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# 125c, Lecture Three : 4/10/16

Last time: density operators.

- $\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

- Given a basis $\{|\phi_a\rangle\}$,

  $\rho_{ab} = \langle\phi_a|\hat{\rho}|\phi_b\rangle.$

- Hermitian: $\hat{\rho}^\dagger = \hat{\rho}$

- $\mathrm{Tr}\,\hat{\rho} = 1.$

Also:

- $\hat{\rho}$ is a <u>positive operator</u>:

  $\forall |\psi\rangle, \quad \langle\psi|\hat{\rho}|\psi\rangle \geq 0.$

Check: $\langle\psi|\hat{\rho}|\psi\rangle = \sum_i p_i \langle\psi|\psi_i\rangle\langle\psi_i|\psi\rangle$

$= \sum_i p_i |\langle\psi|\psi_i\rangle|^2$

$\geq 0.$ ✓

- Expectation values of operators in a mixed state:

(do last trick w/ complete set of states, but backwards.)

$$\langle \hat{O} \rangle_\rho = \sum_i p_i \langle \psi_i | \hat{O} | \psi_i \rangle$$

$$= \sum_{i,a} p_i \langle \psi_i | \hat{O} | \phi_a \rangle \langle \phi_a | \psi_i \rangle$$

$$= \sum_{i,a} p_i \langle \phi_a | \underline{\psi_i \rangle \langle \psi_i} | \hat{O} | \phi_a \rangle$$

$$= \sum_a \langle \phi_a | \hat{\rho} \hat{O} | \phi_a \rangle$$

$$= \mathrm{Tr}(\hat{\rho} \hat{O}) .$$

The expectation value of any operator $\hat{O}$ in the mixed state defined by $\hat{\rho}$ is just the trace of $\hat{\rho}\hat{O}$.

## Why do we describe mixed states using $\hat{\rho} = \sum_i |\psi_i\rangle\langle\psi_i|$?

Classically: $(\vec{p}, \vec{q}) \in \Gamma$, phase space.

Mixture = distribution function

$$f(\vec{p}, \vec{q}) : \Gamma \to \mathbb{R}^+,$$

$$\int f(\vec{p}, \vec{q})\, dp\, dq = 1.$$

We might conjecture a "quantum distribution function," $F(|\psi\rangle) : \mathcal{H} \to \mathbb{R}^+$.

(e.g. for a qubit, a function on the Bloch sphere.)

But we don't!

That would be much more data than $\hat{\rho}$. # of parameters $= \infty$.

whereas, for $\dim \mathcal{H} = d$, $\rho_{ij}$ has

$$\underbrace{2d^2}_{d\times d \text{ complex matrix}} - \underbrace{d^2}_{\text{Hermitian}} - \underbrace{1}_{\mathrm{Tr}=1} = \boxed{d^2 - 1} \text{ real parameters.}$$

Answer: we use $\hat{\rho}$, not $F(|\psi\rangle)$, because that's all we need to predict measurement outcomes.

E.g. what's the probability in $\hat{\rho}$ to measure $\hat{X}$ and obtain answer $|x_0\rangle$?

Pure state: $p_\psi(x_0) = \langle\psi|\hat{\Pi}_{x_0}|\psi\rangle$ $\quad (\hat{\Pi}_{x_0} = |x_0\rangle\langle x_0|)$

Mixed state: 
$$p_{\hat{\rho}}(x_0) = \sum_i p_i \, p_{\psi_i}(x_0)$$
$$= \sum_i p_i \langle\psi_i|\hat{\Pi}_{x_0}|\psi_i\rangle$$
$$= \langle\hat{\Pi}_{x_0}\rangle_{\hat{\rho}}$$
$$= \mathrm{Tr}(\hat{\rho}\,\hat{\Pi}_{x_0}).$$

The density matrix is all we need to calculate expectation values, and measurement probabilities are expectation values of projection operators.

$\therefore$ $\hat{\rho}$ is all we need to describe measurements.

But this hides some subtleties.

E.g. we can construct $\hat{\rho}$ from $\{p_i, |\psi_i\rangle\}$, but not vice-versa.

Consider $\hat{\rho} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$.

Use $|0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$,
$|1\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$.

Then
$$\hat{\rho} = \frac{1}{4}\left[|+\rangle\langle +| + |+\rangle\langle -| + |-\rangle\langle +| + |-\rangle\langle -|\right]$$
$$+ \frac{1}{4}\left[|+\rangle\langle +| - |+\rangle\langle -| - |-\rangle\langle +| + |-\rangle\langle -|\right]$$
$$= \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -|.$$

Same density operator, different "statistical mixture."

$\hat{\rho}$ tells us measurement outcomes, but not which particular states the mixture was originally made from.

# Reduced Density Matrices

$\boxed{A \,|\, B}$

Consider a composite system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$,
and a pure state $|\Psi\rangle = \sum_{ab} \psi_{ab} |\phi_a\rangle_A |\eta_b\rangle_B$.

Even though $|\Psi\rangle$ is pure, entanglement means there is no pure state for subsystem A (or B). Rather, it is described by a density operator.

First, note that any state $|\beta\rangle \in \mathcal{H}_B$ defines a map

$$ {}_B\langle\beta| : \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \longrightarrow \mathcal{H}_A . $$

E.g.

$$ \langle\beta|\Psi\rangle = \sum_a \Big( \sum_b \psi_{ab} \langle\beta|\eta_b\rangle \Big) |\phi_a\rangle \in \mathcal{H}_A . $$

(Keep wits about you to remember what Hilbert space each vector lives in.)

Then define partial trace of an operator:

$$ \mathrm{Tr}_B \, \hat{O} = \sum_b \langle\eta_b| \hat{O} |\eta_b\rangle \in L(\mathcal{H}_A). $$

Lots of notation, but everything basically means what it looks like.

Reduced density matrix for $A$ is the partial trace of $\hat{\rho}$ over B. ⑦

$$\hat{\rho}_A \equiv \mathrm{Tr}_B\, \hat{\rho}.$$

($\hat{\rho}$ itself might be pure, $\hat{\rho} = |\Psi\rangle\langle\Psi|$, or mixed, $\sum_i p_i |\psi_i\rangle\langle\psi_i|$.)

Examples.

① $$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A + |1\rangle_A\right)|0\rangle_B \equiv \frac{1}{\sqrt{2}}\left(|00\rangle + |10\rangle\right)$$

$$\hat{\rho} = |\Psi\rangle\langle\Psi| = \frac{1}{2}\left(|00\rangle + |10\rangle\right)\left(\langle 00| + \langle 10|\right)$$

$$= \frac{1}{2}\left(|00\rangle\langle 00| + |00\rangle\langle 10| + |10\rangle\langle 00| + |10\rangle\langle 10|\right).$$

$$\rightarrow \hat{\rho}_A = \mathrm{Tr}_B\, \hat{\rho} = \sum_b {}_B\langle \eta_b|\hat{\rho}|\eta_b\rangle_B \qquad |\eta_b\rangle \in \{|0\rangle_B, |1\rangle_B\}$$

$$= {}_B\langle 0|\hat{\rho}|0\rangle_B + {}_B\langle 1|\hat{\rho}|1\rangle_B$$

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

$$= \left[\frac{1}{\sqrt{2}}\left(|0\rangle_A + |1\rangle_A\right)\right]\left[\frac{1}{\sqrt{2}}\left({}_A\langle 0| + {}_A\langle 1|\right)\right]$$

$\rightarrow$ unmixed!

What we expect, because original state $|\Psi\rangle$ was unentangled.

Example 2: pure but entangled initial state.

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B\right)$$

$$\equiv \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right).$$

$$\hat{\rho} = |\Psi\rangle\langle\Psi| = \frac{1}{2}\left(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\right)$$

$$\hat{\rho}_A = \mathrm{Tr}_B\, \hat{\rho} = {}_B\langle 0|\hat{\rho}|0\rangle_B + {}_B\langle 1|\hat{\rho}|1\rangle_B$$

$$= \frac{1}{2}\left(|0\rangle_A\langle 0| + |1\rangle_A\langle 1|\right) \quad \checkmark$$

A mixed state! Can't be written as $\hat{\rho}_A = |\psi\rangle_A\langle\psi|$ for any $|\psi\rangle_A$. Unsurprising again, since original $|\Psi\rangle$ was entangled.

<u>Purification</u>: Given $\hat{\rho}_A \in L(\mathcal{H}_A)$, there exist an $\mathcal{H}_B$ and $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ s.t.

$$\hat{\rho}_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi|.$$

Proof: pretty obvious. Write $\hat{\rho}_A = \sum_i p_i |\psi_i\rangle_A\langle\psi_i|$. Then let $|\Psi\rangle = \sum_i \sqrt{p_i}\, |\psi_i\rangle_A |\eta_i\rangle_B$ for as many orthonormal states $\{|\eta_i\rangle_B\}$ as needed.

# Schmidt Decomposition

Consider a pure state

$$|\Psi\rangle = \sum_{ab} \psi_{ab} |\phi_a\rangle |\eta_b\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B .$$

Reduced density matrix for A: $\hat{\rho}_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi|$.

Can always diagonalize:

$$\exists \{|\sigma_a^{(A)}\rangle\} \in \mathcal{H}_A \text{ s.t. } \langle \sigma_a^{(A)} | \hat{\rho}_A | \sigma_b^{(A)} \rangle = p_a \delta_{ab} .$$

Let "Schmidt number" $k$ = # of nonzero eigenvalues $p_a$.

Then $\sum_{a'} |\sigma_{a'}^{(A)}\rangle\langle\sigma_{a'}^{(A)}| = \mathbb{1}_A$, so

$$|\phi_a\rangle = \sum_{a'} \langle \sigma_{a'}^{(A)} | \phi_a \rangle | \sigma_{a'}^{(A)} \rangle .$$

We can therefore expand $|\Psi\rangle$ in the new basis:

$$|\Psi\rangle = \sum_{aa'b} \psi_{ab} \langle \sigma_{a'}^{(A)} | \phi_a \rangle | \sigma_{a'}^{(A)} \rangle |\eta_b\rangle$$

Now define

$$|\sigma_{a'}^{(B)}\rangle = \frac{1}{\sqrt{p_{a'}}} \sum_{ab} \psi_{ab} \langle \sigma_{a'}^{(A)} | \phi_a \rangle |\eta_b\rangle$$

$$\Rightarrow |\Psi\rangle = \sum_{a'=1}^{k} \sqrt{p_{a'}}\, |\sigma_{a'}^{(A)}\rangle |\sigma_{a'}^{(B)}\rangle$$

Schmidt decomposition

Easy to check orthonormality: $\langle \sigma_{a'}^{(B)} | \sigma_{b'}^{(B)} \rangle = \delta_{a'b'}$,

Thus: we have orthonormal "Schmidt Bases"

$$\{ |\sigma_{a'}^{(A)}\rangle \} \in \mathcal{H}_A , \qquad \{ |\sigma_{b'}^{(B)}\rangle \} \in \mathcal{H}_B ,$$

such that our state $|\Psi\rangle = \sum_{ab} \psi_{ab} |\phi_a\rangle |\eta_b\rangle$

becomes "diagonal," $|\Psi\rangle = \sum_{a'=1}^{k} \sqrt{p_{a'}} \, |\sigma_{a'}^{(A)}\rangle |\sigma_{a'}^{(B)}\rangle$.

[strictly speaking, bases for <u>subspaces</u> of $\mathcal{H}_A$ & $\mathcal{H}_B$, since there may not be enough Schmidt vectors to span the spaces.]

Of course Schmidt basis is adapted to $|\Psi\rangle$, not universal.

In Schmidt basis, $\hat{\rho}_A = \sum_{a'=1}^{k} p_{a'} |\sigma_{a'}^{(A)}\rangle\langle \sigma_{a'}^{(A)}|$,

$$\hat{\rho}_B = \sum_{a'=1}^{k} p_{a'} |\sigma_{a'}^{(B)}\rangle\langle \sigma_{a'}^{(B)}| .$$

Note Schmidt number $k \leq \min(\dim \mathcal{H}_A, \dim \mathcal{H}_B)$.

you can't have more entanglement than the dimensionality of the smaller Hilbert space.