} \, e^{-i\frac{\gamma P_3}{N_T}} \right)^{N_T}$$



Trotterization

The larger N_T is, the better the approximation:

$$\lim_{N_T \to \infty} \left(e^{\frac{A}{N_T}} e^{\frac{B}{N_T}} \right)^{N_T} = e^{A+B}$$

Can analytically derive expressions for the error and relationships with time and magnitude of commutator (see Codebook H.8):

$$e^{A+B} = \left(e^{\frac{A}{N_T}} e^{\frac{B}{N_T}} \right)^{N_T} + O\left(\frac{1}{N_T} \right)$$

Can use such relationships to determine N_T for a desired error.

"Higher-order" Trotter formulas also exist, e.g., second order:

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

Lower approximation error, *at cost of more gates*!

Other methods

Trotterization is not the only method, but is most straightforward to understand.

Other methods include:

- Linear combination of unitaries
- Qubitization

See Codebook H.6-H.9.

All these methods are more "long term" algorithms as they require huge amount of computational resources.

Apply QPE and Hamiltonian simulation to estimate ground state energy of a deuteron.

Next time

Content:

- Quiz 9
- Hands-on with variational quantum eigensolver

Action items:

1. Finish assignment 3
2. Work on project

Recommended reading:

- Codebook module H