PHYS 414: 4-17-20

Ensemble:

$$\underbrace{|\psi_1\rangle\ |\psi_1\rangle\ |\psi_1\rangle}_{p_1}\quad \underbrace{|\psi_2\rangle\ |\psi_2\rangle}_{p_2}\quad \underbrace{|\psi_3\rangle}_{p_3}\ \cdots$$

$A \Rightarrow$ measurements on ensemble

mean result $\langle A\rangle = \sum_{n,a} a\, p_n |\langle a|\psi_n\rangle|^2$

$\hat{A}|a\rangle = a|a\rangle$

$$= \sum_{n,a} p_n \langle a|\psi_n\rangle\langle\psi_n|\hat{A}|a\rangle$$

$$= \sum_a \langle a| \underbrace{\left[\sum_n p_n |\psi_n\rangle\langle\psi_n|\right]}_{\equiv\ \hat{\rho}} \hat{A}|a\rangle$$

$\equiv \hat{\rho}$ density operator for our quantum ensemble

$$\boxed{\hat{\rho} = \sum_n p_n |\psi_n\rangle\langle\psi_n|}$$

$$= \sum_a \langle a|\hat{\rho}\hat{A}|a\rangle$$

$$= tr(\hat{\rho}\hat{A})$$

example:

two states: $|0\rangle, |1\rangle$

50% of ens. — 50% of ens.

$$\hat{\rho} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

one state: $|1\rangle$

100%

$$\hat{\rho} = |1\rangle\langle 1|$$

Show eventually:

operator $\hat{\rho}$ encodes all info about ensemble + plays the analogue of classical prob. $\vec{p}$

Note: trace is indep. of basis

$$\mathrm{tr}(\hat{\rho}\hat{A}) = \sum_a \langle a|\hat{\rho}\hat{A}|a\rangle$$

$$= \sum_m \langle m|\hat{\rho}\hat{A}|m\rangle$$ for another basis $\{|m\rangle\}$

$$\sum_m \langle m|\hat{\rho}\hat{A}|m\rangle$$

$$= \sum_{m,a} \langle m|\hat{\rho}\hat{A}|a\rangle\langle a|m\rangle$$

$$= \sum_{m,a} \langle a|m\rangle\langle m|\hat{\rho}\hat{A}|a\rangle$$

$$= \sum_a \langle a|\hat{\rho}\hat{A}|a\rangle$$

Properties of $\hat{\rho}$:

i) $$\mathrm{tr}(\hat{\rho}) = \sum_m \langle m|\hat{\rho}|m\rangle \qquad \{|m\rangle\} \text{ basis}$$

$$= \sum_{m,n} p_n \langle m|\psi_n\rangle\langle\psi_n|m\rangle$$

$|\psi_n\rangle$ are individually norm. (not necessarily forming an orthon. basis)

$$= \sum_{m,n} p_n \langle\psi_n|m\rangle\langle m|\psi_n\rangle$$

$$= \sum_n p_n \underbrace{\langle\psi_n|\psi_n\rangle}_{1} = \underline{\underline{1}}$$

ii) $\hat{\rho}^\dagger = \hat{\rho} \Rightarrow$ Hermitian

$$\hat{\rho}^\dagger = \Big[\sum_n \underset{\substack{\downarrow \\ \text{real}}}{p_n} |\psi_n\rangle\langle\psi_n|\Big]^\dagger = \hat{\rho}$$

$\Rightarrow$ the e-states of $\hat{\rho}$ form a complete basis where $\hat{\rho}$ is diagonal in matrix form

iii) for a <u>pure ensemble</u> (one state in ensemble)

$$\hat{\rho} = |\psi_1\rangle\langle\psi_1|$$

$$\hat{\rho}^2 = |\psi_1\rangle\underbrace{\langle\psi_1|\psi_1\rangle}_{1}\langle\psi_1| = |\psi_1\rangle\langle\psi_1| = \hat{\rho}$$

$\hat{\rho}^2 = \hat{\rho}$ is <u>only</u> valid in a pure ensemble

Anytime this is violated we have a <u>mixed ensemble</u> (more than one state in ensemble)

Proof: let's choose a basis $\{|m\rangle\}$ where $\hat{\rho}$ is diagonal

$$\hat{\rho}^2 = \hat{\rho} \iff \rho_{mm}^2 = \rho_{mm} \text{ for all } m$$

$$\rho_{mm} = 0 \text{ or } 1$$

but since $\sum \rho_{mm} = 1$ $(\mathrm{tr}\,\hat{\rho} = 1)$

$\Rightarrow$ only element $\rho_{mm} = 1$

$$\hat{\rho} = \begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & 1 & & \\ & & & 0 & \\ & & & & 0 \\ & & & & & \ddots \end{pmatrix}$$ in diag. basis

Example: $\hat{\rho} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ in some basis $\{|0\rangle, |1\rangle\}$

since $\hat{\rho}^2 = \hat{\rho}$ $\Rightarrow$ this indeed a pure ensemble

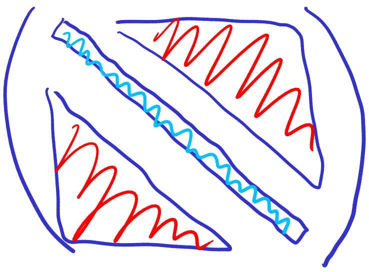
$$\hat{\rho} = |\psi_1\rangle\langle\psi_1| \quad \text{where } |\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$= \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right)\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right)$$

$$= \frac{1}{2}\left(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|\right)$$

matrix repr: $\hat{\rho} = \sum_{m,n} \underbrace{\rho_{mn}}_{\text{elements of } \hat{\rho} \text{ matrix in this basis}} |m\rangle\langle n|$

some repr. of $\hat{\rho}$ in a basis:

$\hat{\rho} =$ 

note: these are basis-dependent

diag elements:

$\rho_{mm} = \langle m|\hat{\rho}|m\rangle$

= "populations"

off-diag elements

$\rho_{mm'} = \langle m|\hat{\rho}|m'\rangle$

$m \neq m'$ = "coherences"

Example: $\hat{\rho} = |\psi_1\rangle\langle\psi_1|$

$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$

$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

$\{|\psi_i\rangle\}$ basis

$$\hat{\rho} = \begin{array}{c c} & \begin{array}{cc} \psi_1 & \psi_2 \end{array} \\ \begin{array}{c} \psi_1 \\ \psi_2 \end{array} & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{array}$$

$\langle\psi_1|\psi_2\rangle = 0 \qquad \langle\psi_i|\psi_i\rangle = 1$

basis where $\hat{\rho}$ is diag.

$\rho_{mn} = \langle m|\hat{\rho}|n\rangle$

$\rho_{11} = \langle\psi_1|\hat{\rho}|\psi_1\rangle = \langle\psi_1|\psi_1\rangle\langle\psi_1|\psi_1\rangle = 1$

$\{|0\rangle, |1\rangle\}$ basis

$$\hat{\rho} = \begin{array}{c c} & \begin{array}{cc} |0\rangle & |1\rangle \end{array} \\ \begin{array}{c} \langle 0| \\ \langle 1| \end{array} & \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \end{array}$$

$\langle 0|\hat{\rho}|0\rangle$

$= \langle 0|\psi_1\rangle\langle\psi_1|0\rangle$

$= \frac{1}{2}\langle 0|\Big[(|0\rangle + |1\rangle)(\langle 0| + \langle 1|)\Big] \cdot |0\rangle$

$= \frac{1}{2}$

Decoherence: over time, all $\rho_{mm'}$ (off-diag.) $\to 0$ in a certain basis due to physical interactions w/ outside environment

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Another example: 2 level system (qubit)

basis: $\{ |0\rangle, |1\rangle \}$

basis: $\{ |\psi_1\rangle, |\psi_2\rangle \}$

ensemble was a 50%/50% mix. of $|0\rangle$, $|1\rangle$

oper. form $\quad \hat{\rho} = \frac{1}{2} |0\rangle\langle 0| + \frac{1}{2} |1\rangle\langle 1| \qquad \hat{\rho} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$

matrix repr. $\quad \underset{\text{basis}}{\underset{\{|0\rangle, |1\rangle\}}{\hat{\rho}}} \to \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \qquad \underset{\text{basis}}{\underset{\{|\psi_1\rangle, |\psi_2\rangle\}}{\hat{\rho}}} \to \begin{pmatrix} \frac{1}{2} & \\ & \end{pmatrix}$

$$\langle \psi_1 | \hat{\rho} | \psi_1 \rangle$$

$$= \frac{1}{2} \left[\langle 0| + \langle 1| \right] \hat{\rho} \left[|0\rangle + |1\rangle \right]$$

$$= \frac{1}{4} \Big(\left[\langle 0| + \langle 1| \right] \left[|0\rangle\langle 0| + |1\rangle\langle 1| \right] \cdot \left[|0\rangle + |1\rangle \right] \Big)$$

$$= \frac{1}{4} \left(\langle 0|0\rangle\langle 0|0\rangle + \langle 1|1\rangle\langle 1|1\rangle \right)$$

$$= \frac{1}{4} (1 + 1) = \frac{1}{2}$$