CPEN 400Q Lecture 16
Mixed states and density matrices

Monday 10 March 2025

Announcements

kraus

☆ Fix grader for order question.

- 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
- TA 3 tomorrow (about VQE)

$$a^{r} \bmod N \equiv 1 \bmod N$$

$r = \text{order}$

$$U_{N,a}|k\rangle = |ka \bmod N\rangle$$

$$(U_{N,a})^r|k\rangle = |k \bmod N\rangle$$

$N = 17$, $a = 15$

$$U_{N,a}|\underbrace{01010}_{10}\rangle \Rightarrow U_{17,15}|10\rangle = |150\rangle$$

$$= |14 \bmod 17\rangle$$

$$= |01110\rangle$$

$(15)^r \equiv 1 \bmod N \Rightarrow$ for idx in range...

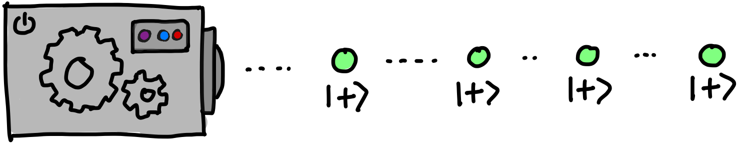
$\Rightarrow r = 8$

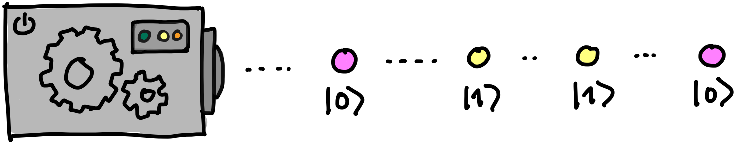
Learning outcomes

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

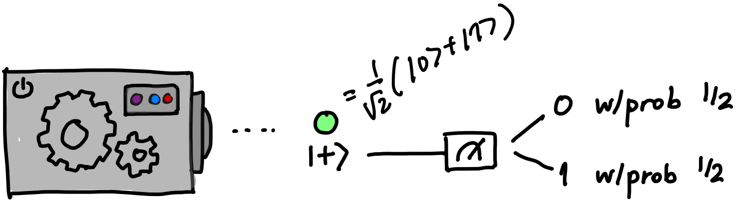
Mixed states

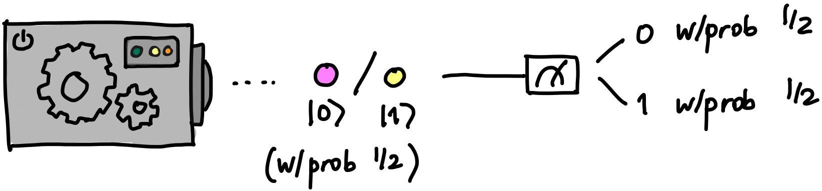
Are these two devices the same?



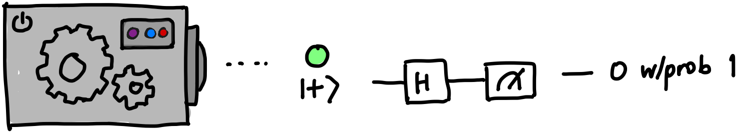


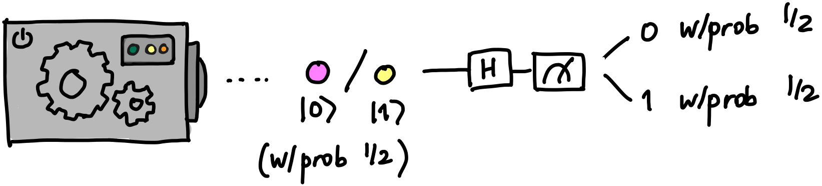
Mixed states





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.,

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

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

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

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

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

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

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

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

eig. vals = 1 , 0

Density matrices

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

$$\rho = \sum_i p_i \underbrace{|\psi_i\rangle\langle\psi_i|}_{\rho_{\psi_i}}, \quad \sum_i p_i = 1.$$

Box: $\frac{1}{2}$ prob $|0\rangle$, $\frac{1}{2}$ prob $|1\rangle$

$$\Rightarrow \rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

Tr $=1$

eigvals $= \frac{1}{2}, \frac{1}{2}$

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

$$|+\rangle\langle +| = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \cdot \frac{1}{\sqrt{2}}(\langle 0| + \langle 1|)$$
$$= \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 1|\right)$$

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

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

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

Density matrices

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

Density matrices have some nice properties.

- they are Hermitian $\rho = \rho^\dagger$
- they have trace 1
- they are positive semi-definite (all eigenvalues are ≥ 0)
- (for pure states only) they are $\underbrace{\text{projectors}}_{\text{relationship w/ proj. measurements}}$, 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
- $\text{Tr}\rho = 5/6 + 1/6 = 1$
- eigenvalues are 0.872678 and 0.127322, both ≥ 0
- not pure, so $\rho^2 \neq \rho$

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

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,

pure state → pure state

$$|\psi\rangle \rightarrow |\psi'\rangle = \underbrace{U|\psi\rangle}$$

As mixed states,

$$\underbrace{|\psi\rangle\langle\psi|}_{\rho_\psi} \rightarrow \underbrace{|\psi'\rangle\langle\psi'|}_{\rho_{\psi'}} = (U|\psi\rangle)(\langle\psi| U^\dagger)$$

$$= U\left(|\psi\rangle\langle\psi|\right)U^\dagger$$

$$\rho_{\psi'} = U \rho_\psi U^\dagger$$

More generally,

$$\rho = \sum p_i \underbrace{|\psi_i\rangle\langle\psi_i|}$$

$\downarrow$

output

$U|\psi_i\rangle\langle\psi_i|U^\dagger$

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

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

mixed state

$\downarrow$

mixed state

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)

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

$$\rho' = H\rho H = \begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \end{pmatrix}$$

$$H\rho H = H\left[\frac{1}{3}|+\rangle\langle+| + \frac{2}{3}|0\rangle\langle 0|\right]H$$

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

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

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...

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

inner product of
$|\psi\rangle$, $(|\varphi\rangle\langle\varphi|)|\psi\rangle$

$\Pi_\varphi = \underline{|\varphi\rangle\langle\varphi|}$ 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)**.

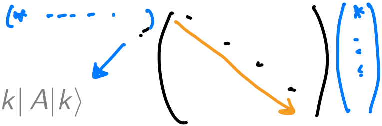
The POVM elements satisfy

$$\sum_i \Pi_i = I$$

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,



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

$$\begin{aligned}
\Pr(\text{outcome i}) &= \mathrm{Tr}(\Pi_i \rho) \\
&= \mathrm{Tr}(\Pi_i |\psi\rangle\langle\psi|) \\
&= \sum_{k=0}^{m-1} \langle k| \Pi_i |\psi\rangle\langle\psi|k\rangle \\
&= \sum_{k=0}^{m-1} \langle\psi|k\rangle\langle k| \Pi_i |\psi\rangle \\
&= \langle\psi| \Bigg(\underbrace{\sum_{k=0}^{m-1} |k\rangle\langle k|}_{=I} \Bigg) \Pi_i |\psi\rangle \\
&= \langle\psi|\Pi_i|\psi\rangle \quad = |\langle\varphi|\psi\rangle|^2 \text{ if } \Pi_i = |\varphi\rangle\langle\varphi|
\end{aligned}$$

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

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

$Tr(|+\rangle\langle+|\rho) + Tr(|-\rangle\langle-|\rho) = 1$

$Tr(|+\rangle\langle+|\rho + |-\rangle\langle-|\rho) = 1$

$\Updownarrow$

$Tr((|+\rangle\langle+| + |-\rangle\langle-|)\rho) = 1$

$\Downarrow$

I

Given a state ρ,

$$\mathsf{Pr}(+) = \mathsf{Tr}(|+\rangle\langle+|\rho)$$
$$\mathsf{Pr}(-) = \mathsf{Tr}(|-\rangle\langle-|\rho)$$

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

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

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 $\Pi_+ = |+\rangle\langle+|$?

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

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)

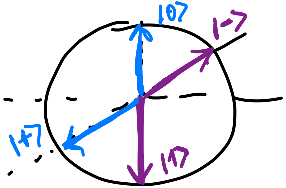
Let $\{M_m\}$ be a set of measurement operators, where the M_m are not necessarily projectors, and

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

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.



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