# Physics 492: Quantum Mechanics II
## Lecture 15: The Density Operator — Generalizing the Quantum State

Coherence: We have seen, numerous times now, that the essential feature of quantum mechanics is the interference between probability amplitudes associated with indistinguishable paths. These probability amplitudes have a definite phase relationship; they are said to be "coherent".

For example, consider, for spin $\frac{1}{2}$

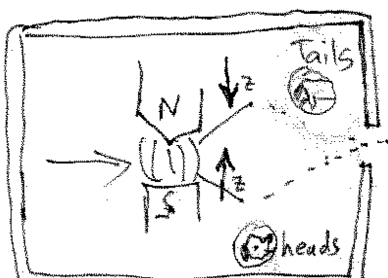
$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}|\uparrow_z\rangle + \frac{1}{\sqrt{2}}|\downarrow_z\rangle$$

$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}}|\uparrow_z\rangle + \frac{i}{\sqrt{2}}|\downarrow_z\rangle$$

In both these states, there is a 50% chance of $|\uparrow_z\rangle$ and 50% $|\downarrow_z\rangle$. However, the phase difference is ~~essential~~ crucial in defining the state. That is the "populations" $|\langle\uparrow_z|\psi\rangle|^2$ and $|\langle\downarrow_z|\psi\rangle|^2$ do not uniquely define the state. Both $|\uparrow_x\rangle$ and $|\uparrow_y\rangle$ are said to be coherent superpositions of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$.

# Statistical mixture vs. coherent superposition

Suppose we have a device rigged with a S-G ~~device~~ analyzer in the $\hat{v}_z$ direction, inside a black box. The box then spits out an atom randomly by flipping a weighted coin: if its heads it outputs a $|\uparrow_z\rangle$ atom, tails $|\downarrow_z\rangle$.




The output is a classical statistical mixture of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$

Although there is a some chance of $|\uparrow_z\rangle$ or $|\downarrow_z\rangle$ the state is not a coherent superposition of the two alternatives. Thus we must add probabilities rather than amplitudes. But how do we describe the quantum state of the atom that comes out of the box? How do we describe this "state of knowledge"?

Suppose we want to calculate the probability of measuring $|\uparrow_x\rangle$ for a spin that exits the box.

$$P_{\uparrow_x} = \underbrace{P_{\downarrow_z} \, |\langle \uparrow_x | \uparrow_z \rangle|^2 + P_{\downarrow_z} \, |\langle \uparrow_x | \downarrow_z \rangle|^2}_{\text{Adding the probabilities for the two alternatives}}$$

$$= P_{\uparrow_z} \langle \uparrow_x | \uparrow_z \rangle \langle \uparrow_z | \uparrow_x \rangle + P_{\downarrow_z} \langle \uparrow_x | \downarrow_z \rangle \langle \downarrow_z | \uparrow_x \rangle$$

$$= \langle \uparrow_x | \underbrace{\left( P_{\uparrow_z} |\uparrow_z\rangle\langle\uparrow_z| + P_{\downarrow_z} |\downarrow_z\rangle\langle\downarrow_z| \right)}_{\equiv \, \hat{\rho}} |\uparrow_x\rangle$$

$$\Rightarrow \boxed{P_{\uparrow_x} = \langle \uparrow_x | \hat{\rho} | \uparrow_x \rangle}$$

The operator $\hat{\rho} = P_{\uparrow_z} |\uparrow_z\rangle\langle\uparrow_z| + P_{\downarrow_z} |\downarrow_z\rangle\langle\downarrow_z|$

is known as the "density operator" (or density matrix when viewed in bases) It represents the most general state of a quantum system.

Generally, state which is a "statistical mixture" of different "pure" quantum states is written

$$\hat{\rho} = \sum_{\psi} P_{\psi} |\psi\rangle\langle\psi|$$

where $P_{\psi}$ is the probability of $|\psi\rangle$ in the mixture

Assuming each $|\psi\rangle$ is normalized $\hat{\rho}$ is normalized when $\sum_{\psi} P_{\psi} = 1$.

The probability of finding state $|\phi\rangle$ is

$$P_{\phi} = \langle\phi|\hat{\rho}|\phi\rangle = \sum_{\psi} P_{\psi} \underbrace{|\langle\phi|\psi\rangle|^2}_{P(\phi|\psi)}$$

A pure state has only one $|\psi\rangle$

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

A mixed state has more than one $|\psi\rangle$

A complete mixed state has equal probability of of $|\psi\rangle$.

Examples:

- Consider the pure state : spin-up along $x$

$$\hat{\rho} = |\uparrow_x\rangle\langle\uparrow_x|$$

Now $|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle + |\downarrow_z\rangle\right)$

$$\Rightarrow \hat{\rho} = \frac{1}{2}|\uparrow_z\rangle\langle\uparrow_z| + \frac{1}{2}|\downarrow_z\rangle\langle\downarrow_z|$$
$$+ \frac{1}{2}\left(|\uparrow_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\uparrow_z|\right)$$

Matrix representation in $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ basis

$$\hat{\rho} \doteq \begin{array}{cc} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} & \begin{array}{l} \langle\uparrow_z| \\ \langle\downarrow_z| \end{array} \end{array}$$

- Contrast this with a 50-50 statistical mixture of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$

$$\hat{\rho} = \frac{1}{2}|\uparrow_z\rangle\langle\uparrow_z| + \frac{1}{2}|\downarrow_z\rangle\langle\downarrow_z|$$

$$\doteq \begin{array}{cc} \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} & \begin{array}{l} \langle\uparrow_z| \\ \langle\downarrow_z| \end{array} \end{array}$$

(completely mixed)

For measurements of $\hat{\sigma}_z$ these two states look identical. However for spin along an arbitrary direction this is not the case.

Consider, for example, $|\uparrow_n\rangle = \cos\frac{\theta}{2}|\uparrow_z\rangle + e^{i\phi}\sin\frac{\theta}{2}|\downarrow_z\rangle$
(spin-up along $\vec{e}_n$ )

$$P_{\uparrow_n} = \langle\uparrow_n|\hat{\rho}|\uparrow_n\rangle$$

- For $\hat{\rho} = |\uparrow_x\rangle\langle\uparrow_x|$ $\quad P_{\uparrow_n} = |\langle\uparrow_n|\uparrow_x\rangle|^2$
$$= \frac{1}{2}\left|\cos\frac{\theta}{2} + e^{i\phi}\sin\frac{\theta}{2}\right|^2$$

- For $\hat{\rho} = \frac{1}{2}|\uparrow_z\rangle\langle\uparrow_z| + \frac{1}{2}|\downarrow_z\rangle\langle\downarrow_z|$

$$\Rightarrow P_{\uparrow_n} = \frac{1}{2}|\langle\uparrow_n|\uparrow_z\rangle|^2 + \frac{1}{2}|\langle\uparrow_n|\downarrow_z\rangle|^2$$
$$= \frac{1}{2}\cos^2\frac{\theta}{2} + \frac{1}{2}\sin^2\frac{\theta}{2} = \boxed{\frac{1}{2}}$$
independent of $\theta, \phi$

Thus, unless $\theta = 0$ or $\theta = \pi$ (ie $\vec{e}_n = \pm\vec{e}_z$)
or $\theta = \frac{\pi}{2}, \phi = \frac{\pi}{2}$ (i.e. $\vec{e}_n = \vec{e}_y$)

these two states <u>do not</u> give the same measurement results. In fact, the completely mixed state gives $\frac{1}{2}$ for prob of finding <u>any</u> spin.

In this basis the mixed state shows zero off-diagonal elements whereas the pure state has large off diagonal elements. These off-diagonal elements of $\hat{\rho}$ are called coherences — they represent the capacity for interference between the two states.

## Off-diagonal elements, coherence, and decoherence

Consider a general pure state for a $d$-dimensional Hilbert space with a basis $\{|e_n\rangle \mid n=1,2,\cdots,d\}$

$$\Rightarrow \quad |\psi\rangle = \sum_{n=1}^{d} c_n |e_n\rangle$$

$$\hat{\rho} = |\psi\rangle\langle\psi| = \sum_{n=1}^{d}\sum_{m=1}^{d} c_n c_m^* \, |e_n\rangle\langle e_m|$$

$$= \sum_{n=1}^{d} |c_n|^2 \, |e_n\rangle\langle e_n| + \sum_{n\neq m} c_n c_m^* \, |e_n\rangle\langle e_m|$$

$\Rightarrow \langle e_n|\hat{\rho}|e_n\rangle = |c_n|^2 =$ Probability of finding $|e_n\rangle$

$$\langle e_n|\hat{\rho}|e_m\rangle = c_n c_m^* = |c_n|\,|c_m| \, \underbrace{e^{i(\phi_n-\phi_m)}}_{\text{Coherence = phase difference}}$$

Now suppose we have a statistical mixture

$$\hat{\rho} = \sum_{\psi} P_{\psi} |\psi\rangle\langle\psi| = \sum_{n=1}^{d} \overline{|c_n|^2} \; |e_n\rangle\langle e_n|$$

$$+ \sum_{n\neq m}' \overline{c_n c_m^*} \; |e_n\rangle\langle e_m|$$

where $\overline{c_n c_m^*} = \sum_{\psi}' P_{\psi} \; \underset{\langle n|\psi\rangle}{\underset{\parallel}{c_n(\psi)}} \; \underset{\langle\psi|m\rangle}{\underset{\parallel}{c_m^*(\psi)}}$

The averaging can remove coherence (wash out the phase difference).

A dynamical process which washes out the phase coherence is known as decoherence.

Decoherence turns a coherent superposition into a statistical mixture $\Longrightarrow$ Measurement!

## Properties of the Density Operator

(1) Born Rule: Given a state $\hat{\rho}$, when we do a projective measurement of an "observable" $\hat{A}$, with eigenvectors $\{|a\rangle\}$, Then the probability of finding outcome a

$$P_a = \langle a|\hat{\rho}|a\rangle = \text{"Population"}$$

(2) The off-diagonal matrix elements of $\hat{\rho}$ w.r.t. some basis are the "coherences". They represent effect of interference on the probability of measurement outcome. For example, Let $|a\rangle = \sum c_i |e_i\rangle$ for some basis $\{|e_i\rangle\}$.

$$\Rightarrow P_a = \langle a|\hat{\rho}|a\rangle = \sum_{i,j} \langle a|e_i\rangle\langle e_i|\hat{\rho}|e_j\rangle\langle e_j|a\rangle = \sum_i \underbrace{|\langle a|e_i\rangle|^2}_{P_{a|i}} \underbrace{\rho_{ii}}_{P_i} + \underbrace{\sum_{i\neq j} \langle e_i|a\rangle\langle a|e_j\rangle \rho_{ij}}_{\text{interference}}$$

The first term is "classical logic" thinking of a statistical mixture of $\{|e_i\rangle\}$. The probability of finding "a" $= \sum$ Probability of finding "a" given "i" $\times$ Prob of finding "i". The second term is the quantum interference term that describes inference between the different possibities $\{|e_i\rangle\}$. these terms depend on $\rho_{ij}$

(3) $\hat{\rho} = \hat{\rho}^\dagger$ is Hermitian. To see this, note $\hat{\rho} = \sum P_i |\psi_i\rangle\langle\psi_i|$. $\{P_i \geq 0 \text{ real}\}$

$\Rightarrow$ Eigen equation: $\hat{\rho}|\lambda\rangle = P_\lambda|\lambda\rangle$ : $\hat{\rho} = \sum P_\lambda |\lambda\rangle\langle\lambda|$ $\Rightarrow$ Eigenvalues $\geq 0$

(4) Trace: $Tr(\hat{\rho}) = \sum_\lambda P_\lambda = 1$ (normalization condition).

## The Bloch Ball

Let us restrict our attention again to spin-½. We have seen that pure states $|\psi\rangle$ are in one-to-one correspondence with a direction on the unit sphere $\vec{e}_n$. The Bloch vector $\vec{e}_n = \langle\psi|\hat{\vec{\sigma}}|\psi\rangle$. We generalize this for mixed states. Consider the decomposition of $\hat{\rho}$ into its eigenvectors. The eigenvectors form a basis for spin-½, thus we can always write this as $\{|\uparrow_n\rangle, |\downarrow_n\rangle\}$ for some $\vec{e}_n$.

$$\hat{\rho} = P_+ |\uparrow_n\rangle\langle\uparrow_n| + P_- |\downarrow_n\rangle\langle\downarrow_n|$$

We thus define the general Bloch vector for an arbitrary spin-½ mixed state as the <u>statistical average</u>:

$$\vec{Q} = P_+ \langle \uparrow_n | \hat{\vec{\sigma}} | \uparrow_n \rangle + P_- \langle \downarrow_n | \hat{\vec{\sigma}} | \downarrow_n \rangle$$
$$= P_+ \vec{e}_n + P_- (-\vec{e}_n) = (P_+ - P_-)\, \vec{e}_n$$

For a pure state $\hat{\rho} = |\uparrow_n\rangle\langle\uparrow_n|$ for some $\vec{e}_n$ $\Rightarrow$ $\vec{Q} = \vec{e}_n$

For a mixed state $P_+ < 1$, $P_- < 1$, $P_+ + P_- = 1$ $\Rightarrow$ $0 \leq |P_+ - P_-| < 1$

where $P_+ = P_- = \frac{1}{2}$ $\Rightarrow$ maximally mixed $\Rightarrow$ $\vec{Q} = 0$ (origin)

$$\Rightarrow \underbrace{0}_{\text{maximally mixed state}} \leq |\vec{Q}| \leq \underbrace{1}_{\text{pure state}}$$

<u>The surface of the Bloch sphere are the pure states</u>

<u>The interior of the Bloch are the mixed states.</u>

The set of all states $\hat{\rho}$ of spin-½ constitute the <u>Bloch Ball</u>