CPEN 400Q Lecture 19
Hamiltonian simulation circuits and Trotterization

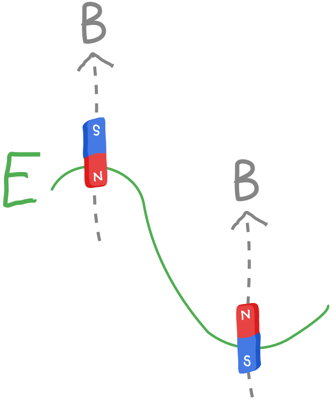
Monday 18 March 2024

Announcements

- Quiz 8 today
- Hands-on 3 due tonight at 23:59
- Assignment 3 due Wednesday at 23:59

Last time

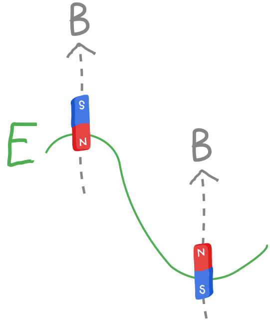
We considered bar magnets in a field as an example physical system to guide our definition of a Hamiltonian.



Every orientation of the magnet has an associated energy.

Image credit: Xanadu Quantum Codebook node H.3

We associated orientations of the magnets with qubit states.



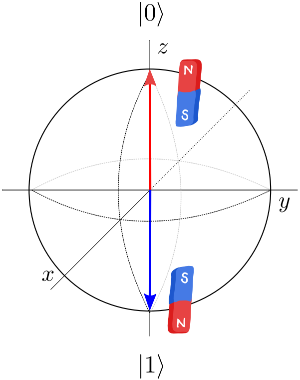


Image credit: Xanadu Quantum Codebook node H.3

Last time

The system energy is the expectation value of a qubit operator called a *Hamiltonian*.

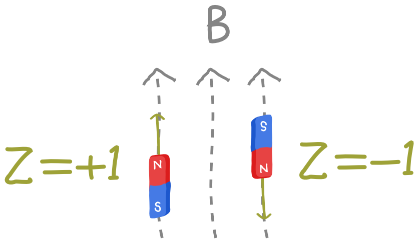


Image credit: Xanadu Quantum Codebook node H.3

Last time

Hamiltonians describe how the parts of a system interact.

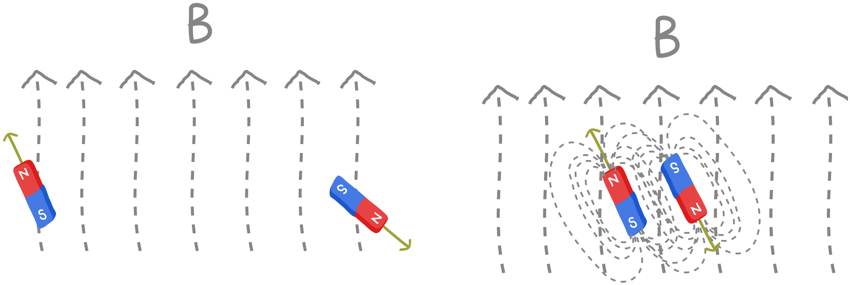
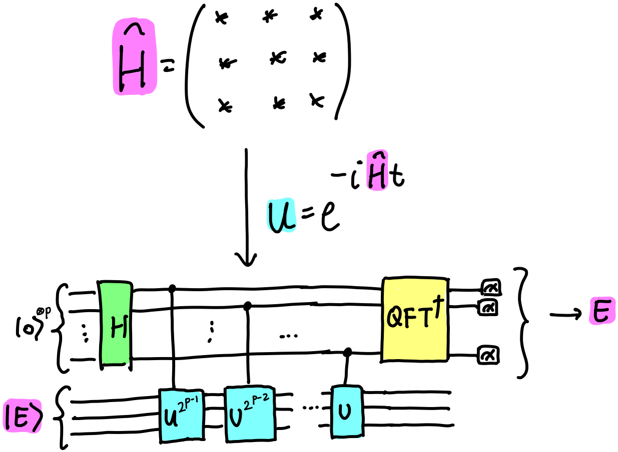


Image credit: Xanadu Quantum Codebook node H.3

Hamiltonians for multi-qubit systems can be expressed as linear combinations of Paulis.

A Hamiltonian of this form has an associated *unitary operator* that describes how the system *evolves over time*:

$U = e^{-i\hat{H}t}$ has eigevalues e^{-iEt}, where E are eigenvalues of $\hat{H}$.



We could do QPE, *if we had a circuit for U*!

Learning outcomes

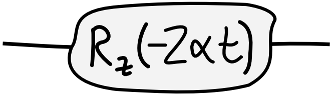
- construct circuits for Hamiltonian simulation
- perform Hamiltonian simulation with Trotterization
- describe pitfalls and consequences encountered in Trotterizing Hamiltonians with many interaction terms

Example: single-qubit

Recall our single-qubit example:

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

The state evolves like



Example: two non-interacting qubits

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

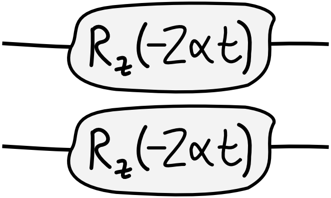


Image credit: Xanadu Quantum Codebook node H.5

Example: three non-interacting qubits

Exercise: What is the circuit for a three-qubit system with the Hamiltonian

$$\hat{H} = -\alpha Z_0 - \beta Y_1 + \gamma X_2$$

Today: more complex interactions

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?

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

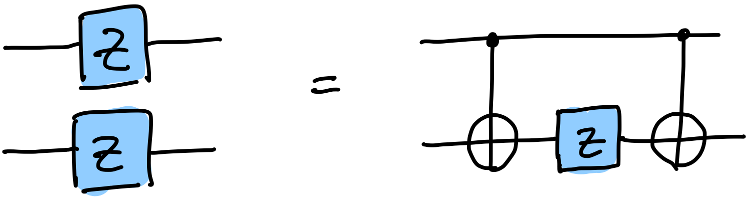
Circuits for individual Pauli terms

We know how to deal with $\hat{H} = -\alpha Z_0$ or $\hat{H} = -\alpha Z_1$ individually:

But how to implement something with an interaction:

Using standard quantum operations, we can turn a Pauli with multiple Z into something with only one Z!

Circuits for individual Pauli terms



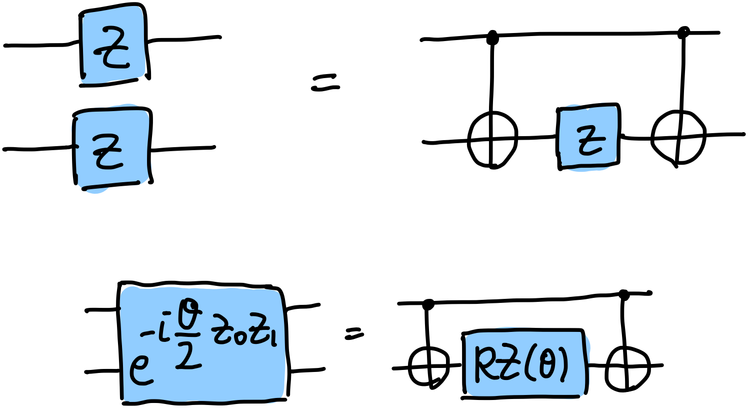
Circuits for individual Pauli terms

We know $Z \otimes Z = CNOT(I \otimes Z)CNOT$:

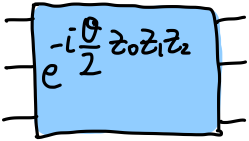
$$U = e^{i\alpha t \cdot CNOT(I \otimes Z)CNOT}$$

This looks worse at first, but:

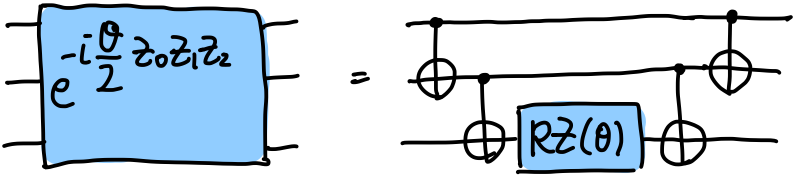
Circuits for individual Pauli terms



Exercise: What does the circuit for this Pauli look like?

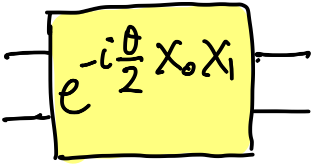


Circuits for individual Pauli terms

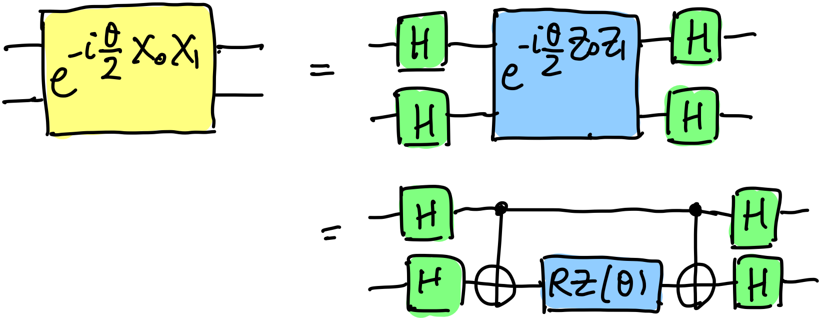


We can deal with any product of Pauli Z in this way.

What strategy can we use for other Paulis?

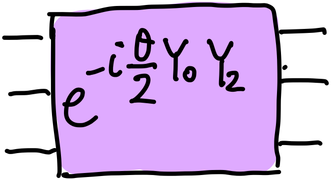


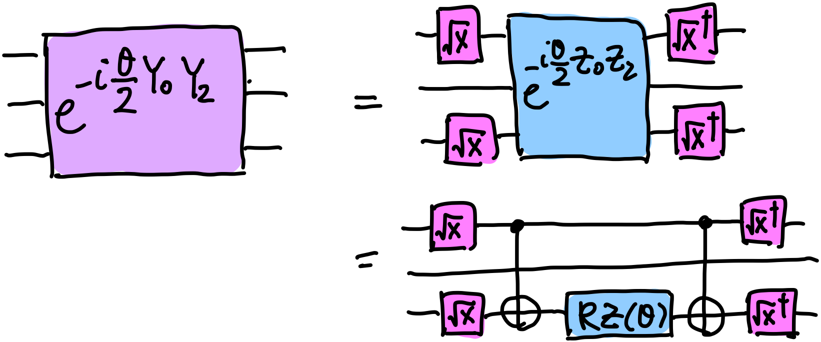
Circuits for individual Pauli terms



Circuits for individual Pauli terms

Exercise: Derive the circuit for





We can do this for arbitrary Paulis with X, Y, and Z terms.

If you use HS instead of $\sqrt{X}$, the operators applied around the Z are elements of the **Clifford group**. Cliffords send Paulis to Paulis.

Today: more complex interactions

1. How do we construct circuits for interaction terms like

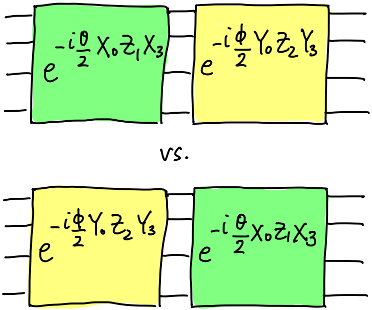
$$\hat{H} = -\alpha Z_0 Z_1$$

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

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

More generally,

When two (or more) Paulis commute, the exponential of their linear combination can be factored exactly:



Dealing with sums of Pauli terms

How to tell if two multi-qubit Paulis commute: 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)

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: Trotterization

When Paulis don't commute, we can *approximate* by applying the **Trotter-Suzuki decomposition**:

where $O(1/N_T)$ is an error term that depends on N_T, the number of **Trotter steps**.

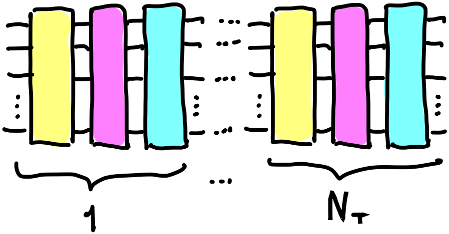
The smaller N_T is, the better the approximation:

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

$$\downarrow$$

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

$$\downarrow$$



Next time

Content:

- Trotterization and error scaling
- Trying QPE for a small system

Action items:

1. Finish hands-on 3 and assignment 3
2. Work on project

Recommended reading:

- Codebook module H