Phys 5701 27 Oct 2020

Today: Density Operator Formalism

[Another "Excursion"]

"Ensemble": Pure or Mixed

$$|\alpha\rangle = e^{-i\alpha/2}\cos(\beta/2)\,|+\rangle + e^{+i\alpha/2}\sin(\beta/2)\,|-\rangle$$

Definite Spin.

"Weights" w_i specify mixed ensembles.

e.g. 50% in $|+\rangle$ and 50% in $|S_x;+\rangle$

$w_1 = 0.5$ $|\alpha^{(1)}\rangle$ $w_2 = 0.5$ $|\alpha^{(2)}\rangle$

Weights w_i are positive real numbers with $\sum_i w_i = 1$

$\Rightarrow$ For some observable A, define "Ensemble Average"

$$\boxed{[A] \equiv \sum_i w_i \langle\alpha^{(i)}|A|\alpha^{(i)}\rangle}$$

Expand $|\alpha^{(i)}\rangle$ in eigenstates of A

$$|\alpha^{(i)}\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha^{(i)}\rangle$$

$$[A] = \sum_i w_i \sum_{a'} \langle\alpha^{(i)}|A|a'\rangle\langle a'|\alpha^{(i)}\rangle$$

$$= \sum_i \sum_{a'} w_i a' |\langle a'|\alpha^{(i)}\rangle|^2$$

Now expand in basis $|b'\rangle$ of B

$$[A] = \sum_i w_i \sum_{b'} \sum_{b''} \langle\alpha^{(i)}|b'\rangle\langle b'|A|b''\rangle\langle b''|\alpha^{(i)}\rangle$$

$$= \sum_{b'} \sum_{b''} \Big[\underbrace{\sum_i w_i \langle b''|\alpha^{(i)}\rangle\langle\alpha^{(i)}|b'\rangle}\Big] \langle b'|A|b''\rangle$$

Define $\rho \equiv \sum_i w_i |\alpha^{(i)}\rangle\langle\alpha^{(i)}|$ Hermitian

$$\langle b''|\rho|b'\rangle = \sum_i w_i \langle b''|\alpha^{(i)}\rangle\langle\alpha^{(i)}|b'\rangle$$

$$\therefore [A] = \sum_{b'} \sum_{b''} \langle b''|\rho|b'\rangle\langle b'|A|b''\rangle$$

$$= \sum_{b''} \langle b'' | \rho A | b'' \rangle$$

$$\boxed{[A] = \mathrm{Tr}(\rho A)}$$

NOTE: $\mathrm{Tr}(\rho) = \sum_{b'} \langle b' | \rho | b' \rangle$

$$= \sum_{b'} \sum_{i} w_i \langle b' | \alpha^{(i)} \rangle \langle \alpha^{(i)} | b' \rangle$$

$$= \sum_{i} \sum_{b'} w_i \langle \alpha^{(i)} | b' \rangle \langle b' | \alpha^{(i)} \rangle$$

$$= \sum_{i} w_i \underbrace{\langle \alpha^{(i)} | \alpha^{(i)} \rangle}_{=1}$$

$$= \sum_{i} w_i = 1$$

i.e. $\boxed{\mathrm{Tr}(\rho) = 1}$

Pure Ensembles

$w_i = 1$ for $i = n$

$\Rightarrow \rho = |\alpha^{(n)}\rangle\langle\alpha^{(n)}|$

$\Rightarrow \rho^2 = |\alpha^{(n)}\rangle \underbrace{\langle\alpha^{(n)}|\alpha^{(n)}\rangle}\langle\alpha^{(n)}|$

$= |\alpha^{(n)}\rangle\langle\alpha^{(n)}| = \rho$

$\Rightarrow \boxed{\rho(\rho-1) = 0}$ i.e. $\rho^2 = \rho$ & $\mathrm{Tr}(\rho^2) = 1$

For Pure Ensembles

BTW: HW Prob 3.11 Prove $0 \leq \mathrm{Tr}(\rho^2) \leq 1$

For matrix of ρ in " basis $\rho|\rho'\rangle = \rho'|\rho'\rangle$

$\langle\rho'''|\rho(\rho-1)|\rho''\rangle = 0$ Pure Ensembles

$= \sum_{\rho'} \langle\rho'''|\rho|\rho'\rangle\langle\rho'|(\rho-1)|\rho''\rangle$

$= \sum_{\rho'} \rho'\langle\rho'''|\rho'\rangle(\rho''-1)\langle\rho'|\rho''\rangle$

$= \rho''\langle\rho'''|\rho''\rangle(\rho''-1) = \rho''(\rho''-1)\,\delta_{\rho'',\rho'''}$

Diagonal! $\Rightarrow \rho'' = 0$

or $\rho'' = 1$

$$\begin{bmatrix} 0 & & & & 0 \\ & 0 & & & \\ & & 1 & & \\ & & & 0 & \\ 0 & & & & 0 \end{bmatrix}$$

Examples with Spin-1/2

1) 100% polarized in S_z+ state

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

Right!! $\rho|+\rangle = +|+\rangle$ $\qquad Tr = 1$

2) 100% polarized in $S_x\pm$ state

$$\rho = |S_x;\pm\rangle\langle S_x;\pm|$$

$$= \frac{1}{\sqrt{2}}\left[|+\rangle \pm |-\rangle\right]\frac{1}{\sqrt{2}}\left[\langle+| \pm \langle-|\right]$$

$$= \frac{1}{2}\left[|+\rangle\langle+| \pm |+\rangle\langle-| \pm |-\rangle\langle+| + |-\rangle\langle-|\right]$$

$$\doteq \begin{pmatrix}1/2 & \pm 1/2\\ \pm 1/2 & 1/2\end{pmatrix} \qquad Tr\,\rho = 1 = \frac{1}{2}+\frac{1}{2}$$

$$\rho^2 \doteq \begin{pmatrix}1/2 & \pm 1/2\\ \pm 1/2 & 1/2\end{pmatrix}\begin{pmatrix}1/2 & \pm 1/2\\ \pm 1/2 & 1/2\end{pmatrix} = \begin{pmatrix}1/2 & \pm 1/2\\ \pm 1/2 & 1/2\end{pmatrix} \doteq \rho$$

Both (1) & (2) are pure ensembles!

3) "Unpolarized beam" Mixed ensemble

$$\rho = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-|$$

$$\doteq \boxed{\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}} = \boxed{\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}$$

$\mathrm{Tr}\,\rho = 1 \qquad \rho^2 \neq \rho\,!! \qquad \underline{\underline{\mathrm{Tr}\,\rho^2 = 1/2}}$

$$= \frac{1}{2}\underline{\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}} + \frac{1}{2}\underline{\begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}}$$

$$\doteq \frac{1}{2}|S_x;+\rangle\langle S_x;+| + \frac{1}{2}|S_x;-\rangle\langle S_x;-|$$

What is the ensemble average of S_i $i=x,y,z$

$$[S_i] = \mathrm{Tr}(\rho S_i)$$

$$= \mathrm{Tr}\left[\frac{1}{2}\mathbb{1}\frac{\hbar}{2}\sigma_i\right]$$

$$= \frac{\hbar}{4}\mathrm{Tr}\,\sigma_i = 0 \quad \text{Right!}$$

4) Partial Polarization

75% S_z+ , 25% S_x+

$$\rho \doteq \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} = \begin{pmatrix} 7/8 & 1/8 \\ 1/8 & 1/8 \end{pmatrix}$$

$$[S_z] = Tr\begin{pmatrix} 7/8 & 1/8 \\ 1/8 & 1/8 \end{pmatrix}\begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix}$$

$$= Tr\begin{pmatrix} 7\hbar/16 & - \\ - & -\hbar/16 \end{pmatrix} = \frac{3\hbar}{8}$$

$$[S_x] = Tr\begin{pmatrix} \hbar/16 & - \\ - & \hbar/16 \end{pmatrix} = \frac{\hbar}{8}$$

$$[S_y] = Tr\begin{pmatrix} 7/8 & 1/8 \\ 1/8 & 1/8 \end{pmatrix}\begin{pmatrix} 0 & -i\hbar/2 \\ i\hbar/2 & 0 \end{pmatrix}$$

$$= Tr\begin{pmatrix} i\hbar/16 & -7i\hbar/16 \\ i\hbar/16 & -i\hbar/16 \end{pmatrix} = 0$$

Time Evolution

$$\rho(t=t_0) = \sum_i w_i \, |\alpha^{(i)}\rangle\langle\alpha^{(i)}|$$

$$i\hbar\frac{\partial}{\partial t}|\alpha^{(i)}, t_0; t\rangle = H\,|\alpha^{(i)}, t_0; t\rangle$$

$$-i\hbar\frac{\partial}{\partial t}\langle\alpha^{(i)}, t_0; t| = \langle\alpha^{(i)}, t_0; t|\,H$$

$$\Rightarrow i\hbar \frac{\partial \rho}{\partial t} = \sum_i w_i \Big[H |\alpha^{(i)}, t_0; t\rangle \langle \alpha^{(i)}, t_0; t|$$
$$- |\alpha^{(i)}, t_0; t\rangle \langle \alpha^{(i)}, t_0; t| H \Big]$$
$$= H\rho - \rho H = -[\rho, H]$$

But $i\hbar \frac{\partial A}{\partial t} = +[A, H]$ "ρ Has wrong sign!"

But "same" as Liouville's theorem
in classical Statistical Mechanics!

Quantum Statistical Mechanics (?)

$$\rho^{\text{Pure}} \doteq \begin{bmatrix} 0 & & & & 0 \\ & 0 & & & \\ & & \ddots & & \\ & & & 1 & \\ 0 & & & & \ddots \; 0 \end{bmatrix} \qquad \rho^{\text{Random}} \doteq \begin{bmatrix} 1/N & & & 0 \\ & 1/N & & \\ & & \ddots & \\ 0 & & & 1/N \end{bmatrix}$$

$$\sigma \equiv -\mathrm{Tr}(\rho \log \rho) = -\sum_i \rho_{ii}^{\text{Diag}} \log \rho_{ii}^{\text{Diag}}$$

≥ 0 in general

$= 0$ for pure ensemble

$$= -N \frac{1}{N} \log \frac{1}{N} = \log N \quad \text{random ensemble}$$

$= \max$ value!

"Entropy" $S = k\sigma$ in QM!!