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:

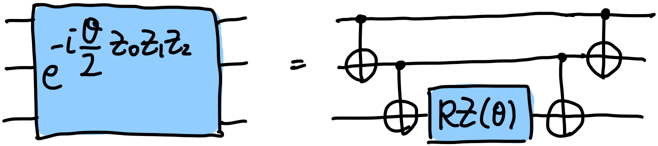
1. How do we construct circuits for interaction terms like

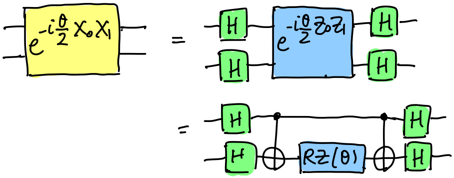
$$\hat{H} = -\alpha Z_0 Z_1$$

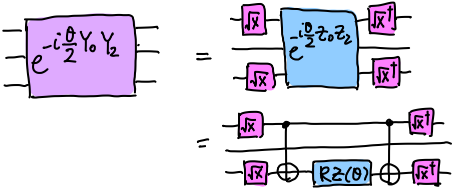
2. How do we construct circuits where a qubit is acted on in more than one term?

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

We answered the first one:

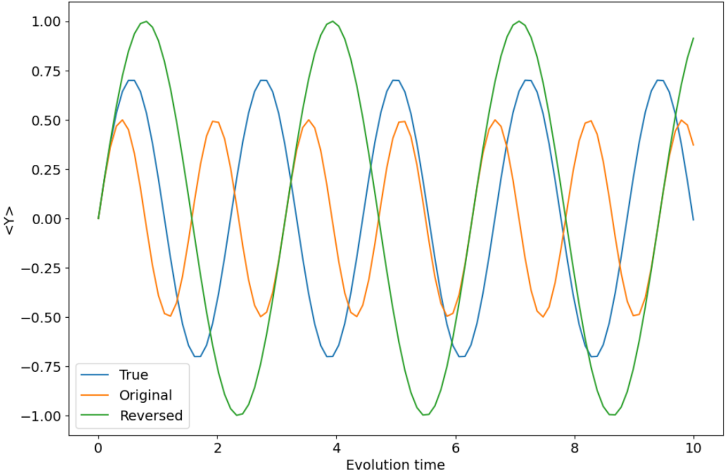






Last time

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

More generally, simulation of something like

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

depends on whether the Paulis *commute*.

$$[A, B] = AB - BA = 0$$

$\xrightarrow{+1}$
XYZ
$\xleftarrow{}$
-1

$$[A,B] = AB - BA \qquad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

- $[X,Y] = 2iZ$
- $[Y,Z] = 2iX$
- $[Z,X] = 2iY$
- $[Y,X] = -2iZ$
- $[Z,Y] = -2iX$
- $[X,Z] = -2iY$

ε_{ijk}

$H = -Z - X$

$XY = iZ$

$YX = -iZ$

$XY - YX = 2iZ$

$$[\sigma_i, \sigma_j] = 2i\underbrace{\varepsilon_{ijk}}\sigma_k$$

$\sigma_i \in \{X, Y, Z\}$

$$(A \otimes B)(C \otimes D) = AC \otimes BD$$

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

$$(X \otimes Y \otimes X)(Z \otimes X \otimes X) = (-iY) \otimes (-iZ) \otimes I = -Y \otimes Z \otimes I$$

$$(Z \otimes X \otimes X)(X \otimes Y \otimes X) = iY \otimes iZ \otimes I = -Y \otimes Z \otimes I$$

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

$$(Z \otimes Y \otimes I \otimes X)(Z \otimes X \otimes Z \otimes I) = I \otimes -iZ \otimes Z \otimes X$$

$$(Z \otimes X \otimes Z \otimes I)(Z \otimes Y \otimes I \otimes X) = I \otimes iZ \otimes Z \otimes X$$

Dealing with sums of Pauli terms

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)

Dealing with sums of Pauli terms

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

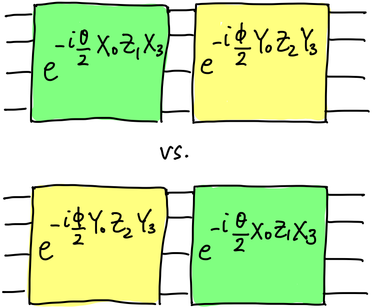
When Paulis commute,

- 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

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

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 $[A, B] = 0$,

Since e^A is sum of powers of A,

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

Dealing with sums of Pauli terms

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

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

Dealing with sums of Pauli terms

Summary:

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

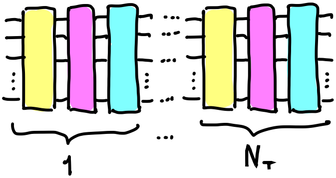
In general, there are extra terms. This is summarized by the **Baker-Campbell-Hausdorff** formula and related Zassenhaus formula:

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

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

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

number of Trotter steps



The ~~smaller~~ 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):

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

big O

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

$$\left| e^{-iHt} - \left(e^{-\frac{P_1}{N_T}} e^{-\frac{P_2}{N_T}} \cdots \right)^{N_T} \right|$$

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

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

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.

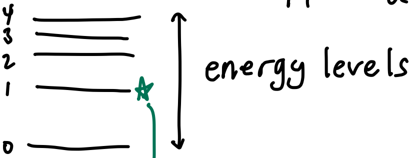
Example

$a_1^\dagger a_0 : |10\cdots0\rangle \to |01\cdots0\rangle$

XX

mapping to qubits

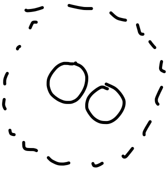
$\hat{H} \sim a_3^\dagger a_2 + a_4^\dagger a_0$



$a_3^\dagger a_3$

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

$\underline{0}\ \underline{1}\ \underline{0}\ \underline{0}\ \underline{0}\ \underline{0}$



$a^\dagger \quad a$: creation, annihilation

$a_3^\dagger$: create deuteron in state 3

a_2 : remove deuteron from state 2

$a_3^\dagger |00000\rangle \sim |00010\rangle$

$a_2 |00100\rangle \sim |00000\rangle$

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