CPEN 400Q Lecture 16
Mixed states and density matrices

Monday 10 March 2025

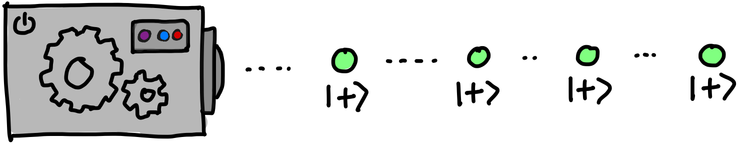
Announcements

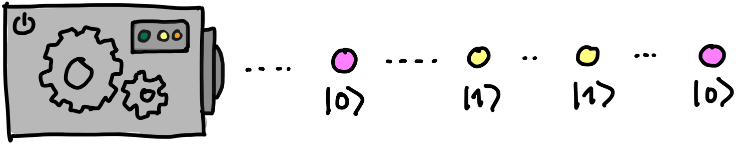
- Quiz 7 today
- Project MT checkpoint report due Friday 12pm
- A3 available (due Tuesday 25 March 23:59). Some reminders regarding academic integrity:
  - collaboration on assignments is allowed, but please honestly fill out contribution statement
  - use of ChatGPT permitted only for spelling/grammar check on literacy assignments; not permitted on other assignments

Learning outcomes

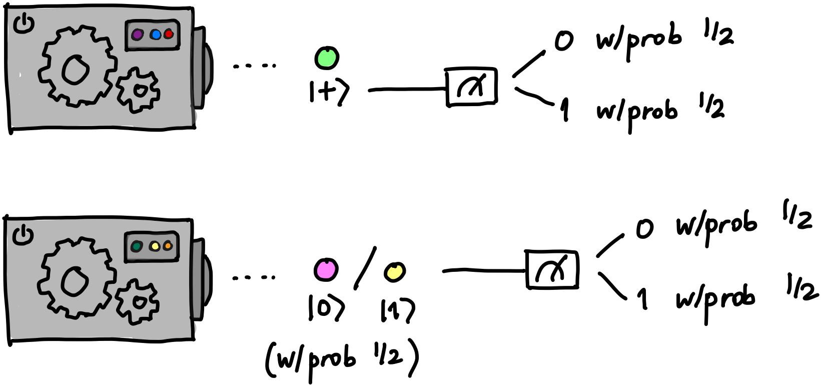
- Define a *mixed state*
- Express quantum states using density matrices
- Perform quantum computation in the density matrix formalism

Are these two devices the same?

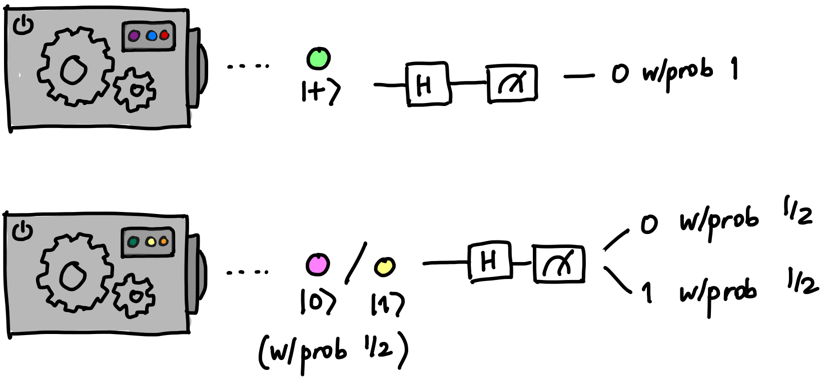




Mixed states



Mixed states



What is the second box doing?

Mixed states

The second box prepares a **mixed state**.

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

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

A **mixed state** is a *probabilistic mixture of pure states*.

$$? = ???$$

Mixed states are represented by **density matrices**.

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

$$\rho = |\psi\rangle\langle\psi|$$

Exercise: what are the density matrices for $|0\rangle$ and $|1\rangle$?

$$\rho_0 = |0\rangle\langle 0| = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$$
$$\rho_1 = |1\rangle\langle 1| = \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix} = \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}$$

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

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad \sum_i p_i = 1.$$

Exercise: A system prepares $|+\rangle$ with probability $1/3$, and $|0\rangle$ with probability $2/3$. What is its state?

$$\begin{aligned}\rho &= \frac{1}{3}|+\rangle\langle+| + \frac{2}{3}|0\rangle\langle 0| \\ &= \frac{1}{3}\cdot\frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} + \frac{2}{3}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} \\ &= \begin{pmatrix}\frac{5}{6} & \frac{1}{6}\\ \frac{1}{6} & \frac{1}{6}\end{pmatrix}\end{aligned}$$

Density matrices

Density matrices have some nice properties.

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

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,

$$|\psi\rangle\langle\psi| \to |\psi'\rangle\langle\psi'| = (U|\psi\rangle)(\langle\psi| U^\dagger)$$

Working with density matrices and mixed states

More generally,

$$
\begin{aligned}
\rho \to \rho' &= U\rho U^\dagger \\
&= U\left(\sum_i p_i|\psi_i\rangle\langle\psi_i|\right)U^\dagger \\
&= \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger \\
&= \sum_i p_i|\psi_i'\rangle\langle\psi_i'|
\end{aligned}
$$

Exercise: what is the output of applying H to our mixed state from the previous exercises? ($|+\rangle$ w/prob. $1/3$, $|0\rangle$ w/prob. $2/3$)

Mixed states and measurements

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

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

We can rewrite this...

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

$\Pi_\varphi = |\varphi\rangle\langle\varphi|$ is the density matrix of $|\varphi\rangle$, which is a *projector*.

In a projective measurement, the $\{\Pi_k\}$ "project" a state down to the consituent eigenstate.

Example: Apply projector Π_0 to $|+\rangle$:

$$\begin{aligned}\Pi_0|+\rangle &= |0\rangle\langle 0| \cdot \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ &= |0\rangle \cdot \frac{1}{\sqrt{2}}(\langle 0|\,|0\rangle + \langle 0|\,|1\rangle) \\ &= \frac{1}{\sqrt{2}}|0\rangle\end{aligned}$$

Apply projector again:

$$\begin{aligned}\Pi_0\Pi_0|+\rangle &= |0\rangle\langle 0|\,|0\rangle\langle 0|\,|+\rangle \\ &= |0\rangle\langle 0|\,|+\rangle \\ &= \frac{1}{\sqrt{2}}|0\rangle\end{aligned}$$

System stays in the state we observed during measurement

Mixed states and measurements

For mixed states, measurement follows the **Born rule**:

$$\Pr(\text{outcome i}) = \mathrm{Tr}(\Pi_i \rho)$$

where $\{\Pi_i\}$ is a **positive operator-valued measure (POVM)**.

The POVM elements satisfy

$$\sum_i \Pi_i = I$$

We can show this is equivalent to a projective measurement when ρ is pure.

Mixed states and measurements

For an $m \times m$ matrix A,

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

$$\begin{aligned}
\Pr(\text{outcome i}) &= \mathrm{Tr}(\Pi_i \rho) \\
&= \mathrm{Tr}(\Pi_i |\psi\rangle \langle\psi|) \\
&= \sum_{k=0}^{m-1} \langle k| \Pi_i |\psi\rangle\langle\psi|k\rangle \\
&= \sum_{k=0}^{m-1} \langle\psi|k\rangle \langle k| \Pi_i |\psi\rangle \\
&= \langle\psi| \left(\sum_{k=0}^{m-1} |k\rangle \langle k| \right) \Pi_i |\psi\rangle \\
&= \langle\psi|\Pi_i|\psi\rangle
\end{aligned}$$

Example: $\{\lvert+\rangle\langle+\rvert, \lvert-\rangle\langle-\rvert\}$.

Given a state ρ,

$$\begin{aligned}\Pr(+) &= \mathrm{Tr}(\lvert+\rangle\langle+\rvert\,\rho)\\ \Pr(-) &= \mathrm{Tr}(\lvert-\rangle\langle-\rvert\,\rho)\end{aligned}$$

Exercise: Show that $\{\lvert+\rangle\langle+\rvert, \lvert-\rangle\langle-\rvert\}$ form a legit POVM.

$$\lvert+\rangle\langle+\rvert + \lvert-\rangle\langle-\rvert = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} + \frac{1}{2}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

Exercise: Suppose we prepare our system in $|+\rangle$ with probability $1/3$ and $|0\rangle$ with probability $2/3$. What is the probability of obtaining the POVM outcome $\Pi_+ = |+\rangle\langle+|$?

$$
\begin{aligned}
\Pr(\Pi_+) &= \mathrm{Tr}(\Pi_+\rho) \\
&= \mathrm{Tr}\left(|+\rangle\langle+|\cdot\left(\frac{1}{3}|+\rangle\langle+| + \frac{2}{3}|0\rangle\langle0|\right)\right) \\
&= \mathrm{Tr}\left(\frac{1}{3}|+\rangle\langle+| + \frac{2}{3}\frac{1}{\sqrt{2}}|+\rangle\langle0|\right) \\
&= \frac{1}{3}\mathrm{Tr}(|+\rangle\langle+|) + \frac{\sqrt{2}}{3}\mathrm{Tr}\left(\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0\\ 1 & 0\end{pmatrix}\right) \\
&= \frac{1}{3} + \frac{1}{3} \\
&= \frac{2}{3}
\end{aligned}
$$

Let's play a game

Suppose I send you a mystery qubit, guaranteed to be either in

$$|\psi_1\rangle = |0\rangle, \quad \text{or} \quad |\psi_2\rangle = |+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

You must correctly determine which state I sent, but *you are only allowed to make one measurement*.

What measurement strategy maximizes your odds of being correct?

Positive operator-valued measures (POVMs)

Let $\{M_m\}$ be a set of measurement operators, where the M_m are not necessarily projectors, and

$$\sum_m M_m^\dagger M_m = I, \qquad p(m) = \langle\psi|\, M_m^\dagger M_m|\psi\rangle.$$

The set of operators

$$E_m = M_m^\dagger M_m$$

constitutes a POVM, and can be used to make a measurement on a quantum system.

Revisit our game

What measurement maximizes odds of distinguishing between

$$|\psi_1\rangle = |0\rangle, \quad \text{or} \quad |\psi_2\rangle = |+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

Choose a set of three POVM elements:

$$\begin{aligned} E_1 &= \frac{\sqrt{2}}{1+\sqrt{2}}|1\rangle\langle 1| \\ E_2 &= \frac{\sqrt{2}}{1+\sqrt{2}}|-\rangle\langle -| \\ E_3 &= I - E_1 - E_2 \end{aligned}$$

	$\Pr(E_1)$	$\Pr(E_2)$	$\Pr(E_3)$
$\lvert\psi_1\rangle = \lvert 0\rangle$	0	$1-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
$\lvert\psi_2\rangle = \lvert +\rangle$	$1-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

Next time

Next class:

- Mixed states and the Bloch sphere
- Quantum channels

Action items:

1. Work on project (MT checkpoint due Friday 12:00)
2. Work on assignment 3 (due Tuesday 25 March 23:59)

Recommended reading:

- Codebook module NT
- Nielsen & Chuang 2.4, 2.2.5-2.2.6