CPEN 400Q Lecture 18
Hamiltonian simulation

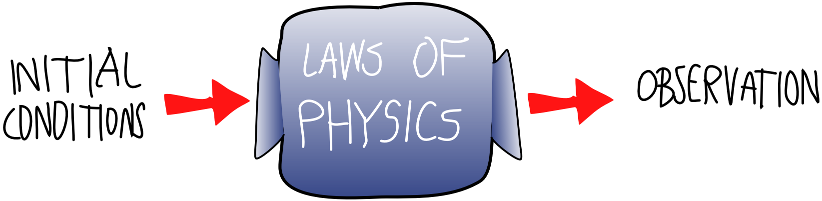
Wednesday 13 March 2024

Announcements

- Hands-on 3 due Monday (18 March) at 23:59
- Assignment 3 due Wednesday (20 March) 23:59
- Quiz 8 on Monday (on today's lecture)

Learning outcomes

- Define a Hamiltonian and describe the relationship between its structure and the energy of a physical system
- Perform time evolution of simple systems in PennyLane



The role of a physicist is to work out what happens in the middle.

Image credit: Xanadu Quantum Codebook node H.1

We can use computers to approximately model or simulate how a system evolves with time. This requires *discretizing* the systems.

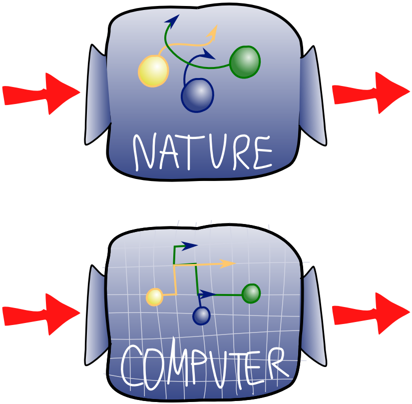


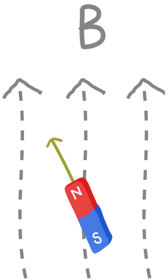
Image credit: Xanadu Quantum Codebook node H.1

To do this on a quantum computer we need:

1. A meaningful way of describing physical systems using qubits
2. A way of manipulating qubits that corresponds to time evolution of that system
3. A way to extract relevant physical quantities

Hamiltonians

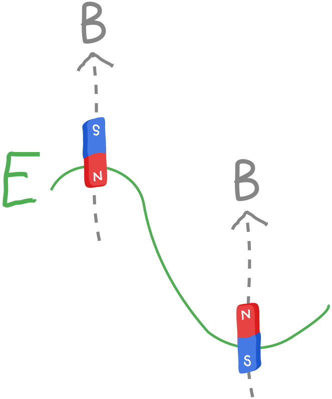
Example: a bar magnet in a magnetic field along the Z direction.



Every orientation of the magnet has an energy associated with it.

Image credit: Xanadu Quantum Codebook node H.3

Bar magnets like to *align* with the external field.



Aligned configuration is the *ground state* (lowest energy state).

Image credit: Xanadu Quantum Codebook node H.3

Magnets have some orientation represented by a vector in 3-dimensional space. We can map this to a qubit.

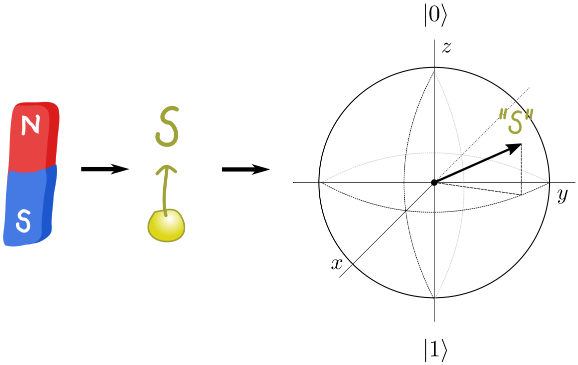
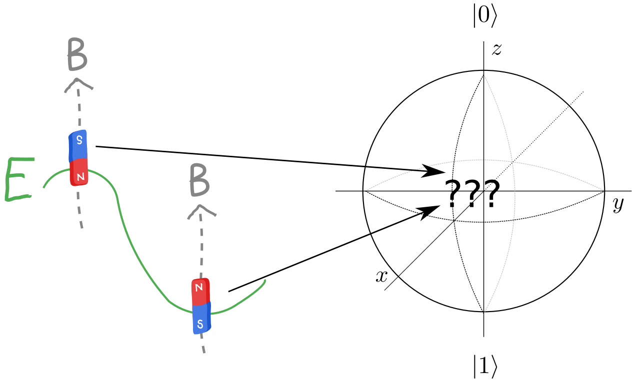


Image credit: Xanadu Quantum Codebook node H.5

Hamiltonians

Can you think of a way to represent these magnets as qubit states?



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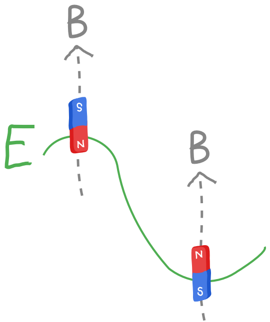
Hamiltonians



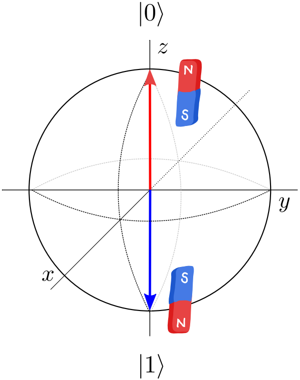
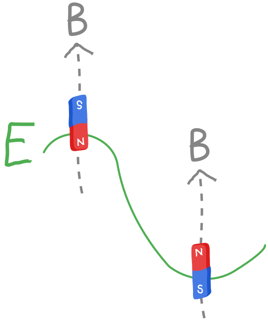


Image credit: Xanadu Quantum Codebook node H.3

What can we use to denote the *energy* of the magnet?



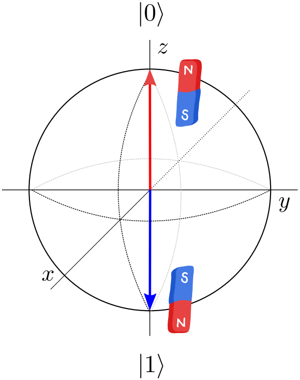
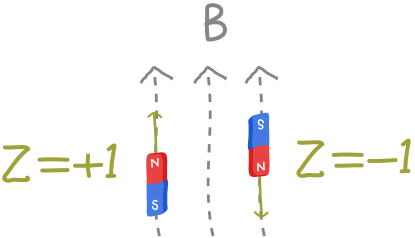


Image credit: Xanadu Quantum Codebook node H.3

A Hermitian operator called a *Hamiltonian* describes the system:

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

where α is a coefficient that depends on physical values.

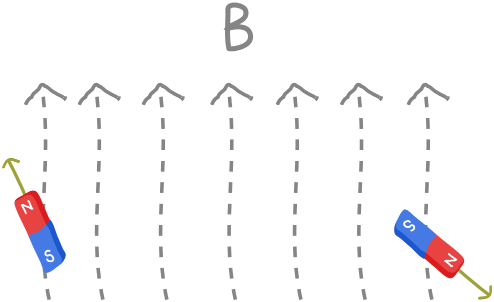


Computing the energy of the system corresponds to *measuring the expectation value of* $\hat{H}$ (which in this case, is just $-\alpha\langle Z \rangle$).

Image credit: Xanadu Quantum Codebook node H.3

Hamiltonians can describe systems with multiple parts. For example, two magnets that are far apart:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = -\alpha Z_0 - \alpha Z_1$$



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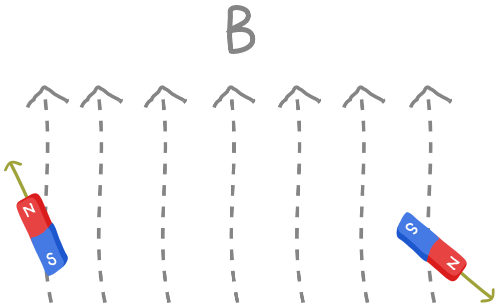


The energy of this system is $\langle \hat{H} \rangle = -\alpha \langle Z_0 \rangle - \alpha \langle Z_1 \rangle$

Image credit: Xanadu Quantum Codebook node H.5

Question: when is the energy of this system minimized?

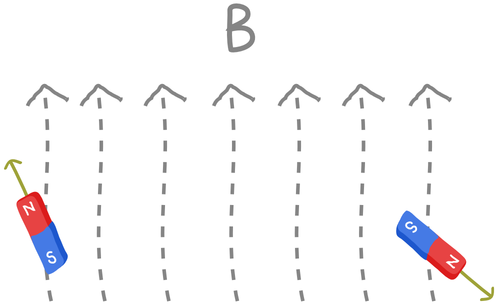
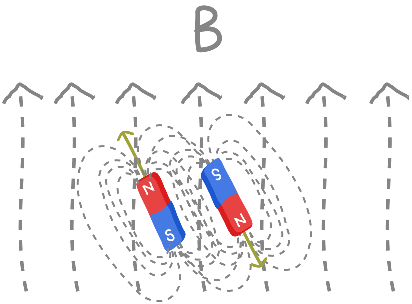


Image credit: Xanadu Quantum Codebook node H.5

If the two magnets are close, we need parts of the Hamiltonian that describe the *interaction*.

$$\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_{01} = -\alpha Z_0 - \alpha Z_1 + \beta(X_0 X_1 + Y_0 Y_1 + Z_0 Z_1)$$



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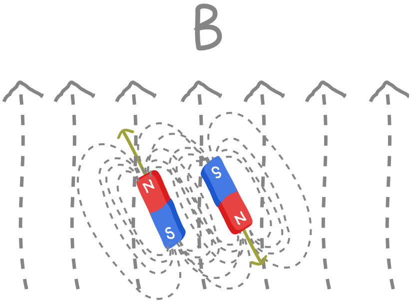
Question: What is the energy? What is the ground state (energy)?

$$\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_{01} = -\alpha Z_0 - \alpha Z_1 + \beta(X_0 X_1 + Y_0 Y_1 + Z_0 Z_1)$$



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More generally, a Hamiltonian can be expressed as

$$\hat{H} = \sum_i c_i P_i, \quad c_i \in \mathbb{R}$$

i.e., as a *linear combination of Pauli operators*.

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Key points:

- An n-qubit Hamiltonian is a giant $2^n \times 2^n$ Hermitian matrix
- The Paulis are a group and form a basis for Hermitian matrices

Hamiltonians

Computation of expectation values is linear:

$$\langle \hat{H} \rangle = \langle \psi | \hat{H} | \psi \rangle$$

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&= \sum_i c_i \, \langle \psi | \, P_i | \psi \rangle \\
&= \sum_i c_i \langle P_i \rangle
\end{aligned}$$

Exercise: Consider two qubits interacting under the Hamiltonian

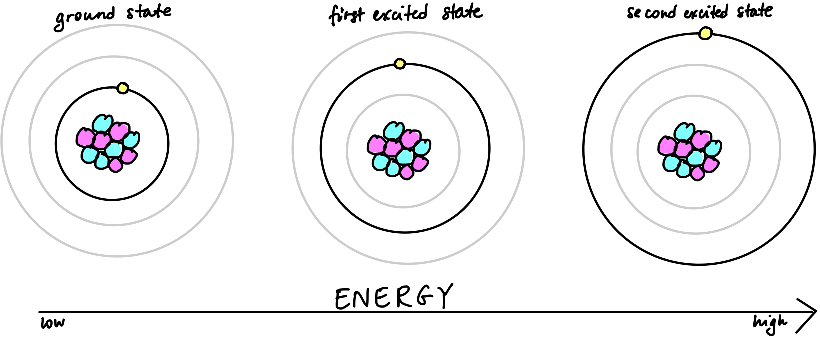
$$\hat{H} = -3(Z_0 + Z_1) + 2Z_0Z_1 + 4(X_0 + X_1)$$

What is the energy of the system if the qubits are in state

$$|\psi\rangle = |+\rangle \otimes |0\rangle$$

Energy of a physical system

Determining energy levels of physical systems is relevant for applications of quantum computing like physics and chemistry.



The energies (and associated configurations) are given by the *eigenvalues* and *eigenvectors* of the system Hamiltonian.

Computing the energy of a Hamiltonian

Given an arbitrary $\hat{H}$, how can we compute its energy?

Option: *exact diagonalization* to find its eigenvalues.

$$\hat{H} = \begin{pmatrix} * & * & * \\ * & * & * \\ * & * & * \end{pmatrix} \xrightarrow{\text{np.linalg.eig}} \{ E_i, |E_i\rangle \}$$

Many other purely classical methods too. But we're more interested in the quantum ones.

Time evolution

The Schrödinger equation from physics describes how the state of a system evolves with time.

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

The solution is:

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle$$

$e^{-i\hat{H}t/\hbar}$ is the *time evolution operator*, and $\hbar$ is a fundamental physical constant (we set it to 1 for simplicity).

Fun fact: if $\hat{H}$ is Hermitian,

$$e^{-i\hat{H}t}$$

is unitary.

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Then

$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle$$

describes how a system evolves with time.

If we can implement U on a quantum computer, we can compute its energy eigenvalues...

Let $\hat{H}$ be a Hamiltonian and $|E\rangle$ an eigenstate with energy E.

$$U|E\rangle = e^{-i\hat{H}t}|E\rangle$$

Computing the energy of a Hamiltonian

Let $\hat{H}$ be a Hamiltonian and $|E\rangle$ an eigenstate with energy E.

$$
\begin{aligned}
U|E\rangle &= e^{-i\hat{H}t}|E\rangle \\
&= \left(I + (-i\hat{H}t) + \frac{1}{2!}(-i\hat{H}t)^2 + \cdots \right) |E\rangle
\end{aligned}
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&= \left(|E\rangle + (-it)\hat{H}|E\rangle + \frac{1}{2!}(-it)^2\hat{H}^2|E\rangle + \cdots \right)
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&= \left(|E\rangle + (-it)E|E\rangle + \frac{1}{2!}(-it)^2E^2|E\rangle + \cdots \right)
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Computing the energy of a Hamiltonian

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&= \left(|E\rangle + (-it)E|E\rangle + \frac{1}{2!}(-it)^2E^2|E\rangle + \cdots\right) \\
&= \left(1 + (-iEt) + \frac{1}{2!}(-iEt)^2 + \cdots\right)|E\rangle
\end{aligned}$$

Computing the energy of a Hamiltonian

Let $\hat{H}$ be a Hamiltonian and $|E\rangle$ an eigenstate with energy E.

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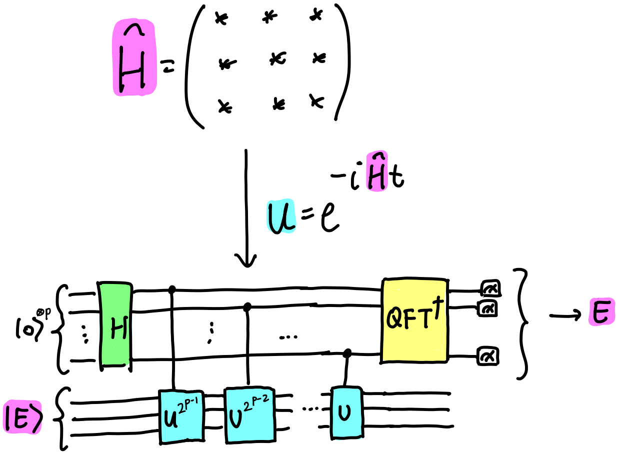
&= e^{-iEt}|E\rangle
\end{aligned}$$

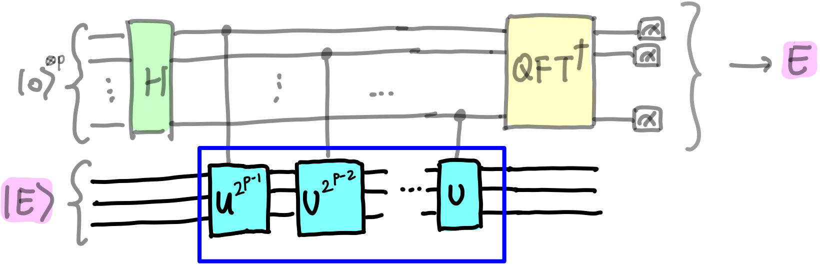
Computing the energy of a Hamiltonian

We can use *quantum phase estimation*!



(In hands-on 4, you will do this with the *variational eigensolver*)

The next challenge: implementing U



$$RZ(\theta) = e^{-i\frac{\theta}{2}Z}$$

Consider just one qubit for now.

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

Exercise: A qubit starts in state $|\psi(0)\rangle$ at time $t = 0$. What is $|\psi(t)\rangle$ for this $\hat{H}$? What quantum operation is this?

$$|\psi(t)\rangle = e^{-i(-\alpha Z_0)t}|\psi(0)\rangle$$

$$= RZ(-2\alpha t)|\psi(0)\rangle$$

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$$\begin{aligned} |\psi(t)\rangle &= e^{-i\hat{H}t}|\psi(0)\rangle \\ &= e^{i\alpha t Z}|\psi(0)\rangle \end{aligned}$$

Example: time evolution

Recall how we expressed RZ as a matrix exponential:

$$RZ(\theta) = e^{-i\frac{\theta}{2}Z}$$

We have

$$\begin{aligned} e^{i\alpha t Z} &= e^{-i\frac{-2\alpha t}{2}Z} \\ &= RZ(-2\alpha t) \end{aligned}$$

Example: time evolution

What about two non-interacting qubits?

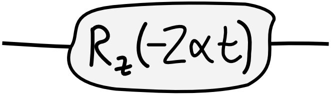
$$\hat{H} = -\alpha Z_0 - \alpha Z_1$$

Exercise: What do you think the quantum circuit for time evolution under this $\hat{H}$ looks like?

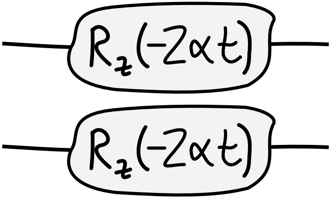
$$\begin{aligned} e^{it(\alpha Z_0 + \alpha Z_1)} &= e^{it\alpha Z_0} e^{it\alpha Z_1} \\ &= RZ(-2\alpha t) \otimes RZ(-2\alpha t) \end{aligned}$$

Example: time evolution

One qubit:



Two qubits:



This makes Hamiltonian simulation looks pretty easy!

Image credit: Xanadu Quantum Codebook node H.5

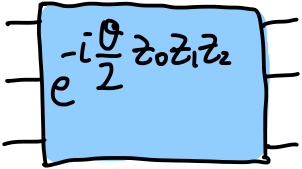
Hamiltonian simulation in general

What happens when

1. we have Paulis that aren't just Z?
2. we have interaction terms?
3. we have combinations of all Paulis and arbitrary interactions?

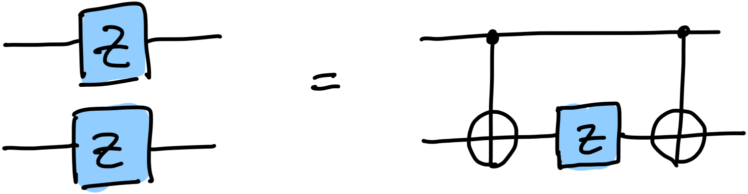
Circuits for individual Pauli terms

Example:

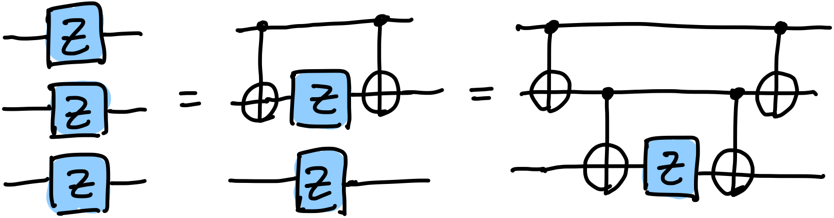


Idea: transform this into an exponential using only single-qubit Pauli Z, then implement those.

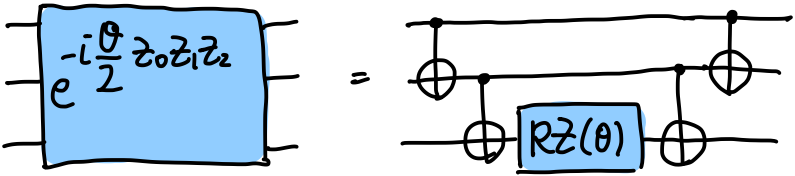
There is a useful circuit identity that relates Z and CNOT:



We can apply this multiple times

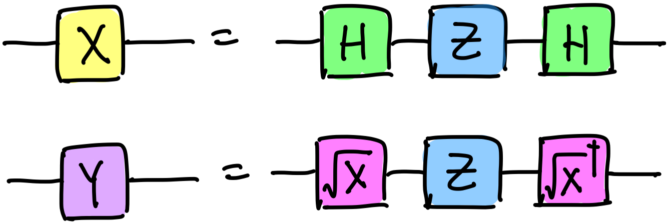


Z is just a special case of RZ though; so this works in general:

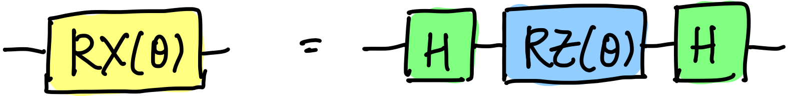


We can deal with any product of Pauli Z in this way.

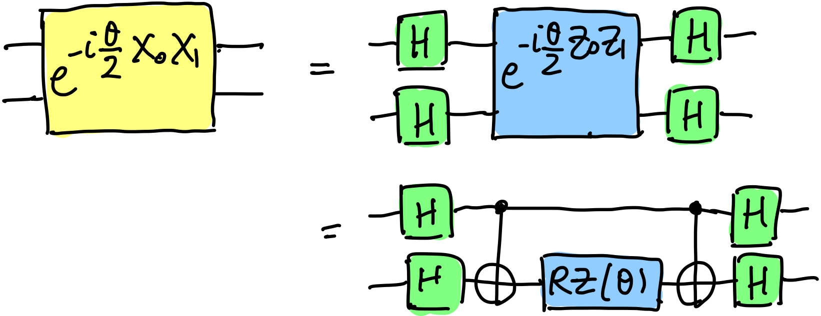
X and Y take a little more work; but they are related to Z in special ways:



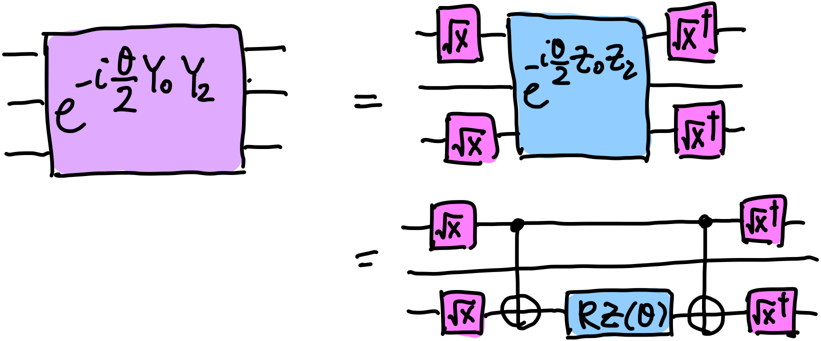
RX has the same relationship:



So when we exponentiate...



Similarly for Y



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

Fun fact: the operators applied on either side of the Z are elements of the **Clifford group**. Cliffords send Paulis to Paulis.

Now for the hard part. What about:

$$e^{-i\alpha Z_0 X_1 - i\beta Z_0 Y_1}$$

More generally,

$$e^{-i\alpha P - i\beta Q}, \quad P, Q \in \mathcal{P}_n$$

Depends whether P, Q commute, i.e., if $[P, Q] = PQ - QP = 0$.

More next time!

Next time

Content:

- Pauli commutation relation
- Hamiltonian simulation with Trotterization
- Error in Hamiltonian simulation

Action items:

1. Assignment 3 and hands-on 3
2. Work on project (remember to fill out weekly surveys)

Recommended reading:

- Codebook module H