Lecture 13: The Density Matrix

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

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

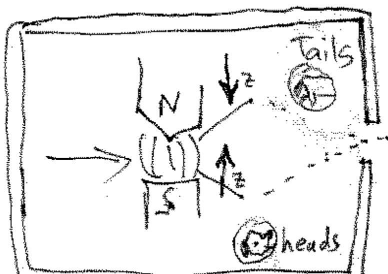
$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}|\uparrow_z\rangle + \frac{1}{\sqrt{2}}|\downarrow_z\rangle$$

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

In both these states, there is a 50% chance of $|\uparrow_z\rangle$ and 50% $|\downarrow_z\rangle$. However, the phase difference is ~~critical~~ <u>crucial</u> 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 <u>coherent superpositions</u> of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$.

Statistical mixture vs. coherent superposition

Suppose we have a device rigged with a S-G 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.

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

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

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

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

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_{ψ} 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 <u>pure state</u> has only one $|\psi\rangle$

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

A <u>mixed state</u> has more than one $|\psi\rangle$

A <u>complete mixed state</u> 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

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

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

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

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

(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 θ, ϕ

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

In this basis the mixed state shows <u>zero</u> <u>off-diagonal</u> elements whereas the pure state has large off diagonal elements.

These off-diagonal elements of $\hat{\rho}$ are <u>called</u> <u>coherences</u> – they represent ~~the~~ capacity for interference between the two states.

<u>Off-diagonal elements, coherence, and decoherence</u>

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

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

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

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

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

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

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

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 $\Rightarrow$ Measurement!