ensemble: $\{\, |\psi_n\rangle$ w/ frac. $p_n \}$ $\quad \sum_n p_n = 1$

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

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

ensemble avg

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

change of basis $\quad |b\rangle = \hat{U}|a\rangle \quad \hat{U}\hat{U}^{+} = \hat{U}^{+}\hat{U} = \hat{I}$

$$\sum_b \langle b|\hat{\rho}\hat{A}|b\rangle = \sum_a \langle a|\hat{U}^{+}\hat{A}\hat{U}|a\rangle$$

$$= tr(\hat{U}^{+}\hat{A}\hat{U})$$

$$= tr(\hat{U}\hat{U}^{+}\hat{A})$$

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

example: i) $\quad$ ensemble: $|0\rangle \quad |1\rangle$

prob: $0.5 \quad 0.5$

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

2D Hilbert space w/ basis $\{|0\rangle, |1\rangle\}$

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

any operator $\quad \hat{\rho} = \sum_{i,j} c_{ij} |i\rangle\langle j| \quad$ c_{ij} comp's of a matrix C

$\{|i\rangle\}$ $\quad c_{ij} = \langle i|\hat{\rho}|j\rangle$

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

$$= \frac{1}{2}\underbrace{\langle 0|0\rangle}_{1}\underbrace{\langle 0|0\rangle}_{1} + \frac{1}{2}\overset{0}{\langle 0|1\rangle}\overset{0}{\langle 1|0\rangle} = \frac{1}{2}$$

ii) ensemble: $\quad |1\rangle$

prob: $\quad 1$

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

properties of $\hat{\rho}$:

i) $\mathrm{tr}(\hat{\rho}) = 1$ $\qquad$ $\{|m\rangle\}$ any basis

proof: $\quad \mathrm{tr}(\hat{\rho}) = \sum_m \langle m|\hat{\rho}|m\rangle$

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

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

$$= \sum_n \langle\psi_n|\psi_n\rangle p_n = \sum_n p_n$$

$$= 1$$

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

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

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

consequence: e-states of $\hat{\rho}$ form a complete basis where $\hat{\rho}$ is diagonal

iii) define pure ensemble:

frac	state
1	$\|\psi_1\rangle$

only one state

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

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

$\hat{\rho}^2 = \hat{\rho}$ iff ensemble is pure: useful test

$\hat{\rho}^2 = \hat{\rho} \Rightarrow$ choose basis where $\hat{\rho}$ is diag.

diag. elements

$$\rho^2_{mm} = \rho_{mm} \quad \text{for all } m$$

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

$$\mathrm{tr}(\hat{\rho}) = 1 \Rightarrow \sum_m \rho_{mm} = 1$$

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

must be pure ensemble

iv) $\mathrm{tr}(\hat{\rho}\hat{A}) = \langle A \rangle$

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

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

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

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

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

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

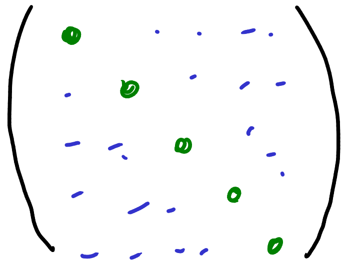
$$= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$ in $\{|0\rangle, |1\rangle\}$ basis

check: $\hat{\rho}^2 = \hat{\rho}$ ✓ pure state

$$= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$ in $\{|\psi_1\rangle, |\psi_2\rangle\}$ basis

definitions: $\hat{\rho}$ in a basis $\{|m\rangle\}$

$$\hat{\rho} = \sum_k p_k |\psi_k\rangle\langle\psi_k| =$$



diag. elements:

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

= "populations"

$\sim$ classical prob. $\rho_{mm} \geq 0$

$$\sum_m \rho_{mm} = 1$$

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

$$= \sum_k p_k \langle m|\psi_k\rangle\langle\psi_k|m\rangle$$

$$= \sum_k \underbrace{p_k}_{\geq 0} \underbrace{|\langle m|\psi_k\rangle|^2}_{\geq 0} \geq 0$$

off-diag elements: $\rho_{mn} = \langle m|\hat{\rho}|n\rangle \quad m \neq n$

= "coherences"

arise when states in ensemble are superpositions of basis states

preview: decoherence: as system interacts w/ env. over time $\rho_{mn} \to 0$ for $m \neq n$ in a particular basis

Summary comparing quantum + classical:

quantum

Hamilt.

energy eigenstates

qu. states $|i\rangle$

$\hat{H}|i\rangle = E_i |i\rangle$

$$\langle H\rangle = \mathrm{tr}(\hat{\rho}\hat{H})$$
$$= \sum_i \langle i|\hat{\rho}\hat{H}|i\rangle$$
$$= \sum_i E_i \langle i|\hat{\rho}|i\rangle$$
$$= \sum_i E_i \rho_{ii}$$

classical

States i

state energies E_i

mean energy

$$E = \sum_i p_i E_i$$

look very similar