Mixed States and Density Matrices

1 Mixed Quantum State

So far we have dealt with pure quantum states
\[ |\psi\rangle = \sum_x \alpha_x |x\rangle. \]

This is not the most general state we can think of. We can consider a probability distribution of pure states, such as
\[ |0\rangle \text{ with probability } \frac{1}{2} \]
and
\[ |1\rangle \text{ with probability } \frac{1}{2} \]
Another possibility is the state
\[ \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \text{ with probability } \frac{1}{2} \]
In general, we can think of mixed state \( \{p_i, |\psi_i\rangle\} \) as a collection of pure states
\[ |\psi_i\rangle \]
each with associated probability \( p_i \), with the conditions \( 0 \leq p_i \leq 1 \) and \( \sum_i p_i = 1 \).

2 Density Matrix

Consider a \( k \)-level quantum system. A pure state of the system can be written as a superposition
\[ |\psi\rangle = \sum_{j=1}^{k} a_j |j\rangle. \]
The most general state of this system is a mixture of pure states: \( |\psi_i\rangle \) with probability \( p_i \). For any such mixture, we can define a density matrix, which is a \( k \times k \) Hermitian matrix \( \rho \). The result of measuring the mixed quantum state can be expressed directly in terms of the matrix \( \rho \). Therefore it follows that if two mixtures have the same density matrix then they cannot be distinguished by any measurement. More specifically, the density matrix associated with the pure state \( |\psi\rangle \) is the outer product \( |\psi\rangle \langle \psi| \), which is the \( k \times k \) matrix
\[
\begin{pmatrix}
  a_1 \\
  a_2 \\
  \vdots \\
  a_k
\end{pmatrix}
\begin{pmatrix}
  \bar{a}_1 & \bar{a}_2 & \cdots & \bar{a}_k
\end{pmatrix}
= \begin{pmatrix}
  a_1\bar{a}_1 & a_1\bar{a}_2 & \cdots & a_1\bar{a}_k \\
  a_2\bar{a}_2 & a_1\bar{a}_2 & \cdots & a_2\bar{a}_k \\
  \vdots & \vdots & \ddots & \vdots \\
  a_k\bar{a}_1 & a_k\bar{a}_2 & \cdots & a_k\bar{a}_k
\end{pmatrix}.
\]
The density matrix \( \rho \) for the mixture \( |\psi_i\rangle \) with probability \( p_i \) is simply a convex combination of the density matrices corresponding to each \( |\psi_i\rangle \):
\[
\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|.
\]
We give some examples. Consider the mixed state $|0\rangle$ with probability 1/2 and $|1\rangle$ with probability 1/2. Then
\[
|0\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},
\]
and
\[
|1\rangle\langle 1| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.
\]
Thus in this case
\[
\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.
\]
Now consider another mixed state, this time consisting of $|+\rangle$ with probability 1/2 and $|-\rangle$ with probability 1/2. This time we have
\[
|+\rangle\langle +| = (1/2) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},
\]
and
\[
|-\rangle\langle -| = (1/2) \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} 1 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.
\]
Thus in this case the offdiagonals cancel, and we get
\[
\rho = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.
\]
Note that the two density matrices we computed are identical, even though the mixed state we started out was different. Hence we see that it is possible for two different mixed states to have the same density matrix.

Nonetheless, the density matrix of a mixture completely determines the effects of making a measurement on the system:

**Theorem:** Suppose we measure a mixed state \(\{p_j, |\psi_j\rangle\}\) in an orthonormal bases \(|\beta_i\rangle\). Then the outcome is \(|\beta_i\rangle\) with probability \(\langle \beta_i | \rho | \beta_i \rangle\).

**proof:** We denote the probability of measuring \(|\beta_i\rangle\) by \(\text{Pr}[i]\). Then
\[
\text{Pr}[i] = \sum_j p_j |\langle \psi_j | \beta_i \rangle|^2
\]
\[
= \sum_j p_j \langle \beta_i | \psi_j \rangle \langle \psi_j | \beta_i \rangle
\]
\[
= \langle \beta_i | \sum_j p_j |\psi_j\rangle \langle \psi_j | \beta_i \rangle
\]
\[
= \langle \beta_i | \rho | \beta_i \rangle.
\]