Quantum Mechanics: Density operator

Density operator formalism

According to the postulates of quantum mechanics, the state of a system is completely described by its quantum state, usually denoted by $|\psi\rangle$. The expectation of an observable $\hat{A}$ is defined as

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle.$$

There exists an alternate formalism, which can be useful in certain situations. This is the density operator formalism, introduced by John von Neumann in 1927. The density operator formalism has proved to be extremely useful in the new field of *quantum information*. For a state $|\psi\rangle$, the density operator is defined as

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

which we will call a *pure state* density operator. The meaning of the term pure state will become clear later. The value of an observable $\hat{A}$ is defined as

$$\langle\hat{A}\rangle = Tr[\hat{\rho}\hat{A}].$$

It is easy to show that this is the same as the expectation value.

$$\begin{aligned}\langle\hat{A}\rangle &= Tr[|\psi\rangle\langle\psi|\hat{A}] \\ &= \sum_n \langle b_n|\psi\rangle\langle\psi|\hat{A}|b_b\rangle \\ &= \sum_n \langle\psi|\hat{A}|b_b\rangle\langle b_n|\psi\rangle = \langle\psi|\hat{A}\sum_n |b_b\rangle\langle b_n|\psi\rangle \\ &= \langle\psi|\hat{A}|\psi\rangle. \qquad (1)\end{aligned}$$

Also easy to see is an important property:

$$\hat{\rho}^2 = |\psi\rangle\langle\psi||\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho}.$$

Density matrix

One can choose a set of basis states to write the density operator in the matrix representation, the *density matrix*

$$\rho_{mn} = \langle b_m|\hat{\rho}|b_n\rangle.$$

Trace of the a density matrix or density operator is given by

$$Tr[\hat{\rho}] = \sum_n \rho_{nn} = \sum_n \langle b_n|\psi\rangle\langle\psi|b_n\rangle = \sum_n \langle\psi|b_n\rangle\langle b_n|\psi\rangle = 1.$$

So the trace of a density operator is always 1. A diagonal element of the density matrix is given by

$$\rho_{kk} = \langle b_k|\psi\rangle\langle\psi|b_k\rangle = |\langle b_k|\psi\rangle|^2.$$

So, the k'th diagonal element of the density matrix represents the probability of finding the system in the state $|b_k\rangle$ (upon a suitable measurement). All diagonal elements of the density matrix are real, irrespective of the basis.

Mixed state density operator

The density operator of the form $\hat{\rho} = |\psi\rangle\langle\psi|$, which we call pure state density operator, can be used to describe either a single quantum system, or an *ensemble* of quantum systems all in identical quantum states. For example, in finding the expectation value of an observable, one has to measure the observable for an ensemble of identical systems. But suppose we have a physical situation in which the systems of the ensemble are produced by some physical process, and (say) one-third of them are in the state $|\psi_1\rangle$, and two-third are in the state $|\psi_2\rangle$. Although each system by itself is in a pure state, one doesn't know if it is $|\psi_1\rangle$ or $|\psi_2\rangle$. There is no way to describe such an ensemble in the quantum mechanics we have studied till now, because the states themselves are occuring probabilistically. Such an ensemble can be described by a *mixed state* density operator defined as

$$\hat{\rho} = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|,$$

where p_1 and p_2 are the probabilities of occurence of the states $|\psi_1\rangle$ and $|\psi_2\rangle$, respectively. It has a straighforward generalization to n states:

$$\hat{\rho} = \sum_{j=1}^{n} p_j|\psi_j\rangle\langle\psi_j|. \tag{2}$$

Note that these different states are not necessarily orthogonal to each other. Even when they *are* orthogonal, it is easy to see the following property

$$\begin{aligned}\hat{\rho}^2 &= \sum_{j=1}^{n} p_j|\psi_j\rangle\langle\psi_j| \sum_{k=1}^{n} p_k|\psi_k\rangle\langle\psi_k| \\ &= \sum_{j=1}^{n} p_j^2|\psi_j\rangle\langle\psi_j| \neq \hat{\rho}.\end{aligned} \tag{3}$$

This suggests an easy check to see if a density operator is pure or mixed. If $\hat{\rho}^2 = \hat{\rho}$, it is pure, if not, it is mixed.

The density matrix for a mixed state would look like the following

$$\rho_{mn} = \sum_{j=1}^{n} p_j\langle b_m|\psi_j\rangle\langle\psi_j|b_n\rangle.$$

The diagonal elements are still probabilities, but a bit more involved

$$\rho_{nn} = \sum_{j=1}^{n} p_j|\langle b_n|\psi_j\rangle|^2.$$

The interpretation is the following - if the state of the system is $|\psi_j\rangle$ the probability of finding it in the state $|b_n\rangle$ is $|\langle b_n|\psi_j\rangle|^2$. However, the state $|\psi_j\rangle$ itself occurs with a probability p_j, so the total probability of finding the system in the state $|b_n\rangle$ would be equal to the weighted average of these individual probabilities.

Notice that in (2) in if $\{|\psi_j\rangle\}$ form an ortho-normal set, and one uses the same states as the basis to write the matrix representation

$$\rho_{mn} = \sum_{j=1}^{n} p_j\langle\psi_m|\psi_j\rangle\langle\psi_j|\psi_n\rangle = p_n\delta_{mn},$$

which is a diagonal matrix with the k'th diagonal term representing the probability of finding a system of the ensemble in the state $|\psi_k\rangle$. So, a mixed state density matrix can be a completely diagonal. On the other hand, a pure state density matrix can never be diagonal, except for the case where there is only *one* nonzero (diagonal) element of the matrix. One can check that if a pure state density operator is given by $\hat{\rho} = |b_k\rangle\langle b_k|$, and one writes its matrix representation using the set $\{|b_j\rangle\}$, the matrix is

$$\rho_{mn} = \delta_{mn}\delta_{nk},$$

and the lone matrix element ρ_{kk} is equal to 1.

Another test of the purity of a density matrix is the trace of $\hat{\rho}^2$. Since for a pure state, $\hat{\rho}^2 = \hat{\rho}$, it is obvious that $Tr[\hat{\rho}^2] = 1$. For a mixed state density matrix in the diagonal form, $Tr[\hat{\rho}^2] = \sum_j p_j^2 < 1$.