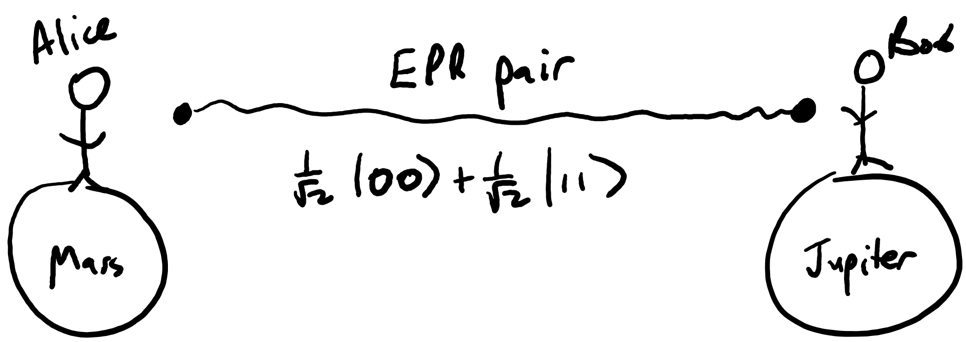
Lecture 21 - Mixed States & Density Matrices

[Starting here, I'll tell you the full truth about what a quantum state is. It's not that I've lied before — it's just that for the sake of mathematical simplicity, haven't told the full story. In fact, the full story — tho seemingly more complicated at first, actually eliminates some mathematical infelicities. Main thing is we need to give full-fledged status to...] **Mixed states** [[prob. dists. over pure quantum states]]

Recall Lecture 6



[Suppose we promise Alice will never hear from Bob again. It should be possible to forget her particle's entanglement, and to ascribe some "state" to Alice's particle that will let us predict outcomes of measurements she might perform. After all, Bob is just staying on Jupiter, not affecting anything....]

Alice's qubit's "state"?

For all we know, Bob measures his qubit.

[["collapses" Alice's qubit to $|0\rangle$ or $|1\rangle$]]

"50% prob. of $|0\rangle$, 50% prob. of $|1\rangle$" ("σ")

Or... maybe Bob measures in $|\pm\rangle$ basis.

We saw: $\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ 1/\sqrt{2} \end{bmatrix} = \frac{1}{\sqrt{2}}|{++}\rangle + \frac{1}{\sqrt{2}}|{--}\rangle$

Alice gets...

"50% prob of $|+\rangle$, 50% prob. of $|-\rangle$". ("σ'")

[[On the face of it, the "mixed" states σ & σ' look very different. But I argued (as did you on homework) that...]]

σ & σ' are "the same" ← <u>no</u> measurement can distinguish them!

[[We'll sketch an analysis of this, & thereby come up with a <u>new</u> representation for quantum states - esp. mixed states - under which σ, σ' are represented by the <u>same</u> math object.]]

[We want to analyze] Mixed state (of a qudit, say)

$\{p_1 \text{ prob. of } |\psi_1\rangle,\ p_2 \text{ prob. of } |\psi_2\rangle, \ldots, p_m \text{ prob. of } |\psi_m\rangle\}$

$\left(\sum_i p_i = 1,\quad |\psi_i\rangle \in \mathbb{C}^d \text{ unit}\right)$

[These arise if: your quantum apparatus flips coins
Or, if it does internal (partial) measurements
but keeps going. Basically we now don't want
to rely on Princ. of Deferred Measurement.]

[We now wish to analyze questions about
"could you use measurements to disting. this
mixed state from that mixed state?"]

Say we measure in basis $|u_1\rangle, |u_2\rangle, \ldots, |u_d\rangle$.

What is $\Pr[\text{readout is "}i\text{"}]$?

It's
$$\sum_{j=1}^{m} \underbrace{p_j}_{\substack{\text{prob. state} \\ \text{is } |\psi_j\rangle}} \underbrace{|\langle u_i|\psi_j\rangle|^2}_{\substack{\text{prob. of measuring "}i\text{"} \\ \text{given that state is} \\ |\psi_j\rangle}}$$

$$\Pr[\text{readout is "}i\text{"}] = \sum_{j=1}^{m} p_j \left|\langle u_i|\psi_j\rangle\right|^2 \quad ☺$$

math trickery: $\bullet\ |z|^2 = zz^*$ $\quad\bullet\ \langle u_i|\psi_j\rangle$ is a 1×1 matrix.

$$\bullet\ \langle u_i|\psi_j\rangle^{\cancel{*}\to\dagger} = \langle\psi_j|u_i\rangle$$

$$\therefore\ ☺ = \sum_{j=1}^{m} p_j \langle u_i|\underbrace{\psi_j\rangle\langle\psi_j}|u_i\rangle$$

[[u_i's don't dep. on j.]]

$\begin{bmatrix}\vdots\end{bmatrix}\begin{bmatrix}\cdots\end{bmatrix}$ ← a $d\times d$ matrix depending on j.

("Projection onto $|\psi_j\rangle$ operator": see HW#2)

$$= \langle u_i|\cdot\underbrace{\left(\sum_{j=1}^{m} p_j|\psi_j\rangle\langle\psi_j|\right)}_{\text{call this } d\times d \text{ matrix } \rho}\cdot|u_i\rangle$$

$$= \langle u_i|\cdot\rho\cdot|u_i\rangle \qquad \begin{bmatrix}\cdots\end{bmatrix}\begin{bmatrix} & & \\ & \rho & \\ & & \end{bmatrix}\begin{bmatrix}\vdots\end{bmatrix}$$

ALL OUTCOME PROBABILITIES DEPEND ONLY ON ρ! [[It encodes all info needed to explain all future measurements.]]

$\rho = \sum_{j=1}^{m} p_j |\psi_j\rangle\langle\psi_j|$ is called the "<u>density matrix</u>"

for mixed state "p_1 prob. of $|\psi_1\rangle, \dots, p_m$ prob. of $|\psi_m\rangle$"

E.g. 1: "50% prob. $|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}$, 50% prob. $|1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$"

has density matrix $.5\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} + .5\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix}$

$$= .5\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + .5\begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}$$

$$= \begin{bmatrix}1/2 & 0\\0 & 1/2\end{bmatrix}$$

[That's it!]

E.g. 2: 50% on $|+\rangle = \begin{bmatrix}1/\sqrt{2}\\1/\sqrt{2}\end{bmatrix}$, 50% on $|-\rangle = \begin{bmatrix}1/\sqrt{2}\\-1/\sqrt{2}\end{bmatrix}$

$$\hookrightarrow \frac{1}{2}\begin{bmatrix}1/\sqrt{2}\\1/\sqrt{2}\end{bmatrix}\begin{bmatrix}1/\sqrt{2} & 1/\sqrt{2}\end{bmatrix} + \frac{1}{2}\begin{bmatrix}1/\sqrt{2}\\-1/\sqrt{2}\end{bmatrix}\begin{bmatrix}1/\sqrt{2} & -1/\sqrt{2}\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1/2 & 1/2\\1/2 & 1/2\end{bmatrix} + \frac{1}{2}\begin{bmatrix}1/2 & -1/2\\-1/2 & 1/2\end{bmatrix}$$

$$= \begin{bmatrix}1/2 & 0\\0 & 1/2\end{bmatrix}.$$

Same! ☺

E.g. 3: "100% prob. of $|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}$": $\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}$.

E.g. 4: "100% prob. of $-|0\rangle = \begin{bmatrix}-1\\0\end{bmatrix}$": $\begin{bmatrix}-1\\0\end{bmatrix}\begin{bmatrix}-1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}$ Same!

[Great! Remember we saw this too: multiplying a state by a "global phase (complex # of magnitude 1)" doesn't affect it for any measurement purposes. So the infelicity that $|0\rangle$ & $-|0\rangle$ & $i|0\rangle$ look dissimilar is fixed when you go to density matrices. ☺]

E.g. 5: "100% of $i|0\rangle = \begin{bmatrix}i\\0\end{bmatrix}$": $\begin{bmatrix}i\\0\end{bmatrix}\begin{bmatrix}-i & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}$ ☺

b/c you take conjugate transpose: $i^* = -i$

Random e.g. 6: "2/3 prob. of $|0\rangle$, 1/3 prob. of $|-\rangle$":

$$\hookrightarrow \frac{2}{3}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} + \frac{1}{3}\begin{bmatrix}1/\sqrt{2}\\-1/\sqrt{2}\end{bmatrix}\begin{bmatrix}1/\sqrt{2} & -1/\sqrt{2}\end{bmatrix} = \frac{2}{3}\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + \frac{1}{3}\begin{bmatrix}1/2 & -1/2\\-1/2 & 1/2\end{bmatrix}$$

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

Qutrit example: "50% of $|1\rangle = \begin{bmatrix}1\\0\\0\end{bmatrix}$,

50% of $\frac{1}{3}|1\rangle + \frac{2}{3}|2\rangle + \frac{2}{3}i\,|3\rangle = \begin{bmatrix}1/3\\2/3\\2/3\,i\end{bmatrix}$"

$$\rho = \frac{1}{2}\begin{bmatrix}1\\0\\0\end{bmatrix}\begin{bmatrix}1 & 0 & 0\end{bmatrix} + \frac{1}{2}\begin{bmatrix}1/3\\2/3\\2/3\,i\end{bmatrix}\begin{bmatrix}1/3 & 2/3 & -\frac{2}{3}i\end{bmatrix}$$

don't forget to conjugate!

$$= \frac{1}{2}\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix} + \frac{1}{2}\begin{bmatrix}1/9 & 2/9 & -\frac{2}{9}i\\ 2/9 & 4/9 & -\frac{4}{9}i\\ \frac{2i}{9} & \frac{4}{9}i & 4/9\end{bmatrix} = \boxed{\begin{bmatrix}5/9 & 1/9 & -i/9\\ 1/9 & 2/9 & -\frac{2}{9}i\\ i/9 & \frac{2}{9}i & \frac{2}{9}\end{bmatrix}}$$

Say we measure in <u>standard basis</u>: $|u_1\rangle = |1\rangle$, $|u_2\rangle = |2\rangle$, $|u_3\rangle = |3\rangle$.

$$\Pr[\text{readout } 1] = \langle u_1|\rho|u_1\rangle = \begin{bmatrix}1&0&0\end{bmatrix}\begin{bmatrix}\ \rho\ \end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix} = \underbrace{\rho_{11}}_{}$$

(5/9 in e.g. above)

$$\Pr[\text{readout } 2] = \langle u_2|\rho|u_2\rangle = \begin{bmatrix}0&1&0\end{bmatrix}\begin{bmatrix}\ \rho\ \end{bmatrix}\begin{bmatrix}0\\1\\0\end{bmatrix} = \underbrace{\rho_{22}}_{}$$

(2/9 in above eg.)

$$\Pr[\text{readout } 3] = \cdots = \rho_{33}$$ (also 2/9 above).

In general: For qudit density mtx ρ, if you measure in std. basis, $\{|1\rangle, \ldots, |d\rangle\}$, $\Pr[\text{"}i\text{"}] = \rho_{ii}$.

Properties of Density Matrices ρ

- They are ~~symmetric~~ Hermitian: $\rho^\dagger = \rho$

  (because $\left(\sum p_i |\psi_i\rangle\langle\psi_i|\right)^\dagger = \sum p_i |\psi_i\rangle\langle\psi_i|$)

- They are positive (aka positive definite, written $\rho \geq 0$ or $\rho \succeq 0$)

  meaning $\langle u|\rho|u\rangle \geq 0 \quad \forall$ unit $|u\rangle \in \mathbb{C}^d$

  ↳ doesn't matter if you include this adjective or not; it's equivalent

  [[Because can extend $|u\rangle$ to a basis to measure in; $\langle u|\rho|u\rangle = \Pr[\text{measuring "}u\text{"}] \geq 0$.]]

- $\underbrace{\sum_{i=1}^{d} \rho_{ii}}$ $= 1$. [Because $\rho_{ii} = \Pr[\text{measuring "}i\text{"}]$ when measuring in std. basis. Probs must add to 1!]

  "trace of matrix ρ", denoted $tr(\rho)$.

[[We'll see: any Hermitian ρ that's positive & has $tr(\rho) = 1$ is the density matrix of some mixed state.]]

def: A d-outcome (d-dim) density matrix is a Hermitian matrix $\rho \in \mathbb{C}^{d \times d}$ with $\rho \geq 0$ & $\sum_{i=1}^{d} \rho_{ii} = 1$

Cf: A d-outcome probability density (prob. dist on $\{1,2,\ldots,d\}$) is a vector $p \in \mathbb{R}^d$ with $p \geq 0$ & $\sum_{i=1}^{d} p_i = 1$.

[Indeed, we'll pursue this analogy very far in future lectures. A quantum (mixed) state can be thought of as a "quantum source of randomness", akin to a classical probability distribution.

Indeed diagonal density matrices

$$\equiv$$

classical prob. distributions,

and "quantum probability theory" will strictly generalize "classical prob. theory".]

Working with density matrices ρ

[[Main thing you can do with a quantum qudit state is apply a unitary transformation to it.]]

quantum mixed state $\xrightarrow{U}$ new mixed state

"p_i prob. of $|\psi_i\rangle$" $(i=1\ldots m)$ → "p_i prob. of $U|\psi_i\rangle$" $(i=1\ldots m)$

density matrix: $\rho = \sum_{i=1}^{m} p_i |\psi_i\rangle\langle\psi_i|$

$$\rho' = \sum_{i=1}^{m} p_i \, U|\psi_i\rangle \underbrace{\cancel{(U|\psi_i\rangle)^\dagger}}_{\langle\psi_i|U^\dagger}$$

$$= U\left(\sum_{i=1}^{m} p_i |\psi_i\rangle\langle\psi_i|\right)U^\dagger$$

$\therefore$ in density mtx world, "applying unitary U" becomes

$$\rho \mapsto U\rho U^\dagger \quad (\text{"conjugating by } U^\dagger\text{"})$$

[[Other main thing you do is "measure in standard basis". Measuring in other bases is, as we know, equiv. to doing a unitary & measuring in std. basis.

Now, after you measure, you are in various (pure) states — $|1\rangle$ with prob. ρ_{11}, $|2\rangle$ with prob. ρ_{22}, etc.

For purposes of further analysis — you're still in a mixed state!!]]

Some mixed qudit state
$\downarrow$
density matrix ρ $\xrightarrow[\text{std. basis}]{\text{measure in}}$ "ρ_{11} prob. of $|1\rangle = \begin{bmatrix}1\\0\\ \vdots\\0\end{bmatrix}$,

ρ_{22} prob. of $|2\rangle = \begin{bmatrix}0\\1\\0\\ \vdots\\0\end{bmatrix}$,

... ρ_{dd} prob. of $|d\rangle$"

density matrix is

$$\rho_{11}|1\rangle\langle 1| + \rho_{22}|2\rangle\langle 2| + \cdots + \rho_{dd}|d\rangle\langle d|$$

$$= \rho_{11}\begin{bmatrix}1 & & 0\\ & 0 & \\ 0 & & \ddots & 0\end{bmatrix} + \rho_{22}\begin{bmatrix}0 & & \\ & 1 & & 0\\ & & 0 & \\ 0 & & & \ddots & 0\end{bmatrix} + \cdots$$

$$= \begin{bmatrix}\rho_{11} & & & 0\\ & \rho_{22} & & \\ & & \ddots & \\ 0 & & & \rho_{dd}\end{bmatrix}$$

<u>Conclusion</u>: Measurement (in std. basis) affects density matrix ρ by <u>zeroing out the off-diagonal entries</u>.

[[You should still think of result as a mixed state.]]

[[We'll later see a unified framework for density matrix transformations that includes conjugations by unitaries & measurements - nice!]]

Linear Algebra Interlude

$d \times d$ ~~symmetric~~ Hermitian matrices M are so great!

Love 'em. [[NB: Unitary matrices aren't always Hermitian :( ]]

Why? <u>Math talk</u>: they have d <u>real</u> eigenvalues, and associated orthonormal eigenvectors.

<u>Real talk</u>: there's an orthonormal basis $|v_1\rangle, \ldots, |v_d\rangle$, and M's action on $\mathbb{C}^d$ is

"<u>stretch by factor $\lambda_i \in \mathbb{R}$ in $|v_i\rangle$ direction</u>"

[[This is the good way to picture any Hermitian M.]]

$$M = \sum_{i=1}^{d} \lambda_i \underbrace{|v_i\rangle\langle v_i|}_{\text{Proj. onto } |v_i\rangle \text{ operator}}$$

[[Annoyance: if λ_i's not all distinct, assoc. $|v_i\rangle$'s not uniquely determined. E.g. suppose $\lambda_1 = \lambda_2 = 5$. So M stretches by factor of 5 in both $|v_1\rangle, |v_2\rangle$ directions. Hence it stretches that whole 2-dim. subspace by 5. So could equivalently replace $|v_1\rangle, |v_2\rangle$ by any 2 orthonormal vectors in that 2-dim. subspace.]]

[[Back to density matrices.]]

Density matrices $\rho \in \mathbb{C}^{d \times d}$ are Hermitian ☺

So they have an associated orthonormal basis $|v_1\rangle, \ldots, |v_d\rangle$ and real stretch factors $\lambda_1, \ldots, \lambda_d$.

Recall: ρ is "positive": $\langle u|\rho|u\rangle \geq 0 \quad \forall$ unit $|u\rangle$

$$\Rightarrow \quad \langle v_i|\rho|v_i\rangle = \langle v_i| \cdot \lambda_i |v_i\rangle = \lambda_i \geq 0.$$

$\Rightarrow$ all λ_i's are nonneg. ⊛

[[Easy to show <u>iff</u>: if Hermitian M has all eigvals ≥ 0, then M is positive.]]

Also: Let U be the unitary moving $|v_1\rangle, \ldots, |v_d\rangle$ to std. basis $|1\rangle, \ldots, |d\rangle$.

Say we apply it to ρ: $\rightsquigarrow \rho' = U\rho U^\dagger$.

On one hand: ρ' has same stretch factors $\lambda_1, \ldots, \lambda_d$, just in another basis

OTOH: ρ' is now a diagonal matrix.

$\therefore$ stretch factors are diag entries ρ_{ii}

But $\sum_{i=1}^{d} \rho_{ii} = 1$.

$\therefore$ λ_i's satisfy $\lambda_1 + \cdots + \lambda_d = 1$ ⊛

So: given any density matrix ρ,
its eigenvals (stretch factors) $\lambda_1, \ldots, \lambda_d$
are real, nonneg., sum to 1
$\Rightarrow$ they form a prob. distribution!

[[Converse also easy: if Hermitian mtx M has eigs nonneg., summing to 1, it's a density matrix.]]

So: any density matrix $\rho \in \mathbb{C}^{d \times d}$ (with distinct eigenvals)
has a "canonical" assoc. mixed state:
"prob. λ_i of state $|v_i\rangle$", $i = 1 \ldots \underline{\underline{d}}$ ← [[dimension many states]]

λ_i: eigs(ρ)

$|v_i\rangle$: orthonormal eigenvecs(ρ)

[[The small print "with distinct eigenvalues" is important. Actually, there's a very common case where we <u>don't</u> have this...]]

def: The <u>maximally</u> <u>mixed state</u> (in d dimensions):

density matrix $\rho = \begin{bmatrix} 1/d & & 0 \\ & 1/d & \\ 0 & & \ddots \; 1/d \end{bmatrix} = \frac{1}{d} \cdot I_{d \times d}$.

[[Hermitian? ✓]]

Stretches by $\frac{1}{d}$ in <u>all</u> directions

(Eigvals are $\frac{1}{d}, \frac{1}{d}, \ldots, \frac{1}{d}$ ← the <u>uniform</u> prob. distribution.)

No "canonical" orthonormal basis. [[All equally the same.]]

Our original example when $d=2$:

" $\frac{1}{2}$ prob. (stretch) on $|0\rangle$, $\frac{1}{2}$ prob. (stretch) on $|1\rangle$ "

=

" $\frac{1}{2}$ prob. on $|+\rangle$, $\frac{1}{2}$ prob. on $|-\rangle$ "

=

$$\begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

[[Maximally mixed state is the "quantum probability" analogue of the uniform prob distribution.]]

[Looking ahead:

There's a whole world of "quantum probability",
(aka noncommutative)

generalizing the usual world of probability you learn as a sophomore.

Besides the randomness in rolling dice & flipping coins, it also models the statistics of microscopic particles.

As you'll see, we get to develop it all again: quantum versions of events, random variables, statistics, information theory, communication complexity, learning....

Quantum computer science is more than just quantum algorithms!]