

PHYS 610: Recent Developments in Quantum Mechanics and Quantum Information  
(Spring 2009)  
Course Notes: The Density Operator

## 1 Density Operator

Traditionally, the **state vector**  $|\psi\rangle$  represents the state of a quantum system. However, we will need a more general object to represent the quantum state for the purposes of studying light-matter interactions. The density operator represents the state of a quantum system in a more general way than the state vector, and equivalently represents an observer's *state of knowledge* of a system. It is particularly important to use the density operator in the quantum theory of *open* systems, where a quantum system interacts with an external system whose evolution is unknown, and in the quantum theory of measurement and information.

When a quantum state can be represented by a state vector  $|\psi\rangle$ , the **density operator** is defined as the product

$$\rho := |\psi\rangle\langle\psi|. \tag{1}$$

(density operator, pure state)

In this case, it is obvious that the information content of the density operator is equivalent to that of the state vector (except for the overall phase, which is not of physical significance).

The state vector can represent states of *coherent* superposition. The power of the density operator lies in the fact that it can represent *incoherent* superpositions as well. For example, let  $|\psi_\alpha\rangle$  be a set of states (without any particular restrictions). Then the density operator

$$\rho = \sum_{\alpha} P_{\alpha} |\psi_{\alpha}\rangle\langle\psi_{\alpha}| \tag{2}$$

(density operator, general)

models the fact that we don't know *which* of the states  $|\psi_\alpha\rangle$  the system is in, but we assign a probability or weight  $P_\alpha$  to the quantum state  $|\psi_\alpha\rangle$  in the mixture defined by  $\rho$ . Note that the weights obey

$$\sum_{\alpha} P_{\alpha} = 1 \tag{3}$$

for proper normalization of the density operator. Another way to say it is this: the state vector  $|\psi\rangle$  represents a certain *intrinsic uncertainty* with respect to quantum observables; the density operator can represent uncertainty *beyond* the minimum required by quantum mechanics. Equivalently, the density operator can represent an *ensemble* of identical systems in possibly different states.

A state of the form (1) is said to be a **pure state**. One that cannot be written in this form is said to be **mixed**.

### 1.1 Example

As a simple example, consider a **qubit**, a two-level system with states  $|0\rangle$  and  $|1\rangle$ . The density operators corresponding to the eigenstates are  $|0\rangle\langle 0|$  and  $|1\rangle\langle 1|$ ; clearly these are pure states. Another pure state is the superposition  $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ , which has the corresponding density operator

$$\rho = \frac{1}{2} \left( |0\rangle\langle 0| + |1\rangle\langle 1| + |0\rangle\langle 1| + |1\rangle\langle 0| \right). \tag{4}$$

The density operator is the sum of the density operators for the eigenstates, plus two extra terms that indicated the *purity* of the state or the *coherence* of the superposition. An example of a mixture of the two eigenstates comes from simply removing these last two terms:

$$\rho = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|). \quad (5)$$

We can clearly regard this as an mixture of the form (2), where the probabilities are  $P_{0,1} = 1/2$  for the eigenstates  $|\psi_0\rangle = |0\rangle$  and  $|\psi_1\rangle = |1\rangle$ . However, we can equally well regard the same mixed state as a different mixture. That is, defining the mixed state

$$\rho' = \frac{1}{2}(|+\rangle\langle +| + |-\rangle\langle -|), \quad (6)$$

where

$$|\pm\rangle := \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle). \quad (7)$$

it is not hard to see that  $\rho = \rho'$ . Thus we see that we have to be a bit careful with our above statement, where we said that a mixed state can be regarded as an association of classical probabilities with being in different pure quantum states. Just given a particular density operator, it is not in general possible to uniquely define pure-state decomposition of the form (2). Thus stating that the state is *really* in a pure state, but we don't quite know *which* one it's in, implies some *extra* information that is not contained in the density operator.

## 1.2 Evolution

Differentiating the density operator and employing the Schrödinger equation  $i\hbar\partial_t|\psi\rangle = H|\psi\rangle$ , we can write down the equation of motion for the density operator:

$$\begin{aligned} \partial_t\rho &= (\partial_t|\psi\rangle)\langle\psi| + |\psi\rangle\partial_t\langle\psi| \\ &= -\frac{i}{\hbar}H\rho + \frac{i}{\hbar}\rho H \\ &= -\frac{i}{\hbar}[H, \rho]. \end{aligned} \quad \begin{array}{l} (8) \\ \text{(Schrödinger–von Neumann equation)} \end{array}$$

This is referred to as the **Schrödinger–von Neumann equation**. The derivation here assumed a pure state but carries through in the obvious way for arbitrary density operators. Of course, the point is that using the density operator allows us to write down more general evolution equations than those implied by state-vector dynamics. The more general forms are referred to as **Liouville–von Neumann equations** or **master equations**, which we can write in the form

$$\partial_t\rho = \mathcal{L}\rho. \quad (9)$$

(master equation, generic form)

Here,  $\mathcal{L}$  is the **Liouvillian superoperator**. We use the term “superoperator” because the Liouvillian represents a higher-dimensional object, since it must represent the commutator above (i.e., it “operates from both sides”). Thinking of the density operator as a two-dimensional matrix as we discuss below, the Liouvillian is effectively a 4-tensor.

### 1.3 Expectation Values

We can compute expectation values with respect to the density operator via the trace operation. The trace of an operator  $A$  is simply the sum over the diagonal matrix elements with respect to any complete, orthonormal set of states  $|\beta\rangle$ :

$$\text{Tr}[A] := \sum_{\beta} \langle \beta | A | \beta \rangle \quad (10)$$

An important property of the trace is that the trace of a product is invariant under cyclic permutations of the product. For example, for three operators,

$$\text{Tr}[ABC] = \text{Tr}[BCA] = \text{Tr}[CAB]. \quad (11)$$

(cyclic permutation invariance)

This amounts to simply an interchange in the order of summations. For example, for two operators, working in the position representation,

$$\begin{aligned} \text{Tr}[AB] &= \int dx \langle x | AB | x \rangle \\ &= \int dx \int dx' \langle x | A | x' \rangle \langle x' | B | x \rangle \\ &= \int dx' \int dx \langle x' | B | x \rangle \langle x | A | x' \rangle \\ &= \int dx' \langle x' | BA | x' \rangle \\ &= \text{Tr}[BA]. \end{aligned} \quad (12)$$

Note that this argument assumes sufficiently “nice” operators (it fails, for example, for  $\text{Tr}[xp]$ ). More general permutations [e.g., of the form (11)] are obtained by replacements of the form  $B \rightarrow BC$ . Using this property, we can obviously write the expectation value with respect to a pure state as

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \text{Tr}[A\rho]. \quad (13)$$

(expectation value, pure state)

This obviously extends to the more general form (2) of the density operator. Taking an additional average over the ensemble of pure states,

$$\langle\langle A \rangle\rangle = \sum_{\alpha} P_{\alpha} \langle \psi_{\alpha} | A | \psi_{\alpha} \rangle = \text{Tr}[A\rho], \quad (14)$$

(expectation value, ensemble)

where the double angle brackets  $\langle\langle \rangle\rangle$  denote the ensemble average over expectation values. For simplicity we will drop the extra brackets and simply use single brackets for expectation values with respect to either a pure state or an ensemble ( $\langle\langle \rangle\rangle \rightarrow \langle \rangle$ ).

### 1.4 The Density Matrix

The physical content of the density operator is more apparent when we compute the elements  $\rho_{\alpha\alpha'}$  of the *density matrix* with respect to a complete, orthonormal basis. The density matrix elements are given by

$$\rho_{\alpha\alpha'} := \langle \alpha | \rho | \alpha' \rangle. \quad (15)$$

(density matrix)

To analyze these matrix elements, we will assume the simple form  $\rho = |\psi\rangle\langle\psi|$  of the density operator, though the arguments generalize easily to arbitrary density operators.

The diagonal elements  $\rho_{\alpha\alpha}$  are referred to as *populations*, and give the measurement probability of the system in the state  $|\alpha\rangle$ :

$$\rho_{\alpha\alpha} = \langle\alpha|\rho|\alpha\rangle = |\langle\alpha|\psi\rangle|^2. \quad (16)$$

The off-diagonal elements  $\rho_{\alpha\alpha'}$  (with  $\alpha \neq \alpha'$ ) are referred to as *coherences*, since they give information about the relative phase of different components of the superposition. For example, if we write the state vector as a superposition with explicit phases,

$$|\psi\rangle = \sum_{\alpha} |c_{\alpha}| e^{i\phi_{\alpha}} |\alpha\rangle, \quad (17)$$

then the coherences are

$$\rho_{\alpha\alpha'} = |c_{\alpha}c_{\alpha'}| e^{i(\phi_{\alpha} - \phi_{\alpha'})}. \quad (18)$$

Notice that for a density operator not corresponding to a pure state, the coherences in general will be the sum of complex numbers corresponding to different states in the incoherent sum. The phases will not in general line up, so that while  $|\rho_{\alpha\alpha'}|^2 = \rho_{\alpha\alpha}\rho_{\alpha'\alpha'}$  for a pure state, we expect  $|\rho_{\alpha\alpha'}|^2 < \rho_{\alpha\alpha}\rho_{\alpha'\alpha'}$  ( $\alpha \neq \alpha'$ ) for a generic mixed state.

## 1.5 Purity

How can we tell a pure state from a mixed one in general? Notice that the diagonal elements of the density matrix form a probability distribution. Proper normalization thus requires

$$\text{Tr}[\rho] = \sum_{\alpha} \rho_{\alpha\alpha} = 1. \quad (19)$$

(normalization)

We can do the same computation for  $\rho^2$ , and we will define the **purity** to be  $\text{Tr}[\rho^2]$ . For a pure state, the purity is simple to calculate, since  $\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = \rho$ :

$$\text{Tr}[\rho^2] = \text{Tr}[\rho] = 1. \quad (20)$$

(purity for pure state)

(In fact  $\rho^n = \rho$  in a pure state for any nonnegative  $n$ .) But for mixed states,  $\text{Tr}[\rho^2] < 1$ . For example, for the density operator in (2),

$$\text{Tr}[\rho^2] = \sum_{\alpha} P_{\alpha}^2, \quad (21)$$

if we assume the states  $|\psi_{\alpha}\rangle$  to be orthonormal. For equal probability of being in  $N$  such states,  $\text{Tr}[\rho^2] = 1/N$ . Intuitively, then we can see that  $\text{Tr}[\rho^2]$  drops to zero as the state becomes more mixed—that is, as it becomes an incoherent superposition of more and more orthogonal states.

To prove that  $\text{Tr}[\rho^2] < 1$  for mixed states, first note that  $\rho$  is a Hermitian operator ( $\rho = \rho^{\dagger}$ ). Thus,  $\rho$  may be diagonalized by a unitary transformation, so we may write

$$\rho' = S\rho S^{\dagger}, \quad (22)$$

where  $\rho'$  is diagonal and  $S^{-1} = S^{\dagger}$ . It is easy to verify that the trace is invariant under unitary transformations, so

$$\text{Tr}[\rho^2] = \text{Tr}[\rho'^2] = \sum_{\alpha} (\rho'_{\alpha\alpha})^2 \leq \left( \sum_{\alpha} \rho'_{\alpha\alpha} \right)^2 = 1, \quad (23)$$

where we used the Cauchy–Schwarz inequality. A diagonal pure state has only a single nonzero diagonal element, while a diagonal mixed state necessarily has more than one nonzero diagonal element. Hence, for a mixed state,  $\text{Tr}[\rho^2] < 1$ . This follows since the diagonal matrix elements are positive,

$$\rho_{\alpha\alpha} = \langle \alpha | \rho | \alpha \rangle = \sum_k P_k |\langle \alpha | \psi \rangle_k|^2 \geq 0, \quad (24)$$

and so the equality occurs only for a single term in the sum.