In this lecture, we will discuss mixed quantum states and density matrices..

1 Mixed Quantum States

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 $|0\rangle$ with probability $1/2$ and $|1\rangle$ with probability $1/2$. Another possibility is the state

$$\begin{cases} |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) & \text{with probability 1/2} \\ |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) & \text{with probability 1/2} \end{cases}$$

In general, we can think of *mixed* state 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 $\sum_i p_i = 1$. One reason we consider such mixed states is because the quantum states are hard to isolate, and hence often entangled to the environment.

2 Density Matrix

Now we consider the result of measuring a mixed quantum state. Suppose we have a mixture of quantum states $|\psi_i\rangle$ with probability p_i. Each $|\psi_i\rangle$ can be represented by a vector in $\mathscr{C}^{2^n}$, and thus we can associate the outer product $|\psi_i\rangle\langle\psi_i| = \psi_i\psi_i^*$, which is an $2^n \times 2^n$ matrix

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \begin{pmatrix} \bar{a}_1 & \bar{a}_2 & \cdots & \bar{a}_N \end{pmatrix} = \begin{pmatrix} a_1\bar{a}_1 & a_1\bar{a}_2 & \cdots & a_1\bar{a}_N \\ a_2\bar{a}_2 & a_1\bar{a}_2 & \cdots & a_2\bar{a}_N \\ \vdots & & & \vdots \\ a_N\bar{a}_1 & a_N\bar{a}_2 & \cdots & a_N\bar{a}_N \end{pmatrix}.$$

We can now take the average of these matrices, and obtain the *density matrix* of the mixture $\{p_i, |\psi_i\rangle\}$:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|.$$

Note that the density matrix is an *operator*.

We give some examples. Consider the mixed state $|0\rangle$ with probability of $1/2$ and $|1\rangle$ with probablity $1/2$. 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. As we now show, this will mean that we cannot distinguish the two states.

Two mixed states can be distinguished if and only if the density matrix ρ are different. This is evident from consideration of the information obtained from a measurement in an orthonormal basis.

Theorem 21.1: *Suppose we measure a mixed state $\{p_j, |\psi_j\rangle\}$ in an orthonormal basis $|\beta_k\rangle$. Then the outcome is $|\beta_k\rangle$ with probability $\langle\beta_k|\rho|\beta_k\rangle$.*

Proof: We denote the probability of measuring $|\beta_k\rangle$ by $\Pr[k]$. Then

$$\begin{aligned} \Pr[k] &= \sum_j p_j |\langle\psi_j|\beta_k\rangle|^2 \\ &= \sum_j p_j \langle\beta_k|\psi_j\rangle\langle\psi_j|\beta_k\rangle \\ &= \left\langle \beta_k \middle| \sum_j p_j |\psi_j\rangle\langle\psi_j| \middle| \beta_k \right\rangle \\ &= \langle\beta_k|\rho|\beta_k\rangle. \end{aligned}$$

□

corollary If we measure the mixed state $\{p_j, |\psi_j\rangle\}$ in the standard basis, we have $\Pr[k] = \rho_{k,k}$, the diagonal entry of the density matrix ρ. Thus we do not obtain any information about the different possible mixed states that give rise to a given density matrix.

We list several more properties of the density matrix:

1. $\mathrm{tr}\rho = 1$. This follows immediately from Corollary **??**, since the probabilities $\Pr[k]$ must add up to 1.
2. $\mathrm{tr}\rho^2 \leq 1$. You can easily prove this by expansion of ρ in an orthonormal basis.
3. ρ is Hermitian. This follows from the fact that ρ is a sum of Hermitian outer products ($(\psi\psi^*)^* = \psi\psi^*$).

4. Eigenvalues of ρ are non-negative. First of all, eigenvalues of a Hermitian matrix is real. Suppose that λ and $|e\rangle$ are corresponding eigenvalue and eigenvector. Then if we measure in the eigenbasis, we have

   $$\Pr[e] = \langle e|\rho|e\rangle = \lambda\langle e|e\rangle = \lambda.$$

   Since the probability must be non-negative, we see that $\lambda \geq 0$.

3 Decoherence, dissipation and the Density Matrix

The diagonal elements ρ_{ii} of the density matrix represent the populations in the chosen basis, i.e., for $\rho = \sum_k p_k |k\rangle\langle k|$ with $|k\rangle = \sum_i c_i^k |i\rangle$, we have

$$\rho_{ii} = \sum_k p_k |c_i^k|^2 \tag{1}$$

as the population in state $|i\rangle$.

The off-diagonal elements ρ_{ij} of the density matrix provide information about interference between the amplitudes of states $|i\rangle$ and $|j\rangle$, i.e., they represent the coherences in the mixed state.

When a qubit is coupled to an environment, this coupling can cause some time dependence of elements of the density matrix. Decay of the off-diagonal elements is referred to as “dephasing” while decay of the diagonal elements is referred to as “relaxation” or “dissipation”.

Note: a pure state $|\psi\rangle$ has a corresponding density matrix $\rho = |\psi\rangle\langle\psi|$. Consider the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{i}{\sqrt{2}}|1\rangle. \tag{2}$$

Writing the density matrix for this state in the standard basis you will find a full 2x2 matrix with off-diagonal coherences. This is very different from the mixed state density matrices in the example above, which are pure diagonal matrices. A pure diagonal density matrix with equal matrix elements on the diagonal is referred to as “the completely mixed state”. You can readily show that the density matrix for a pure state satisfies $\mathrm{tr}\rho^2 = 1$, so the criterion $\mathrm{tr}\rho^2 < 1$ allows you to distinguish a mixed from a pure state density matrix.