CPEN 400Q / EECE 571Q Lecture 16
Mixed states, noise, and quantum channels

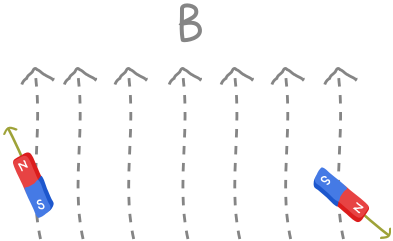
Thursday 10 March 2022

Announcements

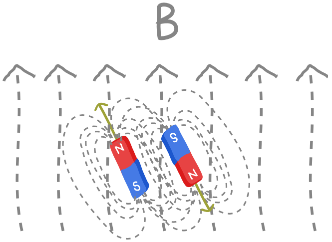
- Assignment 3 due Friday 11 March 23:59
- Project prototype meetings
  - Today: come to my office first (KAIS 3043), and we can snag KAIS 3028 if free
  - Tomorrow: KAIS 3065 booked from 15:00-17:00
  - Both days: Zoom (use my office hours link)

Last time

We introduced the idea of Hamiltonians, Hermitian operators that describe the energy of physical systems. They can be expressed as linear combinations of Pauli operators.



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



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

Image credits: Xanadu Quantum Codebook node H.5

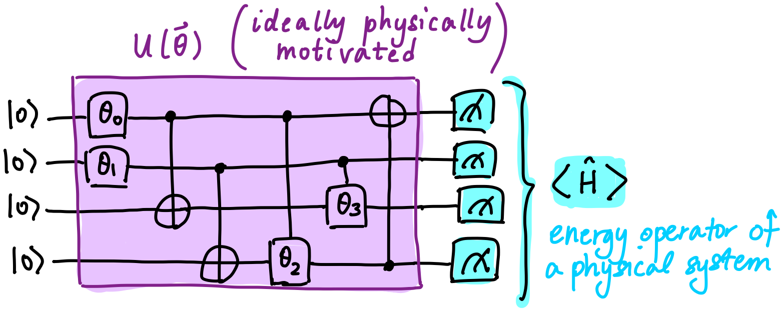
Last time

The energy of a system is the *expectation value of the Hamiltonian*. It is computed as a linear combination of the expectation values of its Pauli constituents.

$$\hat{H} = \sum_i c_i P_i \quad \Rightarrow \quad \begin{aligned} \langle \hat{H} \rangle &= \langle \psi | \hat{H} | \psi \rangle \\ &= \langle \psi | \left(\sum_i c_i P_i \right) | \psi \rangle \\ &= \sum_i c_i \langle \psi | P_i | \psi \rangle \\ &= \sum_i c_i \langle P_i \rangle \end{aligned}$$

Last time

We computed the ground state energy of a small quantum system with a variational eigensolver.



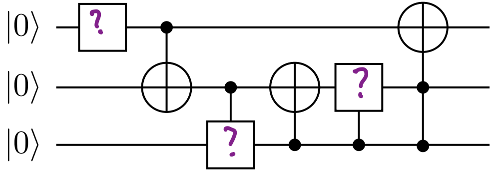
$$\min_{\vec{\theta}} \langle \hat{H} \rangle = \min_{\vec{\theta}} \langle 0 | U^{\dagger}(\vec{\theta})\, \hat{H}\, U(\vec{\theta}) | 0 \rangle \rightarrow E_g$$

(ground state energy)

Use the VQE to determine the ground state energy of

$$\hat{H} = X_0X_1 + 2X_1X_2 + 3X_0X_2 - Z_0 - 2Z_1 - 3Z_2$$

You were given the template circuit

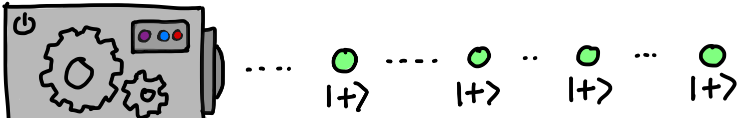


Let's code it up.

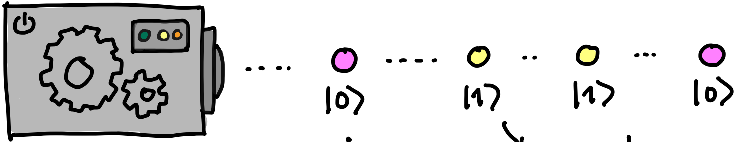
Learning outcomes

- Define a *mixed state*, and express quantum states using density matrices
- Describe the effects of common noise channels on qubit states
- Add noise to quantum circuits in PennyLane

Suppose we have two different "boxes" that shoot particles:



$$= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

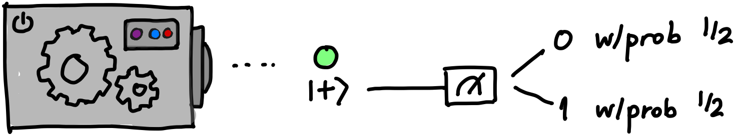


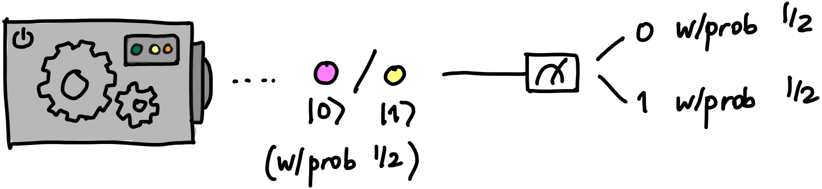
$p(0) = \frac{1}{2}$ $\quad p(1) = \frac{1}{2}$

Are these the same?

Mixed states

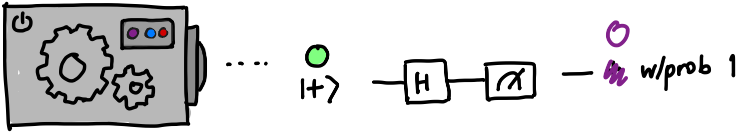
If we measure in the computational basis, it looks like they are.

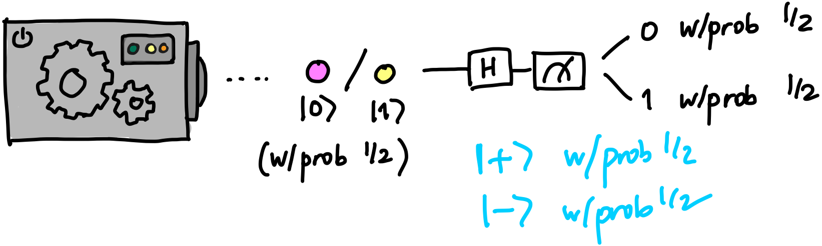




Mixed states

But if we measure in the Hadamard basis, they are not!





What is the second box doing?

Mixed states

The second box is outputting something called a **mixed state**.

A state is a **pure state** if it can be expressed as a single ket vector, e.g.,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$|0\rangle$, $|1\rangle$

$|+\rangle$

A state is a **mixed state** if it can be expressed as a *probabilistic mixture of pure states* (it describes an ensemble of states).

$$? = ???$$

... what does that look like?

Olivia look up

is any mixed state pure in some basis?

Density matrices

Mixed states cannot be represented as ket vectors. Instead, we use a matrix representation called a **density matrix**.

The density matrix of a pure state $|\psi\rangle$ is

rho

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \beta\alpha^* & |\beta|^2 \end{pmatrix}$$

For example,

$$\rho_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\rho_1 = |1\rangle\langle 1| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Density matrices of mixed states are linear combinations of density matrices of pure states:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \qquad \sum_i p_i = 1$$

$$p_0 = \frac{1}{2}, \quad p_1 = \frac{1}{2} \qquad \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

For example, suppose we have a box that prepares $|+\rangle$ with probability $1/3$, and $|0\rangle$ with probability $2/3$:

$$\rho = \frac{1}{3}|+\rangle\langle +| + \frac{2}{3}|0\rangle\langle 0|$$

$$= \frac{1}{3}\cdot\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{2}{3}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 5/6 & 1/6 \\ 1/6 & 1/6 \end{pmatrix}$$

$\mathrm{Tr} = 1$

$$|+\rangle\langle +| = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\rho = |\psi\rangle\langle\psi| \quad \rightarrow \quad \rho^2 = |\psi\rangle\underbrace{\langle\psi|\cdot|\psi\rangle}_{=1}\langle\psi|$$
$$= |\psi\rangle\langle\psi|$$

Density matrices have some nice properties.

- they are Hermitian $\rho^\dagger = \rho$
- they have trace 1
- they are positive semi-definite (all eigenvalues are ≥ 0)
- (for pure states only) they are projectors, i.e., $\rho^2 = \rho$

$$\mathrm{Tr}\left[\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}\right] \quad \Sigma$$

Check with our example:

$$\rho = \begin{pmatrix} \frac{5}{6} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{6} \end{pmatrix}$$

- clearly Hermitian
- $\mathrm{Tr}\rho = 5/6 + 1/6 = 1$
- eigenvalues are 0.872678 and 0.127322, both ≥ 0
- not pure, so $\rho^2 \neq \rho$

Fun activity: show properties hold for general $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$

Working with density matrices and mixed states

We can do all the normal things we do to pure states (i.e., operations, measurements) with mixed states as well.

For a pure state $|\psi\rangle$ and operation U,

$$|\psi\rangle \to |\psi'\rangle = U|\psi\rangle$$

As mixed states,

$$|\psi\rangle\langle\psi| \longrightarrow |\psi'\rangle\langle\psi'| = \left[U|\psi\rangle\right]\left[\langle\psi|U^\dagger\right]$$

$$= U|\psi\rangle\langle\psi|U^\dagger$$

$$\rho \to \rho' = U\rho U^\dagger$$

More generally,

$$\rho \to \rho' = U\rho U^\dagger$$

$$= U\left[\sum_i p_i |\psi_i\rangle\langle\psi_i|\right]U^\dagger$$

$$= \sum_i p_i \underbrace{U|\psi_i\rangle\langle\psi_i|U^\dagger}$$

$$= \sum_i p_i |\psi_i'\rangle\langle\psi_i'|$$

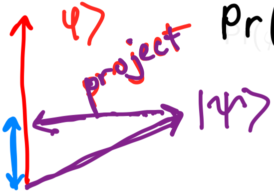
$$= \sum_i p_i \rho_i'$$

What about measurements?

Recall that for a pure state $|\psi\rangle$, the probability of measuring and observing it in state $|\varphi\rangle$ is computed using the inner product:

$$\Pr(\varphi) = |\langle\varphi|\psi\rangle|^2$$

We can rewrite this...



$$\begin{aligned}\Pr(\varphi) &= |\langle\varphi|\psi\rangle|^2 \\ &= \langle\varphi|\psi\rangle \cdot \langle\psi|\varphi\rangle \\ &= \langle\psi|\varphi\rangle\langle\varphi|\psi\rangle \\ &= \langle\psi| \left(|\varphi\rangle\langle\varphi|\right) |\psi\rangle\end{aligned}$$

$|\varphi\rangle\langle\varphi|$ is the density matrix of $|\varphi\rangle$, which is a *projector*. We are projecting $|\psi\rangle$ onto $|\varphi\rangle$, and then measuring the overlap with $|\psi\rangle$.

Mixed states and measurements

Measurement is performed w.r.t. a basis $\{|\varphi_i\rangle\}$; there are multiple possible outcomes:

$$\Pr(\text{outcome } i) = |\langle \varphi_i | \psi \rangle|^2$$

For mixed states, measurement outcome probabilities follow the **Born rule**:

$$\Pr(\text{outcome } i) = \mathrm{Tr}[P_i \cdot \rho]$$

where the set $\{P_i\}$ is called a **positive operator-valued measure (POVM)**. The elements of the POVM satisfy

$$\sum_i P_i = I$$

Can see that this reduces to our original projective measurement in the case where ρ is a pure state...

$$\Pr(\text{outcome } i) = \mathrm{Tr}(P_i \cdot \rho) = \mathrm{Tr}(P_i \cdot |\psi\rangle\langle\psi|)$$

For an $m \times m$ matrix A,

$$\mathrm{Tr}(A) = \sum_{k=0}^{m-1} \langle k|A|k\rangle$$

$$(\cdots 0 1 0 \cdots) \begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix} \begin{pmatrix} \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = (\cdots 0 1 0 \cdots) \begin{pmatrix} & & \\ & \boxed{\;} & \\ & & \end{pmatrix} = A_{kk}$$

Can see that this reduces to our original projective measurement in the case where ρ is a pure state...

$$\Pr(\text{outcome } i) = \mathrm{Tr}(P_i |\psi\rangle\langle\psi|)$$

$$= \sum_{k=0}^{m-1} \underbrace{\langle k| P_i |\psi\rangle}\underbrace{\langle\psi|k\rangle}$$

$$= \sum_{k=0}^{m-1} \langle\psi|k\rangle\langle k| P_i |\psi\rangle$$

$$= \langle\psi| \left[\underbrace{\sum_{k=0}^{m-1} |k\rangle\langle k|}_{=\mathbb{1}} \right] P_i |\psi\rangle$$

$$= \langle\psi| P_i |\psi\rangle$$

$$\downarrow$$

$$|\varphi_i\rangle\langle\varphi_i|$$

$$|0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$|1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sum P_i = I$$

Example POVM: $\{|+\rangle\langle+|, |-\rangle\langle-|\}$. $\quad |+\rangle\langle+| + |-\rangle\langle-| = \mathbb{1}$

First, check the criteria:

$$\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

For a particular ρ,

$$\Pr(+) = \mathrm{Tr}\left(|+\rangle\langle+| \cdot \rho\right)$$
$$\Pr(-) = \mathrm{Tr}\left(|-\rangle\langle-| \cdot \rho\right)$$

Now, remember how we computed expectation values from samples back in one of the early classes:

$$\langle X \rangle = \frac{1 \cdot (\#\ {+1}\ \text{eigvals}) + (-1) \cdot (\#\ {-1}\ \text{eigvals})}{\text{num-samples}}$$

$$= 1 \cdot Pr(+) + (-1) \cdot Pr(-)$$

$$= Tr(|+\rangle\langle+|\rho)$$

We can compute these probabilities in terms of the trace and ρ...

$$\langle X \rangle = Tr(|+\rangle\langle+|\rho) - Tr(|-\rangle\langle-|\rho)$$

$$= Tr\left(\left[|+\rangle\langle+| - |-\rangle\langle-|\right] \cdot \rho\right)$$

$$= Tr(X\rho)$$

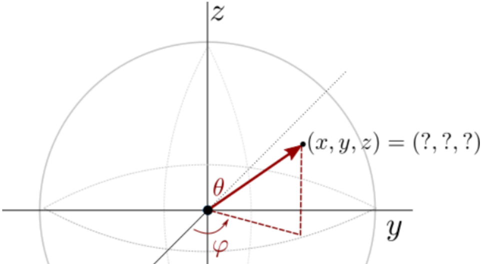
Mixed states and measurements

We can do the same for Y and Z: We can compute these probabilities in terms of the trace and ρ...

$$\langle X \rangle = \mathrm{Tr}(X\rho)$$
$$\langle Y \rangle = \mathrm{Tr}(Y\rho)$$
$$\langle Z \rangle = \mathrm{Tr}(Z\rho)$$

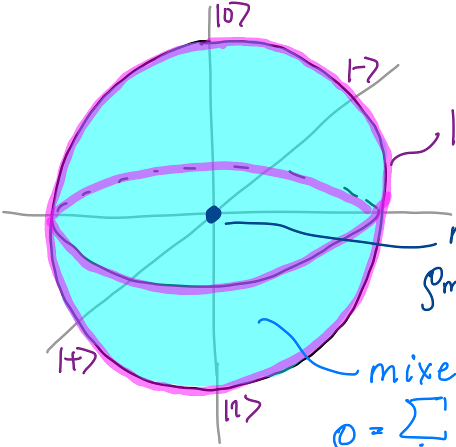
Remember from assignment 1:

Write a function that uses quantum measurements to extract its Bloch vector, i.e., its coordinates in 3-dimensional space, as demonstrated by the following graphic:



Mixed states on the Bloch sphere

Mixed states live *in* the Bloch sphere!



pure states

$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

maximally mixed state

$\rho_{max} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\mathbb{1}$

mixed states

$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

More formally, we can write any ρ as

$$\rho = \frac{1}{2} I + \frac{a_x}{2} X + \frac{a_y}{2} Y + \frac{a_z}{2} Z$$

where $a_P = \mathrm{Tr}(P\rho) = \langle P \rangle$.

(Should know such an expansion is possible since ρ is Hermitian, and Paulis are a basis for Hermitian matrices)

The case where $a_x = a_y = a_z = 0$ is the **maximally mixed state**.

(Note that all of this generalizes to multiple qubits as well)

Quantum channels and noise

Noise occurring in quantum systems is represented by **quantum channels**.

A quantum channel Φ *maps* states to other states.

$$\rho \to \rho' = \Phi(\rho)$$

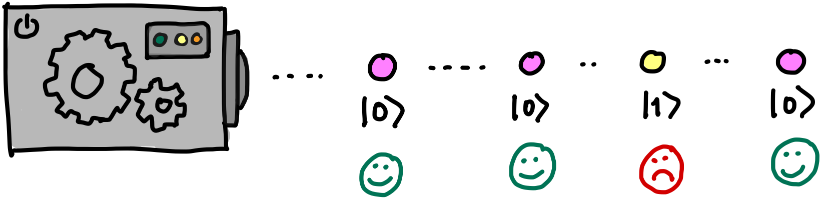
More formally, quantum channels are linear CPTP (Completely Positive, Trace-Preserving) maps.

Example: applying a unitary U is a channel, $\mathcal{U}$.

$$\rho \to \rho' = U \rho U^\dagger = \mathcal{U}(\rho)$$

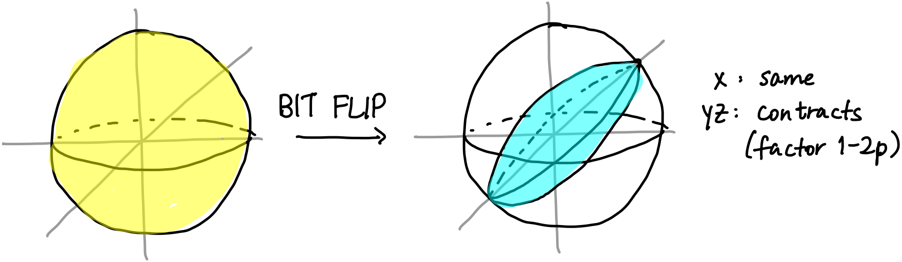
Suppose a "bit flip" (Pauli X) error occurs with probability p.

$$\mathcal{E}(\rho) = (1-p)\cdot\rho + p\cdot X\rho X$$



The bit flip channel

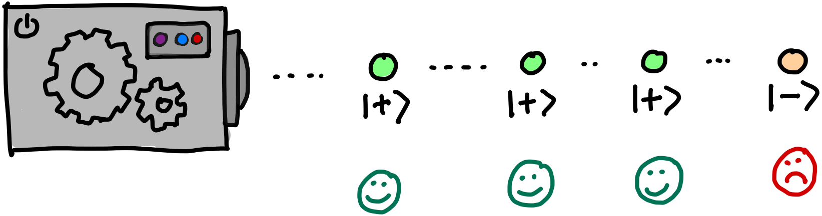
We can visualize the effects of such a channel by observing how it deforms the Bloch sphere.



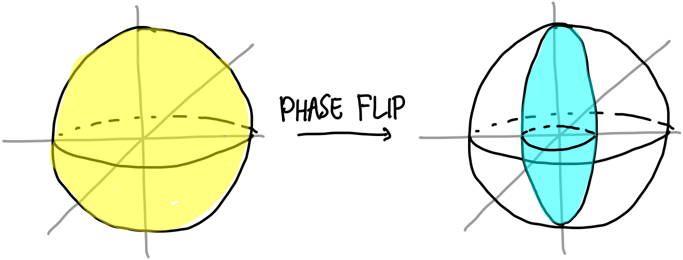
The phase flip channel

Suppose a “phase flip” (Pauli Z) error occurs with probability p.

$$\mathcal{E}(\rho) = (1-p)\cdot\rho + p\cdot Z\rho Z$$



The phase flip channel



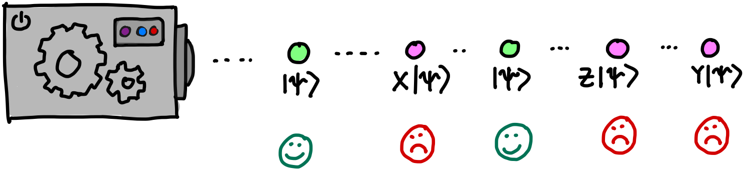
z : same

xy : contracts (factor 1-2p)

The depolarizing channel

Suppose each Pauli error occurs with probability $p/3$. This is called the *depolarizing channel*.

$$\mathcal{E}(\rho) = (1-p)\cdot\rho + \frac{p}{3}\cdot X\rho X + \frac{p}{3} Y\rho Y + \frac{p}{3} Z\rho Z$$



"default. mixed"

The depolarizing channel

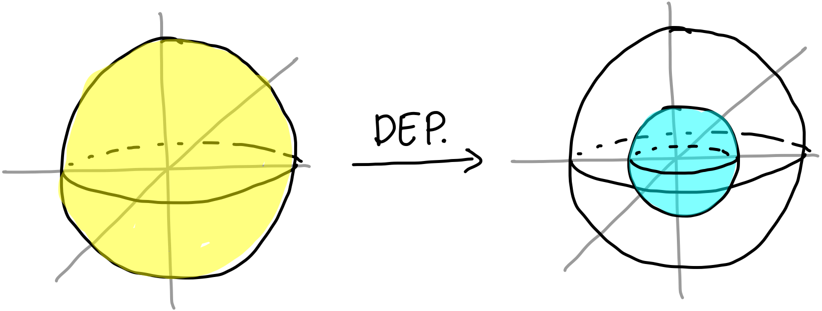
$$\mathcal{E}(\rho) = (1-p)\rho + \frac{p}{3}X\rho X + \frac{p}{3}Y\rho Y + \frac{p}{3}Z\rho Z$$

can also be written as

$$\mathcal{E}(\rho) = (1-p)\rho + p \cdot \frac{I}{2}$$

Think of this as outputting ρ w/probability $1-p$, and maximally mixed state with probability p.

The depolarizing channel



Comparing density matrices

How can we quantify "how much" error occurs? How close is $\sigma = \mathcal{E}(\rho)$ to ρ?

One common metric is the **trace distance**:

$$T(\rho, \sigma) = \frac{1}{2}||\rho - \sigma||_1 = \frac{1}{2}\mathrm{Tr}\left(\sqrt{(\rho - \sigma)^\dagger(\rho - \sigma)}\right)$$

Value of trace distance is bounded by $0 \leq T(\rho, \sigma) \leq 1$, and *lower* trace distance is better.

Comparing density matrices

Another is the **fidelity**:

$$F(\rho, \sigma) = \left(\mathrm{Tr} \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right)^2$$

Value of fidelity is bounded by $0 \leq F(\rho, \sigma) \leq 1$, and *higher* fidelity is better.

Next time

Content:

- VQE part II: VQE for real molecules
- What does *actual* hardware noise look like?
- How do we process noisy results?

Action items:

1. Prototype implementation for project
2. Assignment 3

Recommended reading:

- Nielsen and Chuang Ch. 8