4.1: Mixed States

First, we recall some properties of the trace:

- \( \operatorname{Tr}(a A) = a \operatorname{Tr}(A) \)
- \( \operatorname{Tr}(A + B) = \operatorname{Tr}(A) + \operatorname{Tr}(B) \)

Also remember that we can write the expectation value of \( A \) as

\[
\langle A \rangle = \operatorname{Tr}(|\psi\rangle\langle\psi| A), \tag{4.1}
\]

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 \( A \)

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

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 \(|\lambda_j\rangle\) forms a complete orthonormal basis, \(\sum \lambda_j = 1\), and \(|\psi\rangle \langle \psi|\) is a positive operator.

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. \(\operatorname{Tr}(\rho) = 1\)
3. \(\rho \geq 0\).

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 \(p_k = 1\) 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}{d t} &= i \hbar \frac{d}{d t} \sum_{j} p_{j} \left| \psi_{j} \right\rangle \left\langle \psi_{j} \right| \\
&= i \hbar \sum_{j} \left\{ \frac{d p_{j}}{d t} \left| \psi_{j} \right\rangle \left\langle \psi_{j} \right| + p_{j} \left( \frac{d}{d t} \left| \psi_{j} \right\rangle \right) \left\langle \psi_{j} \right| + \left| \psi_{j} \right\rangle \left( \frac{d}{d t} \left\langle \psi_{j} \right| \right) \right\} \\
&= i \hbar \frac{\partial \rho}{\partial t} + H \rho - \rho H \\
\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 \( \frac{\partial_{t} \rho}{\partial t} = 0 \).