# 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:

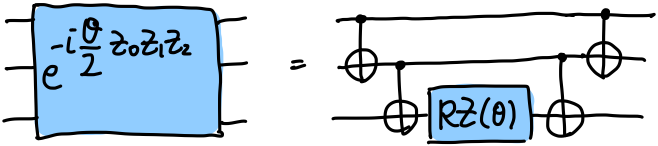
1. How do we construct circuits for interaction terms like

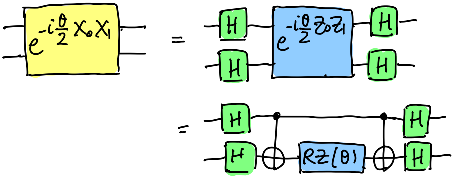
$$\hat{H} = -\alpha Z_0 Z_1$$

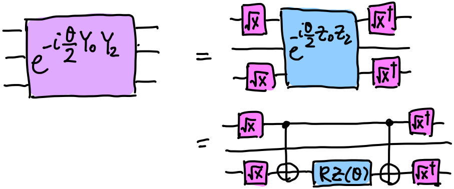
2. How do we construct circuits where a qubit is acted on in more than one term?

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

We answered the first one:

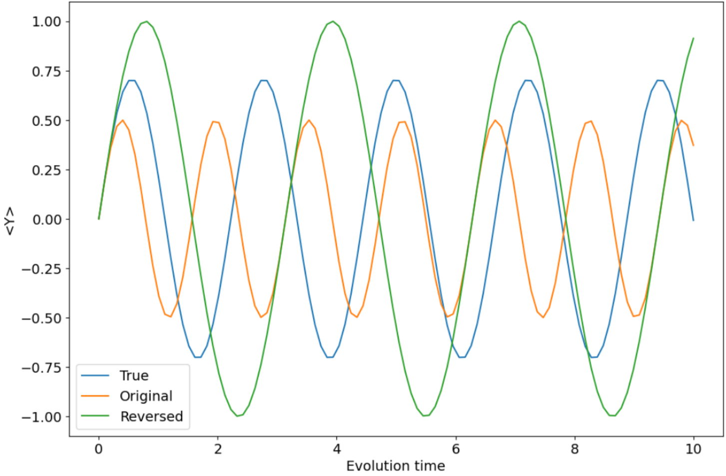


# Last time

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*.

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

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

**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?

## 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 |
| ✓ | ✓ | ✗ | ✗ | ✓ | ✗ | ✓ |

$\# \times = 3 \Rightarrow$ 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,

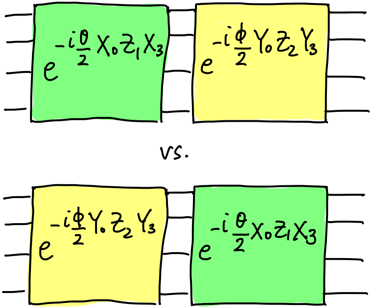
- We can split the exponential of the sum into a product of exponentials
$$e^{-i\alpha P-i\beta Q} = e^{-i\alpha P}e^{-i\beta Q}$$
- We can evolve the terms individually in any order

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

# 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 $[A, B] = 0$,

Since $e^A$ is sum of powers of $A$,

# Dealing with sums of Pauli terms

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

# Dealing with sums of Pauli terms

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

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

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:

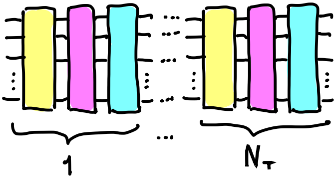
When Paulis don't commute, we can approximate evolution by Trotterizing:

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

$$\downarrow$$

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

$$\downarrow$$



# Trotterization

The smaller $N_T$ is, the better the approximation:

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

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

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

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

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