0.1 lecture VIII

0.1.1 Density Matrix I

Consider a quantum system with two possible outcomes following a measurement. The Hilbert space basis vectors are chosen to be $|+>$ and $|->$ whose eigenvalues, for S_z, are $\pm\hbar/2$ respectively.

We now suppose the quantum system is in the state

$$|\Psi>=\frac{1}{\sqrt{2}}(|+>+|->). \tag{1}$$

We make repeated measurements on an ensemble of **identical** states given above. Using the postulates of QM we find that 50 percent of the measurements result in the value $\hbar/2$ and the other half $-\hbar/2$. Measurements performed on a system in a given quantum state (also, called a pure state or coherent state) is called a *pure ensemble*. We shall simply mean by state a vector in Hilbert space and shall banish the use of the term *mixed state*. However, we do consider the notion of a *mixed ensemble*.

Suppose we make a measurement on a quantum system but are uncertain of which quantum state the system is in. Suppose the system is in state $|+>$ 50 % of the time and in state $|->$ for the remainder. Taking measurements on this *mixed ensemble* of states with instrument S_z yields values for the measurements that have an identical distribution with that obtained from the pure ensemble.

Lets take the expectation value for the measurements. Keeping in mind that we are allowing for a mixed ensemble, the mean value of the measurements, with operator $\hat{A}$, is

$$<\hat{A}>=\sum_i p_i <\Psi_i|\hat{A}|\Psi_i> \tag{2}$$

where p_i is the probability for the system to be in state $|\Psi_i>$, and $<\Psi_i|\hat{A}|\Psi_i>$ is the expectation value for $\hat{A}$ when the system is in state $|\Psi_i>$. It is clear that Eq. (2) allows for both types of ensembles. A pure ensemble is the special case where all but one of the probabilities $p_i = 0$.

Getting back to the example in the first paragraph we get

$$<\hat{S}_z>=<\Psi|\hat{S}_z|\Psi>=0 \tag{3}$$

for the pure ensemble, and

$$< \hat{S}_z >= \frac{1}{2} < +|\hat{S}_z|+ > +\frac{1}{2} < -|\hat{S}_z|- >= 0 \tag{4}$$

for the mixed ensemble. Both pure and mixed ensembles give identical results for the expectation value of $\hat{S}_z$ so the question arises, if the two ensembles give identical results for the expectation value of $\hat{S}_z$, in what sense do they describe different physics? To find the answer lets calculate the expectation value of a different operator but using the same ensembles. Lets perform measurements using $\hat{S}_x$ when the system is described by the pure state $|\Psi>$. Thus,

$$< \hat{S}_z >=< \Psi|\hat{S}_z|\Psi >= \hbar/2 \tag{5}$$

where we used the matrix representation, in this basis, of $\hat{S}_z$ and the matrix representation of

$$|\Psi >= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{6}$$

to obtain this result. For the mixed ensemble

$$< \hat{S}_x >= \frac{1}{2} < +|\hat{S}_x|+ > +\frac{1}{2} < -|\hat{S}_x|- >= 0 \tag{7}$$

thus, for this measurement, we clearly see that the pure and mixed ensembles describe different physics.

In order to work with both pure and mixed ensembles, von Neumann introduced the concept of a density matrix. Lets define the density operator

$$\hat{\rho} \equiv \sum_i p_i|\Psi_i >< \Psi_i|$$
$$\sum_i p_i = 1 \tag{8}$$

which corresponds to a given ensemble

$$\{p_i, |\Psi_i >\}. \tag{9}$$

Consider an operator $\hat{A}$ which in Hilbert space is spanned by vectors

$$|v_i > \tag{10}$$

and can be written

$$\hat{A} = \sum_{mn} a_{mn}|v_m >< v_n|$$
$$a_{nm} =< v_n|A|v_m > \tag{11}$$

where a_{mn} are, by definition, the matrix elements of the matrix representation of $\hat{A}$ in this basis. Since $\hat{\rho}$ is an operator we can also rewrite

$$\rho = \sum_{mn} \rho_{mn}|v_m >< v_n| \tag{12}$$

Comparing with the definition of $\hat{\rho}$, we get

$$\rho_{mn} \equiv \sum_i p_i < v_m|\Psi_i >< \Psi_i|v_n > \tag{13}$$

Now

$$\hat{\rho}\hat{A} = \sum_k \rho_{mk} a_{kn}|v_m >< v_n| \tag{14}$$

and if we take the matrix elements of the matrix representation of operator $[\hat{\rho}\hat{A}]_{mn} = \sum_k \rho_{mk} a_{kn}$ we get

$$Trace[\sum_k \rho_{mk} a_{kn}] \equiv \sum_n \sum_k \rho_{nk} a_{kn} \tag{15}$$

Inserting the values for ρ_{nk} and a_{kn} into the expression above we obtain for the r.h.s of this expression

$$\sum_n \sum_k \sum_i p_i < v_n|\Psi_i >< \Psi_i|v_k >< v_k|A|v_n > \tag{16}$$

Using the completeness property $\sum_k |v_k >< v_k| = 1$, we get

$$\sum_n \sum_i p_i < v_n|\Psi_i >< \Psi_i|A|v_n > \; = \; \sum_n \sum_i p_i < \Psi_i|A|v_n >< v_n|\Psi_i >=$$
$$\sum_i p_i < \Psi_i|A|\Psi_i > \tag{17}$$

where we have, once again used completeness of the basis. Thus

$$Tr(\hat{\rho}\hat{A}) = \sum_i p_i < \Psi_i|A|\Psi_i >=< \hat{A} > . \tag{18}$$

The left hand side is short-hand notation for the trace of the matrix representation of $\hat{\rho}\hat{A}$. It is important to stress that the above result is independent of basis representation. So even though the density matrix depends on the choice of basis (representation) as does the matrix representation for $\hat{A}$, the ensemble average $Tr(\hat{\rho}\hat{A})$ does not.

Given a density matrix ρ (we shall use density operator and matrix interchangeably now, but in all practical calculations it is useful to express it as a matrix), how do we know if it describes a pure or mixed ensemble? We know that

$$\hat{\rho} = |\Psi_i >< \Psi_i| \tag{19}$$

for any normalized state $|\Psi_i>$is a pure state (why?). Then

$$\hat{\rho}^2 = |\Psi_i >< \Psi_i||\Psi_i >< \Psi_i| = |\Psi_i >< \Psi_i| = \hat{\rho} \tag{20}$$

Now for a pure state $\hat{\rho}_i$

$$[\hat{\rho}_i]_{mn} =< m|\Psi_i >< \Psi_i|n > \tag{21}$$

and thus

$$\begin{aligned} Tr[\hat{\rho}] &= \sum_m \rho_{mm} = \sum_m < m|\Psi_i >< \Psi_i|m > \\ &= \sum_m < \Psi_i|m >< m|\Psi_i >=< \Psi_i|\Psi_i >= 1 \end{aligned} \tag{22}$$

Therefore

$$Tr[\hat{\rho}^2] = Tr[\hat{\rho}] = 1 \tag{23}$$

We now consider the density matrix describing a mixed ensemble

$$\hat{\rho} = \sum_i p_i|\Psi_i >< \Psi_i| \tag{24}$$

we make a simplifying assumption that the states $|\Psi_i >$ are orthonormal, then

$$\hat{\rho}^2 \sum_i p_i^2|\Psi_i >< \Psi_i| = \sum_i p_i^2 \hat{\rho}_i \tag{25}$$

where we have made use of the fact that $< \Psi_j|\Psi_i >= \delta_{ij}$. Thus

$$Tr[\hat{\rho}^2] = \sum_i p_i^2 Tr[\hat{\rho}_i] = \sum_i p_i^2 \tag{26}$$

Since $\sum_i p_i = 1$ it follows

$$\sum_i p_i^2 < 1 \tag{27}$$

if more than one $p_i \neq 0$, or

$$Tr[\hat{\rho}^2] \leq 1. \tag{28}$$

The equality is satisfied if $\hat{\rho}$ describes a *pure ensemble* and the inequality follows if $\hat{\rho}$ describes a *mixed ensemble*. Since the $Tr[\hat{\rho}]$ is independent of representation the above inequality can be used to answer the question posed above. We proved relation (28) using ensembles created by orthogonal states, however the general result holds even if the $|\Psi_i >$ are not orthogonal.

One final note, suppose we want to construct a density matrix in which the system is found in state $|+>$, 25 % of the time and in state $|->$, 75 % of the time. Thus

$$\hat{\rho} = 1/4|+><+| + 3/4|-><-|. \tag{29}$$

Lets define the states

$$\begin{aligned} |a >&= \sqrt{1/4}|+> + \sqrt{3/4}\,|-> \\ |b >&= \sqrt{3/4}|+> - \sqrt{1/4}\,|-> \end{aligned} \tag{30}$$

and construct

$$\hat{\rho}' = 1/2|a><a| + 1/2|b><b| \tag{31}$$

which describes a density matrix in which the system has equal probability to be in states $|a>, |b>$. By substitution of $|a>, |b>$ into Eq. (31) we find that $\hat{\rho} = \hat{\rho}'$. So different mixed ensembles can lead to the same density matrix, or a density matrix may not define a unique mixed ensemble.