Lecture 34: The `Density Operator'

Phy851 Fall 2009



The QM `density operator'

- HAS NOTHING TO DO WITH MASS PER UNIT VOLUME
- The density operator formalism is a generalization of the **Pure State** QM we have used so far.
- New concept: Mixed state
- Used for:
 - Describing open quantum systems
 - Incorporating our ignorance into our quantum theory
- Main idea:
 - We need to distinguish between a `statistical mixture' and a `coherent superposition'
 - Statistical mixture: it is either a or b, but we don't know which one
 - No interference effects
 - Coherent superposition: it is both a and b at the same time
 - Quantum interference effects appear

Pure State quantum Mechanics

- The goal of quantum mechanics is to make predictions regarding the outcomes of measurements
- Using the formalism we have developed so far, the procedure is as follows:
 - Take an initial state vector
 - Evolve it according to Schrödinger's equation until the time the measurement takes place
 - Use the projector onto eigenstates of the observable to predict the probabilities for different results
 - To confirm the prediction, one would prepare a system in a known initial state, make the measurement, then re-prepare the same initial state and make the same measurement after the same evolution time. With enough repetitions, the results should show statistical agreement with the results of quantum theory



Expectation Value

• The expectation value of an operator is defined (with respect to state $|\psi\rangle$) as:

$$\langle A \rangle \equiv \langle \psi | A | \psi \rangle$$

The interpretation is the average of the results of many measurements of the observable *A* on a system prepared in state |ψ⟩.

- Proof:
$$\langle A \rangle \equiv \langle \psi | A | \psi \rangle$$

$$= \sum_{n} \langle \psi | a_{n} \rangle \langle a_{n} | A | \psi \rangle$$

$$= \sum_{n} \langle \psi | a_{n} \rangle a_{n} \langle a_{n} | \psi \rangle$$

$$= \sum_{n} \langle a_{n} | \psi \rangle \langle \psi | a_{n} \rangle a_{n}$$

$$= \sum_{n} |\langle \psi | a_{n} \rangle|^{2} a_{n}$$

$$= \sum_{n} p(a_{n}) a_{n}$$

This is clearly the weighted average of all possible outcomes

Statistical mixture of states

- What if we cannot know the exact initial quantum state of our system?
 - For example, suppose we only know the temperature, T, of our system?
- Suppose I know that with probability P_1 , the system is in state $|\psi_1\rangle$, while with probability P_2 , the system is in state $|\psi_2\rangle$.
 - This is called a statistical mixture of the states $|\psi_1\rangle$ and $|\psi_2\rangle$.
- In this case, what would be the probability of obtaining result a_n of a measurement of observable A?
 - Clearly, the probability would be $\langle \psi_I | a_n \rangle \langle a_n | \psi_I \rangle$ with probability p_1 , and $\langle \psi_2 | a_n \rangle \langle a_n | \psi_2 \rangle$ with probability p_2 .

 $P(a_n) = P(a_n | \psi_1) P(\psi_1) + P(a_n | \psi_2) P(\psi_2)$

 Thus the frequency with which a_n would be obtained over many repetitions would be

$$p(a_n) = \left| \left\langle a_n \left| \psi_1 \right\rangle \right|^2 P_1 + \left| \left\langle a_n \left| \psi_2 \right\rangle \right|^2 P_1 \right|^2$$



The Density `Operator'

 For the previous example, Let us define a `density operator' for the system as:

$$\rho = |\psi_1\rangle \langle \psi_1|P_1 + |\psi_2\rangle \langle \psi_2|P_2$$

This will describe the state of the system, in place of a wavefunction

• The probability to obtain result *a_n* could then obtained in the following manner:

$$P(a_n) = Tr\{\rho I(a_n)\} \qquad I(a_n) = |a_n\rangle\langle a_n|$$

Proof: $P(a_{n}) = Tr \{ \rho I(a_{n}) \} \qquad \{|m\rangle\} \text{ is a complete basis}$ $= \sum_{m} \langle m | \rho | a_{n} \rangle \langle a_{n} | m \rangle$ $= \sum_{m} \langle m | (P_{1} | \psi_{1} \rangle \langle \psi_{1} | + P_{2} | \psi_{2} \rangle \langle \psi_{2} |) a_{n} \rangle \langle a_{n} | m \rangle$ $= \sum_{m} \langle a_{n} | m \rangle \langle m | (P_{1} | \psi_{1} \rangle \langle \psi_{1} | + P_{2} | \psi_{2} \rangle \langle \psi_{2} |) a_{n} \rangle$ $= \langle a_{n} | (P_{1} | \psi_{1} \rangle \langle \psi_{1} | + P_{2} | \psi_{2} \rangle \langle \psi_{2} |) a_{n} \rangle$ $= \langle a_{n} | (P_{1} | \psi_{1} \rangle \langle \psi_{1} | + P_{2} | \psi_{2} \rangle \langle \psi_{2} |) a_{n} \rangle$ $= P_{1} \langle a_{n} | \psi_{1} \rangle \langle \psi_{1} | a_{n} \rangle + P_{2} \langle a_{n} | \psi_{2} \rangle \langle \psi_{2} | a_{n} \rangle$ $= | \langle a_{n} | \psi_{1} \rangle |^{2} P_{1} + | \langle a_{n} | \psi_{2} \rangle |^{2} P_{2}$

Generic Density Operator

 For a 'statistical mixture' of the states $\{|\psi_i\rangle\}$ with respective probabilities $\{P_i\}$, the density operator is thus:

$$\rho = \sum_{j} P_{j} |\psi_{j}\rangle \langle \psi_{j} |$$

- The sum of the P_j 's is Unity: $\sum_i P_j = 1$
- The $|\psi_i\rangle$'s are required to be normalized to one, but are not necessarily orthogonal
 - For example, we could say that with 50% probability, an electron is in state $|\uparrow\rangle$, and the other 50% of the time it is in state $(|\uparrow\rangle+|\downarrow\rangle)/\sqrt{2}$

$$\begin{split} \rho &= \frac{1}{2} |\uparrow\rangle \langle\uparrow| + \frac{1}{2} \frac{\left(|\uparrow\rangle + |\downarrow\rangle\right)}{\sqrt{2}} \frac{\left(\langle\uparrow| + \langle\downarrow|\right)}{\sqrt{2}} \\ &= \frac{3}{4} |\uparrow\rangle \langle\uparrow| + \frac{1}{4} |\uparrow\rangle \langle\downarrow| + \frac{1}{4} |\downarrow\rangle \langle\uparrow| + \frac{1}{4} |\downarrow\rangle \langle\downarrow| \end{split}$$

This state is only `partially mixed', meaning interference effects are reduced, but not eliminated



Density matrix of a pure state

• Every pure state has a density matrix description:

$$\rho = |\psi\rangle \langle \psi|$$

- Every density matrix does not have a pure state description
 - Any density matrix can be tested to see if it corresponds to a pure state or not:
- Test #1:
 - If it is a pure state, it will have exactly one non-zero eigenvalue equal to unity
 - Proof:

• Start from:
$$\rho = |\psi\rangle\langle\psi|$$

- Pick any orthonormal basis that spans the Hilbert space, for which $|\psi\rangle$ is the first basis vector
- In any such basis, we will have the matrix elements
 (1 0 0 ····)

Testing for purity cont.

- Test #2:
 - In any basis, the pure state will satisfy for every *m*,*n*:

$$\rho_{mn}\rho_{nm} = \rho_{mm}\rho_{nn}$$

 A partially mixed state will satisfy for at least one pair of *m*,*n* values:

$$0 < \rho_{mn} \rho_{nm} < \rho_{mm} \rho_{nn}$$

 And a totally mixed state will satisfy for at least one pair of *m*, *n* values:

$$\rho_{mn} = \rho_{nm} = 0 \quad and \quad \rho_{mm} \rho_{nm} \neq 0$$

Probabilities and `Coherence'

- In a given basis, the diagonal elements are always the probabilities to be in the corresponding states:
- The off diagonals are a measure of the 'coherence' between any two of the basis states.

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix} \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}$$

$$pord pord pord pord rotally mixed$$

– Coherence is maximized when:

$$\rho_{mn}\rho_{nm} = \rho_{mm}\rho_{nn}$$



Rule 1: Normalization

• Consider the trace of the density operator $\rho = \sum P_j |\psi_j\rangle \langle \psi_j|$

$$Tr\{\rho\} = \sum_{j} P_{j} \langle \psi_{j} | \psi_{j} \rangle$$
$$= \sum_{j} P_{j}$$

 $Tr\{\rho\} = 1$

Since the *P*_j's are probabilities, they must sum to unity



Rule 2: Expectation Values

• The expectation value of any operator *A* is defined as:

 $\langle A \rangle = Tr\{\rho A\}$

• For a pure state this gives the usual result:

$$\langle A \rangle = Tr\{|\psi\rangle\langle\psi|A\}$$

= $\langle\psi|A|\psi\rangle$

• For a mixed state, it gives:

$$\langle A \rangle = Tr \left\{ \sum_{j} p_{j} | \psi_{j} \rangle \langle \psi_{j} | A \right\}$$
$$= \sum_{j} p_{j} \langle \psi_{j} | A | \psi_{j} \rangle$$



Rule 3: Equation of motion

• For a closed system:

$$\rho = |\psi\rangle \langle \psi|$$

$$\frac{d}{dt} \rho = \left(\frac{d}{dt}|\psi\rangle\right) \langle \psi| + |\psi\rangle \left(\frac{d}{dt} \langle \psi|\right)$$

$$= -\frac{i}{\hbar} H|\psi\rangle \langle \psi| + \frac{i}{\hbar}|\psi\rangle \langle \psi|H$$

$$\dot{\rho} = -i\hbar [H,\rho]$$

- Pure state will remain pure under Hamiltonian evolution
- For an open system, will have additional terms:
 - Called 'master equation'
 - Example: 2 –level atom interacting with quantized electric field.

$$\dot{\rho} = -\frac{i}{\hbar} [H,\rho] - \frac{\Gamma}{2} (|e\rangle \langle e|\rho + \rho|e\rangle \langle e|) + \Gamma |g\rangle \langle e|\rho|e\rangle \langle g|$$

- Master equation describes state of system only, not the `environment', but includes effects of coupling to environment
- Pure state can evolve into mixed state

Example: Interference fringes

Consider a system which is in either a coherent, or incoherent (mixture) superposition of two momentum states k, and -k:

- Coherent superposition:

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|k\rangle + |-k\rangle\right)$$

$$\rho = \frac{1}{2} |k\rangle \langle k| + \frac{1}{2} |k\rangle \langle -k| + \frac{1}{2} |-k\rangle \langle k| + \frac{1}{2} |-k\rangle \langle -k|$$

$$P(x) = \operatorname{Tr}\left\{\rho |x\rangle \langle x|\right\} = \langle x |\rho| x\rangle$$

$$P(x) = 1 + \cos(2kx)$$
 Fringes!

- Incoherent mixture:

$$|\psi\rangle = NA$$

$$\rho = \frac{1}{2}|k\rangle\langle k| + \frac{1}{2}|-k\rangle\langle -k|$$

$$P(x) = 1$$
No fringes!



Entanglement Gives the Illusion of decoherence

• Consider a small system in a pure state. It is initially decoupled from the environment:

$$|\psi\rangle^{(s,e)} = \left(\sum_{s} c_{s}|s\rangle^{(s)}\right) \otimes |\phi\rangle^{(e)}$$

• Then turn on coupling to the environment:

$$\left|\psi'\right\rangle^{(s,e)} = U^{(s,e)} \left|\psi(0)\right\rangle^{(s,e)}$$

- Let the interaction be *non-dissipative*
 - System states do not decay to lower energy states

$$U^{(s,e)}|s\rangle^{(s)} \otimes |\phi\rangle^{(e)} = |s\rangle^{(s)} \otimes |\phi_s\rangle^{(e)}$$

• Strong interaction: assume that different $|s\rangle$ states drive $|\phi\rangle$ into orthogonal states

$$\left\langle \phi_{s} \left| \phi_{s'} \right\rangle^{(e)} = \delta_{s,s'}$$



The `reduced system density operator'

- Suppose we want to make predictions for system observables only
 - Definition of `system observable':

$$A_s = A^{(s)} \otimes I^{(e)}$$

• Take expectation value:

$$\langle A_s \rangle = Tr \left\{ \rho^{(s,e)} A^{(s)} \otimes I^{(e)} \right\}$$

= $\sum_{m,n} \langle m |^{(s)} \otimes \langle n |^{(e)} \rho^{(s,e)} A^{(s)} \otimes I^{(e)} | m \rangle^{(s)} \otimes | n \rangle^{(e)}$
= $\sum_m \langle m |^{(s)} \sum_n \langle n |^{(e)} \rho^{(s,e)} | n \rangle^{(e)} A^{(s)} | m \rangle^{(s)}$

 Define the `reduced system density operator':

$$\rho^{(s)} = \sum_{n} \langle n | {}^{(e)} \rho^{(s,e)} | n \rangle^{(e)} = Tr_e \left\{ \rho^{(s,e)} \right\}$$

(s)

• Physical predictions regarding system observables depend only on $\rho^{(s):}$

$$\langle A_s \rangle = \sum_m \langle m | {}^{(s)} \rho^{(s)} A^{(s)} | m \rangle$$
$$\langle A_s \rangle = Tr_s \{ \rho^{(s)} A^{(s)} \}$$

Entanglement mimics <u>`collapse'</u>

Return to our entangled state of the system + environment:

$$|\psi\rangle^{(s,e)} = \sum_{s} c_{s} |s\rangle^{(s)} \otimes |\phi_{s}\rangle^{(e)}$$

• Compute density matrix:

$$\rho = |\psi\rangle \langle \psi|^{(s,e)}$$
$$= \sum_{s,s'} c_s c_{s'}^* |s\rangle^{(s)} \otimes |\phi_s\rangle^{(e)} \langle s'|^{(s)} \otimes \langle \phi_{s'}|^{(e)}$$

• Compute the reduced system density operator:

$$\rho^{(s)} = Tr_e \left\{ |\psi\rangle \langle \psi|^{(s,e)} \right\}$$

= $\sum_{s,s'} c_s c_{s'}^* Tr_e \left\{ |s\rangle^{(s)} \otimes |\phi_s\rangle^{(e)} \langle s'|^{(s)} \otimes \langle \phi_{s'}|^{(e)} \right\}$
= $\sum_{s,s'} c_s c_{s'}^* |s\rangle \langle s'|^{(s)} \langle \phi_{s'} |\phi_s\rangle$
= $\sum_{s} |c_s|^2 |s\rangle \langle s|^{(s)}$



'Collapse' of the state

$$\rho^{(s)} = \sum_{s} |c_{s}|^{2} |s\rangle \langle s|^{(s)}$$

- **Conclusion:** Any subsequent measurement on the system, will give results *as if* the system were in only one of the $|s\rangle$, chosen at random, with probability $P_s = |c_s|^2$
 - This is also how we would describe the `collapse' of the wavefunction
- Yet, the true state of the whole system is not `collapsed':

$$|\psi\rangle^{(s,e)} = \sum_{s} c_{s} |s\rangle^{(s)} \otimes |\phi_{s}\rangle^{(e)}$$

- We see that the entanglement between system and env. mimics `collapse'
 - Is collapse during measurement real or illusion?
- Pointer States: for a measuring device to work properly, the assumption, ⟨φ_s |φ_{s'}⟩ = δ_{s,s'} will only be true if the system basis states, {|s⟩}, are the eigenstates of the observable being measured

