# 4.1: Mixed States

First, we recall some properties of the trace:

- $\mathrm{Tr}(aA) = a\,\mathrm{Tr}(A)$,
- $\mathrm{Tr}(A+B) = \mathrm{Tr}(A) + \mathrm{Tr}(B)$.

Also remember that we can write the expectation value of $A$ as

$$\langle A\rangle = \mathrm{Tr}(|\psi\rangle\langle\psi|A), \tag{4.1}$$

where $|\psi\rangle$ is the state of the system. It tells us everything there is to know about the system. But what if we don't know everything?

As an example, consider that Alice prepares a qubit in the state $|0\rangle$ or in the state $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ depending on the outcome of a balanced (50:50) coin toss. How does Bob describe the state before any measurement? First, we cannot say that the state is $\frac{1}{2}|0\rangle + \frac{1}{2}|+\rangle$, because this is not normalized!

The key to the solution is to observe that the expectation values must behave correctly. The expectation value $\langle A\rangle$ is the average of the eigenvalues of $A$ for a given state. If the state is itself a statistical mixture (as in the example above), then the expectation values must also be averaged. So for the example, we require that for any A

$$\begin{aligned}\langle A\rangle &= \frac{1}{2}\langle A\rangle_0 + \frac{1}{2}\langle A\rangle_+ = \frac{1}{2}\mathrm{Tr}(|0\rangle\langle 0|A) + \frac{1}{2}\mathrm{Tr}(|+\rangle\langle +|A) \\ &= \mathrm{Tr}\left[\left(\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|+\rangle\langle +|\right)A\right] \\ &\equiv \mathrm{Tr}(\rho A),\end{aligned} \tag{4.2}$$

where we defined

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|+\rangle\langle +|. \tag{4.3}$$

The statistical mixture is therefore properly described by an operator, rather than a simple vector. We can generalize this as

$$\rho = \sum_k p_k\,|\psi_k\rangle\,\langle\psi_k|\,, \tag{4.4}$$

where the $p_k$ are probabilities that sum up to one $(\sum_k p_k = 1)$ and the $|\psi_k\rangle$ are normalized states (not necessarily complete or orthogonal). Since $\rho$ acts as a weight, or a density, in the expectation value, we call it the density operator. We can diagonalize $\rho$ to find the spectral decomposition

$$\rho = \sum_j \lambda_j\,|\lambda_j\rangle\,\langle\lambda_j|\,, \tag{4.5}$$

where $\{|\lambda_j\rangle\}_j$ forms a complete orthonormal basis, $0 \le \lambda_j \le 1$, and $\sum_j \lambda_j = 1$. We can also show that $\rho$ is a positive operator:

$$\begin{aligned}\langle\psi|\rho|\psi\rangle &= \sum_{jk} c_j^* c_k\,\langle\lambda_j|\rho|\lambda_k\rangle = \sum_{jk} c_j^* c_k \left\langle \lambda_j \middle| \sum_l \lambda_l \middle| \lambda_l \right\rangle \langle\lambda_l \mid \lambda_k\rangle \\ &= \sum_{jkl} c_j^* c_k \lambda_l\,\langle\lambda_j \mid \lambda_l\rangle\,\langle\lambda_l \mid \lambda_k\rangle = \sum_{jkl} c_j^* c_k \lambda_l \delta_{jl}\delta_{lk} \\ &= \sum_l \lambda_l |c_l|^2 \\ &\ge 0\end{aligned} \tag{4.6}$$

In general, an operator $\rho$ is a valid density operator if and only if it has the following three properties:

1. $\rho^\dagger = \rho$,
2. $\mathrm{Tr}(\rho) = 1$,
3. $\rho \ge 0$.

The density operator is a generalization of the state of a quantum system when we have incomplete information. In the special case where one of the $p_j = 1$ and the others are zero, the density operator becomes the projector $|\psi_j\rangle\,\langle\psi_j|$. In other words, it is completely determined by the state vector $|\psi_j\rangle$. We call these pure states. The statistical mixture of pure states giving rise to the density operator is called a **mixed state**.

The unitary evolution of the density operator can be derived directly from the Schrödinger equation $i\hbar\partial_t|\psi\rangle = H|\psi\rangle$:

$$\begin{aligned} i\hbar\frac{d\rho}{dt} &= i\hbar\frac{d}{dt}\sum_j p_j\,|\psi_j\rangle\,\langle\psi_j| \\ &= i\hbar\sum_j\left\{\frac{dp_j}{dt}|\psi_j\rangle\,\langle\psi_j| + p_j\left[\left(\frac{d}{dt}|\psi_j\rangle\right)\langle\psi_j| + |\psi_j\rangle\left(\frac{d}{dt}\langle\psi_j|\right)\right]\right\} \\ &= i\hbar\frac{\partial\rho}{\partial t} + H\rho - \rho H \\ &= [H,\rho] + i\hbar\frac{\partial\rho}{\partial t} \end{aligned} \tag{4.7}$$

This agrees with the Heisenberg equation for operators, and it is sometimes known as the Von Neumann equation. In most problems the probabilities $p_j$ have no explicit time-dependence, and $\partial_t\rho = 0$.