lecture 23 II

If $|\psi\rangle$ is indeterminate then we an ensemble of replicas of the states $|\psi\rangle$ of the ensemble systems are distributed with probability P_ψ then [a fraction of the members in the ensemble is characterized by the $|\psi\rangle$ with prob. P_ψ]

$$\hat{\rho} = \sum_\psi P_\psi |\psi\rangle\langle\psi| \quad \nearrow \text{projection representation}$$

[$\hat{\rho}$ is a mixture of the states $|\psi\rangle$ with probability P_ψ]

with $\sum_\psi P_\psi = 1$

$$T_r\{\hat{\rho}\} = \sum_\psi P_\psi T_r\{|\psi\rangle\langle\psi|\} = \sum_\psi P_\psi = 1$$

$$\langle\hat{A}\rangle = T_r\{\hat{\rho}\hat{A}\} = \sum_\psi P_\psi \langle\psi|\hat{\rho}\hat{A}|\psi\rangle =$$

$$= \sum_\psi P_\psi \langle\psi|\hat{A}|\psi\rangle$$

Example

an electron beam generated at a cathode has an isotropic distribution of spins

$$\langle S_x\rangle = \langle S_y\rangle = \langle S_z\rangle = 0$$

Find the density matrix with this property which makes $\hat{S}_z$ diagonal

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$\hat{S}_y = \frac{i\hbar}{2}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$$

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

The probability of finding S_z" with values $\pm\frac{\hbar}{2}$ is $\frac{1}{2}$.

recall $\rho_{nn} = |\langle\psi|n\rangle|^2 = c_n^* c_n = P_n$

which implies that the diagonal elements of $\hat{\rho}$ are $\frac{1}{2}$

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

$$\langle S_z\rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{S}_z\} = \frac{\hbar}{4}\,\mathrm{Tr}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = 0$$

same for $\langle S_y\rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{S}_y\} = 0 = \langle S_x\rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{S}_x\}$

S_z is diagonal with states

$$|\alpha\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|\beta\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\hat{\rho} = \frac{1}{2} |\alpha\rangle\langle\alpha| + \frac{1}{2} |\beta\rangle\langle\beta|$$

$$\langle S_x\rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{S}_x\} = \langle\alpha|\hat{\rho}\,\hat{S}_x|\alpha\rangle + \langle\beta|\hat{\rho}\,\hat{S}_x|\beta\rangle =$$

$$= \frac{1}{2}\langle\alpha|\hat{S}_x|\alpha\rangle + \frac{1}{2}\langle\beta|\hat{S}_x|\beta\rangle =$$

$$= \frac{\hbar}{4}\left[(1\ 0)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + (0\ 1)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right] = 0$$

Pure ensembles

$$P_{\psi_i} = 1 \quad P_{\psi_j} = 0 \quad \forall j \neq i$$

$$\hat{\rho} = |\psi_i\rangle\langle\psi_i|$$

$$(\hat{\rho})^2 = |\psi_i\rangle\langle\psi_i|\psi_i\rangle\langle\psi_i\rangle = |\psi_i\rangle\langle\psi_i| = \hat{\rho}$$

$$(\hat{\rho})^2 = \hat{\rho} \Rightarrow \hat{\rho}(\hat{\rho} - 1) = 0$$

$$\mathrm{Tr}(\hat{\rho}^2) = \mathrm{Tr}(\hat{\rho}) = 1$$

The eigenvalues of the density operator for a pure ensemble are zero or one.

when diagonalized $\rho = \begin{pmatrix} 0 & & & & & & & \hat{0} & \\ & 0 & & & & & & & \\ & & 0 & & & & & & \\ & & & 1 & & & & & \\ & & & & 0 & & & & \\ & \hat{0} & & & & 0 & & & \\ & & & & & & 0 & & \\ & & & & & & & 0 & \\ & & & & & & & & 0 \end{pmatrix}$

It can be proven that for a mixed ensemble $\mathrm{Tr}\{\hat{\rho}^2\} < 1$.