P4410 LECTURE 11

Properties of density matrix:

① Normalization condition is on trace:

$$tr(\hat{\rho}) = \sum_{j=1}^{N} \rho_{jj} = \sum_i w_i \sum_{j=1}^{N} \langle \alpha_j | i \rangle \langle i | \alpha_j \rangle$$

$$= \sum_i w_i \left[\sum_{j=1}^{N} \langle i | \alpha_j \rangle \langle \alpha_j | i \rangle \right]^*$$

$$= \sum_i w_i \left[\langle i | i \rangle \right]^*$$ But $|i\rangle$ is normalized.

$$= \sum_i w_i (1^*) = \sum_i w_i$$

$$\boxed{= 1.}$$

② Density matrix is Hermitian. This is easy to show:

$$\hat{\rho}^\dagger = \sum_i w_i^* \left(|i\rangle\langle i| \right)^\dagger$$

$$= \sum_i w_i^* |i\rangle\langle i|$$ but w_i are real, so

$$= \sum_i w_i^* |i\rangle\langle i|$$

$$= \hat{\rho} .$$

Density matrix for a coherent ensemble: One $w_i = 1$, all others are 0: $w_n = 1$, $w_{i \neq n} = 0$

so $\hat{\rho} = |n\rangle\langle n|$ ⟶ just the projection operator!

For this case, what is $\hat{\rho}^2$?

$$\hat{\rho}^2 = |n\rangle \underbrace{\langle n|n\rangle}_{1} \langle n| = \hat{\rho} \quad . \quad \longleftarrow \text{pure (coherent) ensembles only!}$$

How to calculate $P(A=a)$? (i.e. probability of measuring an eigenvalue)

For single system:

$$P(A=a) = |\langle a|\psi\rangle|^2 = \langle\psi|a\rangle\langle a|\psi\rangle = \langle\, |a\rangle\langle a|\,\rangle$$

So, for ensemble, prob. of finding $A=a$ for a random member of the ensemble is $\langle \overline{P(A=a)} \rangle$

$$= \langle\, \overline{|a\rangle\langle a|}\,\rangle$$

$$= tr\left(|a\rangle\langle a|\hat{\rho}\right)$$

Time evolution of ensembles.

Let's say $\hat{\rho}(t_0) = \sum_i w_i |i\rangle\langle i|$

If the ensemble isn't disturbed (i.e. by measurements, etc.) the w_i will be constant and time evolution will be confined to the $|i\rangle$ evolution; these obey the Schrödinger equation.

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = i\hbar \frac{\partial}{\partial t}\left[\sum_i w_i |i\rangle\langle i|\right]$$

$$= \sum_i w_i \left[i\hbar \left(\frac{\partial}{\partial t}|i\rangle\right)\langle i| + i\hbar |i\rangle \left(\frac{\partial}{\partial t}\langle i|\right) \right]$$

$$= \sum_i w_i \left[\hat{H}|i\rangle\langle i| - |i\rangle\langle i|\hat{H} \right]$$

so $$i\hbar \frac{\partial \hat{\rho}}{\partial t} = -[\hat{\rho}, \hat{H}] .$$

Some examples of density matrices:

① A beam of polarized electrons in the z direction:

$$\hat{\rho} = |+\rangle\langle +| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

② A beam of polarized electrons in the X direction:

$$\hat{\rho} = |+_x\rangle\langle +_x| = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

③ An unpolarized beam (equal mixture of $|+\rangle$ and $|-\rangle$):

$$\hat{\rho} = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| = \frac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

④ Is this a pure or mixed (coherent or incoherent) ensemble?

$$\hat{\rho} = \begin{pmatrix} \frac{1}{4} & \frac{-i\sqrt{3}}{4} \\ \frac{i\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix}$$

What is $\hat{\rho}^2$? $$\begin{pmatrix} \frac{1}{4} & \frac{-i\sqrt{3}}{4} \\ \frac{i\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix}\begin{pmatrix} \frac{1}{4} & \frac{-i\sqrt{3}}{4} \\ \frac{i\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{16}+\frac{3}{16} & \frac{-i\sqrt{3}}{16} \frac{-3i\sqrt{3}}{16} \\ \frac{i\sqrt{3}}{16}+\frac{3i\sqrt{3}}{16} & \frac{3}{16}+\frac{9}{16} \end{pmatrix} = \begin{pmatrix} & \\ & \end{pmatrix} = \hat{\rho}$$

turns out $\sqrt{\frac{1}{4}}|+\rangle + i\sqrt{\frac{3}{4}}|-\rangle$.

Continuum generalization: $\cancel{\hat{\rho} = \sum_i w_i |\psi\rangle\langle\psi|}$ ~~(still!)~~

$$\langle \bar{A} \rangle = \int dx' \int dx'' \, \langle x''|\hat{\rho}|x'\rangle \langle x'|\hat{A}|x''\rangle$$

where $$\langle x''|\hat{\rho}|x'\rangle = \langle x''|\left(\sum_i w_i |i\rangle\langle i|\right)|x'\rangle$$

$$= \sum_i w_i \, \psi_i(x'')\psi_i^*(x')$$