

Physics 566 - Lecture 6

Quantum Coherence and the Density Matrix

A two-level system in a state $|\psi\rangle = c_{\uparrow_z} |\uparrow_z\rangle + c_{\downarrow_z} |\downarrow_z\rangle$ is in one-to-one correspondence with the Bloch vector $\vec{Q} = \langle \psi | \hat{\sigma} | \psi \rangle = (u, v, w)$

$$u = \langle \psi | \hat{\sigma}_x | \psi \rangle = \text{Re}(c_{\uparrow_z} c_{\downarrow_z}^*) = \text{Re}(|c_{\uparrow_z}| |c_{\downarrow_z}| e^{i(\phi_{\uparrow} - \phi_{\downarrow})})$$

$$v = \langle \psi | \hat{\sigma}_y | \psi \rangle = \text{Im}(c_{\uparrow_z} c_{\downarrow_z}^*) = \text{Im}(|c_{\uparrow_z}| |c_{\downarrow_z}| e^{i(\phi_{\uparrow} - \phi_{\downarrow})})$$

$$w = \langle \psi | \hat{\sigma}_z | \psi \rangle = |c_{\uparrow_z}|^2 - |c_{\downarrow_z}|^2$$

The $u+v$ components tell us something about *coherences* between $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$, since they involve the relative phase between the probability amplitudes c_{\uparrow_z} and c_{\downarrow_z} .

The w component tells us about the *"population"*, i.e., the relative probability of \uparrow_z vs. \downarrow_z .

The Bloch vector representation motivates us to characterize the state by a matrix *bilinear* in the probability amplitudes, with matrix elements

$$\rho_{\alpha\beta} = c_{\alpha} c_{\beta}^* : \text{Elements of the "density matrix"}$$

Diagonal matrix element $\rho_{\alpha\alpha} = |c_{\alpha}|^2 = \text{Probability to be in state } |\alpha\rangle$

$$\text{Normalization } \sum_{\alpha} \rho_{\alpha\alpha} = 1$$

Off-diagonal matrix element $\rho_{\alpha\beta} = |c_{\alpha}| |c_{\beta}| e^{i(\phi_{\alpha} - \phi_{\beta})} = \text{Coherence between } |\alpha\rangle \text{ and } |\beta\rangle$

$$\rho = \begin{bmatrix} |c_{\uparrow}|^2 & c_{\uparrow} c_{\downarrow}^* \\ c_{\downarrow} c_{\uparrow}^* & |c_{\downarrow}|^2 \end{bmatrix} = \begin{bmatrix} c_{\uparrow} \\ c_{\downarrow} \end{bmatrix} \otimes \begin{bmatrix} c_{\uparrow}^* & c_{\downarrow}^* \end{bmatrix}$$

$$|c_{\uparrow}|^2 + |c_{\downarrow}|^2 = \text{Tr}(\rho) = 1$$

The density matrix is basis-dependent, here written in the $|\uparrow_z\rangle, |\downarrow_z\rangle$ basis.

We can see this as the matrix representation of the density operator:

$$\rho_{\alpha\beta} = c_\alpha c_\beta^* = (\langle\alpha|\psi\rangle) (\langle\beta|\psi\rangle)^* = \langle\alpha|\psi\rangle \langle\psi|\beta\rangle = \langle\alpha|\hat{\rho}|\beta\rangle$$

$$\Rightarrow \text{Density operator for state } |\psi\rangle: \quad \hat{\rho} = |\psi\rangle\langle\psi|$$

The off-diagonal elements of $\hat{\rho}$ are the coherences in a given basis. They determine the possibility of quantum interference with respect to the distinguishable alternatives of the basis.

$$\text{Consider } \hat{\rho} = |\uparrow_x\rangle\langle\uparrow_x| = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}}_{\text{In the basis } \{|\uparrow_x\rangle, |\downarrow_x\rangle\}}$$

In the basis $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$

The state has coherence between $|\uparrow_z\rangle, |\downarrow_z\rangle$. This implies that there can be quantum interference between these alternatives.

Consider the probability of finding $|\downarrow_x\rangle$ given the state was prepared $|\uparrow_x\rangle$

$$P(\downarrow_x|\uparrow_x) = \langle\downarrow_x|\hat{\rho}|\downarrow_x\rangle$$

$$= \langle\downarrow_x|(|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\downarrow_z|) \hat{\rho} (|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\downarrow_z|)|\downarrow_x\rangle$$

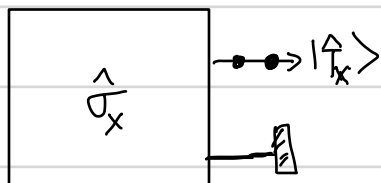
$$= \underbrace{|\langle\downarrow_x|\uparrow_z\rangle|^2}_{P(\downarrow_x|\uparrow_z)} \rho_{\uparrow_z\uparrow_z} + \underbrace{|\langle\downarrow_x|\downarrow_z\rangle|^2}_{P(\downarrow_x|\downarrow_z)} \rho_{\downarrow_z\downarrow_z} + \underbrace{\langle\downarrow_x|\uparrow_z\rangle\langle\downarrow_z|\downarrow_x\rangle \rho_{\uparrow_z\downarrow_z} + \langle\downarrow_x|\downarrow_z\rangle\langle\uparrow_z|\downarrow_x\rangle \rho_{\downarrow_z\uparrow_z}}_{\text{Quantum Interference?}}$$

$$= \left(\frac{1}{2}\right)\left(\frac{1}{2}\right) + \left(\frac{1}{2}\right)\left(\frac{1}{2}\right) + \left(+\frac{1}{\sqrt{2}}\right)\left(-\frac{1}{\sqrt{2}}\right)\left(\frac{1}{2}\right) + \left(-\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{2}\right)$$

$$= \frac{1}{4} + \frac{1}{4} - \frac{1}{4} - \frac{1}{4} = 0 \quad \text{Destructive interference between } |\uparrow_z\rangle \text{ and } |\downarrow_z\rangle$$

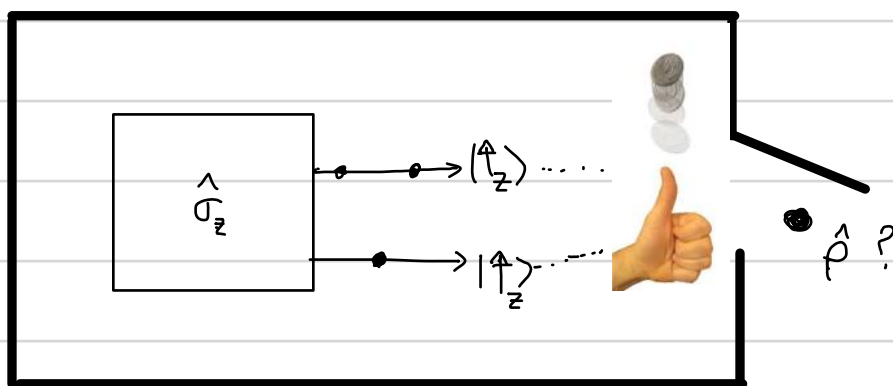
Pure States vs. Mixed States

So far, all the states of a quantum mechanical system that we have discussed have been pure states, $|\psi\rangle \Rightarrow \hat{\rho} = |\psi\rangle\langle\psi|$. A pure state implies we have maximum possible knowledge of the system, e.g., we prepared the system $|\uparrow_x\rangle$ as the output of a Stern-Gerlach apparatus



The bizarre thing about quantum mechanics is that even with maximal possible knowledge of the system, we have imperfect ability to predict future outcomes, e.g. when we measure $\hat{\sigma}_z$, we have 50-50 to see $|\uparrow_z\rangle$ vs. $|\downarrow_z\rangle$.

Consider another preparation scheme. Suppose the preparer has a Stern-Gerlach device inside a black box that she selects either $|\uparrow_z\rangle$ or $|\downarrow_z\rangle$ spins. She then flips a coin and decides which spin to set to measure.



The preparer tells us the weighting of the coin: with probability p_{\uparrow_z} she sends $|\uparrow_z\rangle$, with probability p_{\downarrow_z} she sends $|\downarrow_z\rangle$. The state $\hat{\rho}$ is not a pure state. It is a statistical mixture of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$. We say $\hat{\rho}$ is a mixed state.

If we measure $\hat{\sigma}_z$, then we know that we will find $|\uparrow_z\rangle$ or $|\downarrow_z\rangle$ with probabilities p_{\uparrow_z} and p_{\downarrow_z} respectively. If this were a fair coin $p_{\uparrow_z} = p_{\downarrow_z} = \frac{1}{2}$, then these are the same outcomes we would see for the pure state $|\uparrow_x\rangle = \frac{1}{\sqrt{2}}|\uparrow_z\rangle + \frac{1}{\sqrt{2}}|\downarrow_z\rangle$. But

$|\uparrow_x\rangle$ is a coherent superposition of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$, whereas the state $\hat{\rho}$ out of the black box is a statistical mixture with no quantum coherence between $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$. To calculate the probability of say $|\downarrow_x\rangle$ given the state out of the black box:

$$P(\downarrow_x) = p_{\uparrow_z} P(\downarrow_x | \uparrow_z) + p_{\downarrow_z} P(\downarrow_x | \downarrow_z) = p_{\uparrow_z} |\langle \downarrow_x | \uparrow_z \rangle|^2 + p_{\downarrow_z} |\langle \downarrow_x | \downarrow_z \rangle|^2$$

$$= \frac{1}{2}(p_{\uparrow_z} + p_{\downarrow_z}) = \frac{1}{2} \quad \text{No interference between } |\uparrow_z\rangle \text{ and } |\downarrow_z\rangle$$

We can assign a density operator to this statistical mixture that represents the state

$$\text{Note: } P(\downarrow_x) = p_{\uparrow_z} \langle \downarrow_x | \uparrow_z \rangle \langle \uparrow_z | \downarrow_x \rangle + p_{\downarrow_z} \langle \downarrow_x | \downarrow_z \rangle \langle \downarrow_z | \downarrow_x \rangle$$

$$= \langle \downarrow_x | (p_{\uparrow_z} |\uparrow_z\rangle \langle \uparrow_z| + p_{\downarrow_z} |\downarrow_z\rangle \langle \downarrow_z|) | \downarrow_x \rangle$$

$$\Rightarrow P(\downarrow_x) = \langle \downarrow_x | \hat{\rho} | \downarrow_x \rangle \quad \hat{\rho} = p_{\uparrow_z} |\uparrow_z\rangle \langle \uparrow_z| + p_{\downarrow_z} |\downarrow_z\rangle \langle \downarrow_z|$$

Statistical mixture of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$

Consider $\langle \uparrow_x | \hat{\rho} | \downarrow_x \rangle = \text{coherence between } |\uparrow_x\rangle \text{ and } |\downarrow_x\rangle$

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

$$= p_{\uparrow_z} \left(\frac{1}{\sqrt{2}}\right) \left(\frac{1}{\sqrt{2}}\right) + p_{\downarrow_z} \left(\frac{1}{\sqrt{2}}\right) \left(-\frac{1}{\sqrt{2}}\right) = \frac{1}{2} (p_{\uparrow_z} - p_{\downarrow_z})$$

\Rightarrow for a 50-50 statistical mixture of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$ there is no coherence between $|\uparrow_x\rangle$ and $|\downarrow_x\rangle$. In fact there is no coherence between any two orthogonal states since

$$\hat{\rho} = \frac{1}{2} (|\uparrow_z\rangle \langle \uparrow_z| + |\downarrow_z\rangle \langle \downarrow_z|) = \frac{1}{2} \hat{1} = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ in any basis}$$

Since the off-diagonal elements of $\hat{\rho}$ are 0 in all bases, this state has no coherence. It is said to be the maximally mixed state.

A state is mixed when we don't have complete information about the state. The example we gave is somewhat contrived, involving preparers flipping coins. Mixed states occur naturally when we have an open quantum system, i.e. a quantum system is interacting with another system (e.g. the environment), whose degrees of freedom we do not or cannot keep track of. For example, let us consider collisions between our two level atoms. A elastic collision will induce a phase shift on one state

$$|\psi\rangle = c_g |g\rangle + c_e |e\rangle \Rightarrow c_g e^{i\phi} |g\rangle + c_e |e\rangle.$$

But if we don't know the phase shift we must take the statistical average of the possible phases

$$\begin{aligned} \Rightarrow \hat{\rho} &= \int d\phi P(\phi) (c_g e^{i\phi} |g\rangle + c_e |e\rangle) (c_g^* e^{-i\phi} \langle g| + c_e^* \langle e|) \\ &= \int d\phi P(\phi) (|c_g|^2 |g\rangle\langle g| + |c_e|^2 |e\rangle\langle e| + c_g c_e^* e^{i\phi} |g\rangle\langle e| + c_e c_g^* e^{-i\phi} |e\rangle\langle g|) \\ &= |c_g|^2 |g\rangle\langle g| + |c_e|^2 |e\rangle\langle e| + \overline{c_g c_e^* e^{i\phi}} |g\rangle\langle e| + \overline{c_e c_g^* e^{-i\phi}} |e\rangle\langle g| \end{aligned}$$

The statistical mixture of random phases \Rightarrow loss of coherence between $|g\rangle$ & $|e\rangle$. This dephasing process is the quantum analogy of collision dephasing of the Lorentz oscillator that we studied classically.

Generally, if we expect the state is one of an ensemble of possible states $|\psi_i\rangle$ with probability p_i we assign the mixed state

$$\hat{\rho} \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i| \quad \text{Statistical mixture of } \{|\psi_i\rangle\}$$

$$\rho_{\alpha\beta} = \sum_i p_i c_{\alpha}^{(i)} c_{\beta}^{(i)*} = \overline{c_{\alpha} c_{\beta}^*} \quad \leftarrow \text{Ensemble average}$$

- A statistical mixture should be distinguished from a coherent superposition
- The states in the ensemble need not be orthogonal, e.g. statistical mixture of $|F_x\rangle$ and $|F_z\rangle$.
- The ensemble decomposition is not unique; different mixtures lead to the same $\hat{\rho}$.

More generally, for an "open quantum system," information about one quantum subsystem that is part of the whole system is not generally a pure state. This can be true even if the state of the whole is pure. E.g. bipartite $A+B$: $|\Psi\rangle_{AB}$ pure, but $\hat{\rho}_A, \hat{\rho}_B$ mixed. This is a uniquely quantum phenomenon: entanglement. We can have maximum possible information about the whole but an incomplete description of the parts. We will revisit this in much greater detail in the next semester.

Formal Properties of the Density Operator

- Hermitian $\hat{\rho}^\dagger = \hat{\rho}$
- Positive: $\hat{\rho} \geq 0 \Rightarrow \langle \phi | \hat{\rho} | \phi \rangle \geq 0 \Rightarrow$ The eigenvalues of $\hat{\rho}$
- Normalization: $\text{Tr}(\hat{\rho}) = 1$
- Diagonalization: $\hat{\rho} = \sum_{i=1}^d \lambda_i |e_i\rangle \langle e_i| =$ Unique ensemble decomposition into orthogonal vectors $\{|e_i\rangle\}$ with probabilities $\{\lambda_i\}$, $\sum \lambda_i = 1$

Pure vs. mixed state:

A pure state $\Rightarrow \exists |\psi\rangle$ s.t. $\hat{\rho} = |\psi\rangle \langle \psi| \Rightarrow$ One eigenvector $|e_1\rangle = |\psi\rangle$, eigenvalue 1
All other eigenvalues are 0

$$\hat{\rho}_{\text{pure}} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix}$$

For a mixed states $\hat{\rho} = \sum \lambda_i |e_i\rangle \langle e_i|$, where $\lambda_i < 1 \forall i$ "purity"

$$\Rightarrow \hat{\rho}^2 = \sum \lambda_i^2 |e_i\rangle \langle e_i| \Rightarrow \text{Tr}(\hat{\rho}^2) = \sum \lambda_i^2 < 1 \text{ for mixed states}$$

Maximally mixed \Rightarrow Equal mixture of all basis states, $\lambda_i = \frac{1}{d} \forall i \Rightarrow \text{Tr}(\hat{\rho}^2)_{\text{min}} = \frac{1}{d}$

Using $\hat{\rho}$ to make predictions

Aside: The trace operation: $\text{Tr}(\hat{A}) = \sum_i \langle e_i | \hat{A} | e_i \rangle$ (independent of basis $\{|e_i\rangle\}$)

$$\text{Tr}(|\psi\rangle\langle\phi| \hat{A}) = \langle\phi| \hat{A} |\psi\rangle$$

$$\text{Tr}(\hat{A}\hat{B}\hat{C}) = \text{Tr}(\hat{C}\hat{A}\hat{B}) = \text{Tr}(\hat{B}\hat{C}\hat{A})$$

} See homework

From these properties it follows

• Probability to find outcome $|a\rangle$: $P_a = \langle a | \hat{\rho} | a \rangle = \text{Tr}(\hat{\rho} |a\rangle\langle a|)$

• Expectation value of an observable:

$$\langle \hat{A} \rangle = \sum_a a P_a = \sum_a a \text{Tr}(|a\rangle\langle a| \hat{\rho}) = \text{Tr}(\sum_a a |a\rangle\langle a| \hat{\rho}) \Rightarrow \langle \hat{A} \rangle = \text{Tr}(\hat{\rho} \hat{A})$$

Schrödinger Eqn for $\hat{\rho}$

The Heisenberg equation of motion for an operator (Heisenberg picture)

$$\frac{\partial}{\partial t} \hat{A} = -\frac{i}{\hbar} [\hat{A}, \hat{H}] \Rightarrow \frac{\partial}{\partial t} \langle \hat{A} \rangle = -\frac{i}{\hbar} (\langle \hat{A} \hat{H} \rangle - \langle \hat{H} \hat{A} \rangle)$$

$$\Rightarrow \frac{\partial}{\partial t} \text{Tr}(\hat{\rho} \hat{A}) = -\frac{i}{\hbar} [\text{Tr}(\hat{A} \hat{H} \hat{\rho}) - \text{Tr}(\hat{H} \hat{A} \hat{\rho})] = -\frac{i}{\hbar} [\text{Tr}(\hat{A} \hat{\rho} \hat{A}) - \text{Tr}(\hat{\rho} \hat{H} \hat{A})] = -\frac{i}{\hbar} \text{Tr}([\hat{\rho}, \hat{H}] \hat{A})$$

\Rightarrow In the Schrödinger picture \hat{A} is constant and

$$\frac{\partial}{\partial t} \hat{\rho} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}]$$

$$\hat{\rho}(t) = \hat{U}(t) \hat{\rho}(0) \hat{U}^\dagger(t)$$

Why is $\hat{\rho}$ called the density operator?

Classical Mechanics: State of the system: $P(\vec{q}, \vec{p}, t)$: Probability density on phase space.

Liouville Eqn of motion: $\frac{\partial}{\partial t} P(\vec{q}, \vec{p}, t) = \{H(\vec{q}, \vec{p}), P(\vec{q}, \vec{p}, t)\} \leftarrow$ Poisson Bracket

$\hat{\rho}$ is the quantum mechanical analog of $P(\vec{q}, \vec{p})$. $\frac{\partial \hat{\rho}}{\partial t} = -i[\hat{H}, \hat{\rho}]$ is sometimes called the Liouville eqn. We will study representations of $\hat{\rho}$ in phase space in great detail when we study the contrasts of classical vs. nonclassical light.

Density Matrix for a Qubit

Consider a two-level system (a qubit) in an arbitrary state $\hat{\rho}$. Like any operator acting on \mathbb{C}^2 :

$$\hat{\rho} = \frac{1}{2} [\text{Tr}(\hat{\rho}) \hat{1} + \text{Tr}(\hat{\sigma} \hat{\rho}) \cdot \hat{\sigma}]$$

$$\hat{\rho} = \frac{1}{2} [\hat{1} + \vec{Q} \cdot \hat{\sigma}], \quad \vec{Q} = \langle \hat{\sigma} \rangle = \text{Tr}(\hat{\rho} \hat{\sigma}) = \text{Bloch vector}$$

For a pure state, $\vec{Q} = \vec{e}_n$: unit vector on the sphere $\Rightarrow \hat{\rho} = \frac{1}{2} (\hat{1} + \hat{\sigma}_n) = |\uparrow_n\rangle\langle\uparrow_n|$ as expected

Generally, $\vec{Q} = (u, v, w)$

$$u = \text{Tr}(\hat{\rho} \hat{\sigma}_x) = \text{Tr}(\hat{\rho} (|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)) = \rho_{\downarrow\uparrow} + \rho_{\uparrow\downarrow} = 2 \text{Re}(\rho_{\downarrow\uparrow})$$

$$v = \text{Tr}(\hat{\rho} \hat{\sigma}_y) = \text{Tr}(\hat{\rho} (-i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow|)) = -i(\rho_{\downarrow\uparrow} - \rho_{\uparrow\downarrow}) = 2 \text{Im}(\rho_{\downarrow\uparrow})$$

$$w = \text{Tr}(\hat{\rho} \hat{\sigma}_z) = \text{Tr}(\hat{\rho} (|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)) = \rho_{\uparrow\uparrow} - \rho_{\downarrow\downarrow} \quad (\text{Normalization: } \rho_{\uparrow\uparrow} + \rho_{\downarrow\downarrow} = 1)$$

The (u, v) components determine the off-diagonal matrix elements (coherences) between \uparrow & \downarrow .
The w components determine the relative size of diagonal matrix elements (populations).

Pure vs. Mixed State

$$\text{Tr}(\hat{\rho}^2) = \frac{1}{2} (1 + |\vec{Q}|^2) \quad (\text{see homework})$$

$$\frac{1}{4} \leq \text{Tr}(\hat{\rho}^2) \leq \frac{1}{2}$$

maximally mixed pure state

$$\Rightarrow 0 \leq |\vec{Q}| < 1, \quad |\vec{Q}| = 1 \text{ (pure)} \quad |\vec{Q}| < 1 \text{ (mixed)}, \quad |\vec{Q}| = 0 \quad \hat{\rho} = \frac{1}{2} \hat{1} \text{ (maximally mixed)}$$

The set of Bloch vectors $\{\vec{Q} \mid |\vec{Q}| \leq 1\} \equiv \text{Unit Ball} : \text{"Bloch Ball"}$

