3.6: Density Operators

We now introduce the **density operator**, which helps to streamline many calculations in multi-particle quantum mechanics.

Consider a quantum system with a d-dimensional Hilbert space $\mathscr{H}$. Given an arbitrary state $|\psi\rangle \in \mathscr{H}$, define

$$\hat{\rho} = |\psi\rangle\,\langle\psi|. \tag{3.6.1}$$

This is just the projection operator for $|\psi\rangle$, but in this context we call it a "density operator". Some other authors call it a **density matrix**, based on the fact that linear operators can be represented as matrices. It has the following noteworthy features:

1. It is Hermitian.
2. Suppose $\hat{Q}$ is an observable with eigenvalues $\{q_\mu\}$ and eigenstates $\{|\mu\rangle\}$ (where μ is some label that enumerates the eigenstates. If we do a $\hat{Q}$ measurement on $|\psi\rangle$, the probability of obtaining q_μ is

$$P_\mu = \left|\langle\mu|\psi\rangle\right|^2 = \langle\mu|\,\hat{\rho}\,|\mu\rangle. \tag{3.6.2}$$

3. Moreover, the expectation value of the observable is

$$\langle Q\rangle = \sum_\mu q_\mu P_\mu = \sum_\mu q_\mu \langle\mu|\hat{\rho}|\mu\rangle = \mathrm{Tr}\left[\,\hat{Q}\,\hat{\rho}\,\right]. \tag{3.6.3}$$

   In the last equality, $\mathrm{Tr}[\cdots]$ denotes the trace, which is the sum of the diagonal elements of the matrix representation of the operator. The value of the trace is basis-independent.

Now consider, once again, a composite system consisting of two subsystems A and B, with Hilbert spaces $\mathscr{H}_A$ and $\mathscr{H}_B$. Let's say we are interested in the physical behavior of A, that is to say the outcome probabilities and expectation values of any measurements performed on A. These can be calculated from $|\psi\rangle$, the state of the combined system; however, $|\psi\rangle$ also carries information about B, which is not relevant to us as we only care about A.

There is a more economical way to encode just the information about A. We can define the density operator for subsystem A (sometimes called the **reduced density operator**):

$$\hat{\rho}_A = \mathrm{Tr}_B\left[\,\hat{\rho}\,\right]. \tag{3.6.4}$$

Here, $\mathrm{Tr}_B[\cdots]$ refers to a **partial trace**. This means tracing over the $\mathscr{H}_B$ part of the Hilbert space $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$, which yields an operator acting on $\mathscr{H}_A$.

To better understand Equation (3.6.4), let us go to an explicit basis. Let $\hat{Q}_A$ be an observable for $\mathscr{H}_A$ with eigenbasis $\{|\mu\rangle\}$, and let $\hat{Q}_B$ be an observable for $\mathscr{H}_B$ with eigenbasis $\{|\nu\rangle\}$. If the density operator of the combined system is $\hat{\rho} = |\psi\rangle\langle\psi|$, then

$$\hat{\rho}_A = \sum_\nu \left(\hat{I}\otimes\langle\nu|\right)\,|\psi\rangle\langle\psi|\,\left(\hat{I}\otimes|\nu\rangle\right). \tag{3.6.5}$$

This is a Hermitian operator acting on the $\mathscr{H}_A$ space. In the $\{|\mu\rangle\}$ basis, its diagonal matrix elements are

$$\begin{aligned}\langle\mu|\hat{\rho}_A|\mu\rangle &= \sum_\nu \left(\langle\mu|\langle\nu|\right)\,|\psi\rangle\langle\psi|\,\left(|\mu\rangle|\nu\rangle\right)\\ &= \langle\psi|\,\left[|\mu\rangle\langle\mu|\otimes\left(\sum_\nu|\nu\rangle\langle\nu|\right)\right]\,|\psi\rangle\\ &= \langle\psi|\,\left(|\mu\rangle\langle\mu|\otimes\hat{I}_B\right)|\psi\rangle.\end{aligned} \tag{3.6.6}$$

According to the rules of partial measurements discussed in Section 3.2, this is precisely the probability of obtaining q_μ when measuring $\hat{Q}_A$ on subsystem A:

$$P_\mu = \langle\mu|\hat{\rho}_A|\mu\rangle. \tag{3.6.7}$$

It follows that the expectation value for observable $\hat{M}$ is

$$\langle Q_A\rangle = \sum_\mu q_\mu \langle\mu|\hat{\rho}_A|\mu\rangle = \mathrm{Tr}\Big[\hat{Q}_A\,\hat{\rho}_A\Big]. \tag{3.6.8}$$

These results hold for any choice of basis. Hence, knowing the density operator for A, we can determine the outcome probabilities of *any* partial measurement performed on A.

To better understand the properties of $\hat{\rho}_A$, let us write $|\psi\rangle$ explicitly as

$$|\psi\rangle = \sum_{\mu\nu}\psi_{\mu\nu}|\mu\rangle|\nu\rangle, \tag{3.6.9}$$

where $\sum_{\mu\nu}|\psi_{\mu\nu}|^2 = 1$. Then

$$\begin{aligned}\hat{\rho} &= \sum_{\mu\mu'\nu\nu'}\psi_{\mu\nu}\psi^*_{\mu'\nu'}\;|\mu\rangle|\nu\rangle\;\langle\mu'|\langle\nu'|\\ \hat{\rho}_A &= \sum_{\mu\mu'\nu}\psi_{\mu\nu}\psi^*_{\mu'\nu}|\mu\rangle\langle\mu'|\\ &= \sum_\nu\left(\sum_\mu\psi_{\mu\nu}|\mu\rangle\right)\left(\sum_{\mu'}\psi^*_{\mu'\nu}\langle\mu'|\right)\\ &= \sum_\nu|\varphi_\nu\rangle\langle\varphi_\nu|,\quad\text{where}\quad|\varphi_\nu\rangle = \sum_\mu\psi_{\mu\nu}|\mu\rangle.\end{aligned} \tag{3.6.10}$$

But $|\varphi_\nu\rangle$ is not necessarily normalized to unity: $\langle\varphi_\nu|\varphi_\nu\rangle = \sum_\mu|\psi_{\mu\nu}|^2 \le 1$. Let us define

$$|\tilde{\varphi}_\nu\rangle = \frac{1}{\sqrt{P_\nu}}|\varphi_\nu\rangle,\quad\text{where}\;\;P_\nu = \sum_\mu|\psi_{\mu\nu}|^2. \tag{3.6.11}$$

Note that each P_ν is a non-negative real number in the range $[0,1]$. Then

$$\hat{\rho}_A = \sum_\nu P_\nu\,|\tilde{\varphi}_\nu\rangle\langle\tilde{\varphi}_\nu|,\quad\text{where}\;\left\{\begin{array}{l}\text{each } P_\nu \text{ is a real number in } [0,1],\text{ and}\\ \text{each } |\tilde{\varphi}_\nu\rangle\in\mathscr{H}_A,\;\;\text{with}\;\;\langle\tilde{\varphi}_\nu|\tilde{\varphi}_\nu\rangle = 1.\end{array}\right. \tag{3.6.12}$$

In general, we can define a density operator as any operator that has the form of Equation (3.6.12), regardless of whether or not it was formally derived via a partial trace. We can interpret it as describing a ensemble of quantum states weighted by a set of classical probabilities. Each term in the sum consists of (i) a weighting coefficient P_ν which can be regarded as a probability (the coefficients are all real numbers in the range $[0,1]$, and sum to 1), and (ii) a projection operator associated with some normalized state vector $|\tilde{\varphi}_\nu\rangle$. Note that the states in the ensemble do not have to be orthogonal to each other.

From this point of view, a density operator of the form $|\psi\rangle\langle\psi|$ corresponds to the special case of an ensemble containing only one quantum state $|\psi\rangle$. Such an ensemble is called a **pure state**, and describes a quantum system that is not entangled with any other system. If an ensemble is not a pure state, we call it a **mixed state**; it describes a system that is entangled with some other system.

We can show that any linear operator $\hat{\rho}_A$ obeying Equation (3.6.12) has the following properties:

1. $\hat{\rho}_A$ is Hermitian.
2. $\langle\varphi|\hat{\rho}_A|\varphi\rangle \ge 0$ for any $|\varphi\rangle\in\mathscr{H}_A$ (i.e., the operator is positive semidefinite).
3. For any observable $\hat{Q}_A$ acting on $\mathscr{H}_A$,

$$\begin{aligned}\langle Q_A\rangle &\equiv \sum_\nu P_\nu\langle\tilde{\varphi}_\nu|\hat{Q}_A|\tilde{\varphi}_\nu\rangle\\ &= \sum_{\mu\nu}P_\nu\,\langle\tilde{\varphi}_\nu|\mu\rangle\,\langle\mu|\hat{Q}|\tilde{\varphi}_\nu\rangle\quad\big(\text{using some basis }\{|\mu\rangle\}\big)\\ &= \sum_\mu\langle\mu|\hat{Q}\left(\sum_\nu|\tilde{\varphi}_\nu\rangle\langle\tilde{\varphi}_\nu|\right)|\mu\rangle\\ &= \mathrm{Tr}\left[\hat{Q}\,\hat{\rho}_A\right].\end{aligned} \tag{3.6.13}$$

This property can be used to deduce the probability of obtaining any measurement outcome: if $|\mu\rangle$ is the eigenstate associated with the outcome, the outcome probability is $\langle\mu|\hat{\rho}_A|\mu\rangle$, consistent with Equation (3.6.7). To see this, take $\hat{Q} = |\mu\rangle\langle\mu|$ in Equation (3.6.13).

4. The eigenvalues of $\hat{\rho}_A$, denoted by $\{p_1, p_2, \ldots, p_{d_A}\}$, satisfy

$$p_j \in \mathbb{R} \quad \text{and} \quad 0 \le p_j \le 1 \quad \text{for} \quad j = 1, \ldots, d_A, \quad \text{with} \quad \sum_{j=1}^{d_A} p_j = 1. \tag{3.6.14}$$

In other words, the eigenvalues can be interpreted as probabilities. This also implies that $\mathrm{Tr}[\hat{\rho}_A] = 1$.

This property follows from Property 3 by taking $\hat{Q} = |\varphi\rangle\langle\varphi|$, where $|\varphi\rangle$ is any eigenvector of $\hat{\rho}_A$, and then taking $\hat{Q} = \hat{I}_A$.