ensemble: $\{ |\psi_n\rangle$ w/ frac. $p_n \}$

$$\Downarrow$$

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

e-vecs of $\hat{A}$

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

avg. in ensemble $= \mathrm{tr}(\hat{\rho}\hat{A})$

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

prob: 0.5 0.5

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

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

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

(i,j) comp. of matrix

$$\hat{\rho} = \sum_{ij} C_{ij} |i\rangle\langle j|$$

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

ii) ensemble: $|1\rangle$

prob: 1

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

properties of $\hat{\rho}$:

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

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

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

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

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

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

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

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

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

iii) define <u>pure ensemble</u>: only one state

frac	state
1	$\lvert\psi_1\rangle$

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

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

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

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

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

$\rho_{mm} = 0$ or 1

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

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

must be pure ensemble

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

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

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

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

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

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

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

check: $\hat{\rho}^2 = \hat{\rho}$ ✓

pure state

$$\langle i | j \rangle = \delta_{ij}$$

$$\hat{O} = |i\rangle\langle j| \qquad \hat{O}|k\rangle = |i\rangle\langle j|k\rangle = \delta_{jk}|i\rangle$$

$$\hat{A} = \sum_{i,j} a_{ij} |i\rangle\langle j|$$

$$= \begin{array}{cc} & j \\ i & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & a_{ij} & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \end{array}$$

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

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

$$= \begin{pmatrix} \bullet & \cdot & \cdot & \cdot & \cdot \\ \cdot & \bullet & \cdot & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \cdot & \bullet & \cdot \\ \cdot & \cdot & \cdot & \cdot & \bullet \end{pmatrix}$$

diag. elements:

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

= "populations"

~ class. probabilities

$\sum_m \rho_{mm} = 1$

clue: ensemble was prepared w/ superpositions of your basis states

off-diag elements:

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

= "coherences"

decoherence : as system interacts w/ env. over time $\rho_{mn} \rightarrow 0$ for $m \neq n$

↓ (we will develop theory for this!)

in a certain basis!

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

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

$\sum_m \rho_{mm} = 1$ ≥ 0

$\Rightarrow$ ρ_{mm} looks like class. prob.

will show: as decoherence occurs

quantum dynamics $\Rightarrow$ classical master equation

Hamilt. ↓ quantum	classical
$\hat{H}\,|i\rangle = E_i\,|i\rangle$	state energies: E_i
$\langle H\rangle = \mathrm{tr}(\hat{\rho}\hat{H})$	mean energy
$= \sum_i \langle i|\hat{\rho}\hat{H}|i\rangle$	$E = \sum_i p_i E_i$
$= \sum_i E_i \langle i|\hat{\rho}|i\rangle$	
$= \sum_i \rho_{ii} E_i$	look very similar!

complication: usually an infinite # of ways to prepare an ensemble that give you the same operator $\hat{\rho}$

$\Rightarrow$ "decompositions" of $\hat{\rho}$

example: ensemble A

frac	state
p	$\|0\rangle$
$1-p$	$\|1\rangle$

$$\Rightarrow \quad \hat{\rho} = p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1|$$

ensemble B

frac	state
$\frac{1}{2}$	$\|u\rangle$
$\frac{1}{2}$	$\|v\rangle$

$$|u\rangle = \sqrt{p}\,|0\rangle + \sqrt{1-p}\,|1\rangle$$
$$|v\rangle = \sqrt{p}\,|0\rangle - \sqrt{1-p}\,|1\rangle$$

$$\hat{\rho} = \frac{1}{2}|u\rangle\langle u| + \frac{1}{2}|v\rangle\langle v|$$
$$= p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1|$$

same as ensemble A

$\Rightarrow$ no way to distinguish these two ensembles by any physical measurements, b/c $tr(\hat{\rho}\hat{A})$ is the same for both for any observable A

$\Rightarrow$ in quantum stat. mech we have to build a dynamical <u>theory</u> for $\hat{\rho}$ (fundamental quantity) rather than probabilities

preview: in classical stat. mech

entropy $S(t) = -k_B \sum_n p_n(t) \ln p_n(t)$

how do we define this in QM, if probabilities depend on decomposition?