Complications: usually an ∞ number of ways to prepare an ensemble that gives you the same $\hat{\rho}$

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

example: ensemble A

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

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

ensemble B

frac	state
$1/2$	$\|u\rangle$
$1/2$	$\|v\rangle$

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

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

$$= \text{algebra} = p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1|$$

same $\hat{\rho}$ as ensemble A

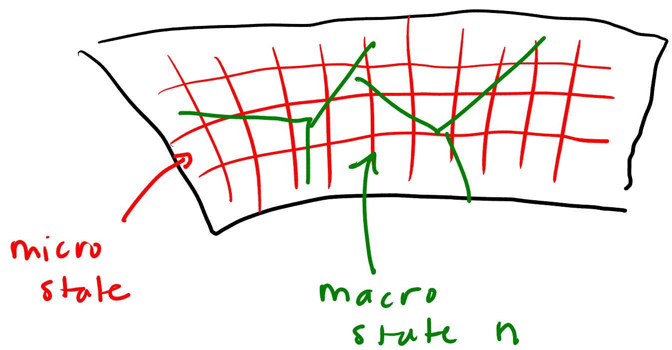
ensembles A & B are two decomp's of $\hat{\rho}$

$\Rightarrow$ there is no way to distinguish these two ensembles by any physical ensemble avg's b/c $\mathrm{tr}(\hat{\rho}\hat{A}) = \langle A \rangle$ is the same for all observables A

In quantum stat. mech we have to build our dynamical theory for $\hat{\rho}$ (fund. quantity) rather than (non-unique) ensemble probabilities

How do we define entropy?

classical recap:



tot = sys + env

Surface w/ const. energy E_{tot}

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

prob. of n at time t

problem: in quantum how to assign entropy to a $\hat{\rho}$?

Von Neumann solution: choose one special decomp $\Rightarrow$ orthonormal decomp. (OD)

$\hat{\rho}$ is Hermitian $\Rightarrow$ complete orthon. basis of e-states of $\hat{\rho}$

$\{|\phi_n\rangle\}$

$\hat{\rho}|\phi_n\rangle = \lambda_n|\phi_n\rangle$

in that basis $\hat{\rho}$ is diagonal:

$$\hat{\rho} = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_N \end{pmatrix}$$

proved last time: $\lambda_i \geq 0 \quad \sum_{i=1}^{N} \lambda_i = 1$

the λ_i look like classical probabilities

$$= \sum_n \lambda_n |\phi_n\rangle\langle\phi_n|$$

interpret these as ensemble fractions: $p_n \equiv \lambda_n$

von Neumann entropy: $S(\hat{\rho}) = -\sum_n p_n \ln p_n$

note: k_B usually left out

e-vals of $\hat{\rho}$

to calculate: i) find $\hat{\rho}$

ii) find e-vals of $\hat{\rho} \Rightarrow \lambda_n = p_n$

iii) calculate $S(\hat{\rho})$

motivation: $|\phi_n\rangle$ are distinguishable:

a measurement that us we are in $|\phi_n\rangle \Rightarrow$ all subsequent measurements cannot give $|\phi_m\rangle$ $m \neq n$

because $\langle \phi_n | \phi_m \rangle = \delta_{nm}$

example: ensemble

frac.	state
1	$\|\psi\rangle = \frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)$

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

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

diagonalize: e-vals $1, 0$

$$S(\hat{\rho}) = -1 \ln 1 - 0 \ln 0$$

$$= 0$$ (will be true for any pure state)

Time evolution of $\hat{\rho}(t)$:

Simplest case: isolated system (no interactions w/ outside) described by Hamiltonian $\hat{H}(t)$

closed quantum system

wavefunction $|\psi(t)\rangle$: $\quad i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle$

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$$

unitary operator: propagator

$$\hat{U}^{+}(t)\,\hat{U}(t) = \hat{U}(t)\,\hat{U}^{+}(t) = \hat{I}$$

Special case: $\hat{H}(t) = \hat{H}$ $\Rightarrow$ $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$

time-indep.

ensemble: focus on OD ensemble

$t=0$ $\rightsquigarrow$ increasing time $\rightsquigarrow$ $t>0$

frac ($t=0$)	state ($t=0$)	frac. ($t>0$)	State ($t>0$)
p_1	$|\phi_1(0)\rangle$	p_1	$|\phi_1(t)\rangle = \hat{U}(t)|\phi_1(0)\rangle$
p_2	$|\phi_2(0)\rangle$	p_2	$|\phi_2(t)\rangle = \hat{U}(t)|\phi_2(0)\rangle$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

$$\hat{\rho}(t) = \sum_n p_n |\phi_n(t)\rangle\langle\phi_n(t)|$$

$$= \sum_n p_n \hat{U}(t)|\phi_n(0)\rangle\langle\phi_n(0)|\hat{U}^{+}(t)$$

$$= \hat{U}(t)\,\hat{\rho}(0)\,\hat{U}^{+}(t)$$

$$\boxed{\hat{\rho}(t) = \hat{U}(t)\,\hat{\rho}(0)\,\hat{U}^{+}(t)}$$

dynamics of $\hat{\rho}$ for any closed qu. system at $t=0$ we started in OD ensemble

claim: at all $t>0$ we will remain in OD ensemble

proof: $$\langle \phi_n(t) | \phi_m(t) \rangle = \langle \phi_n(0) | \hat{U}^\dagger(t) \hat{U}(t) | \phi_m(0) \rangle$$
$$= \langle \phi_n(0) | \phi_m(0) \rangle$$
$$= \delta_{nm}$$

$\hat{\rho}(t)$ started diag at $t=0$ remains diag. at $t>0$

$p_1, p_2, \ldots$ stay same at $t \geq 0$

$$\boxed{S(\hat{\rho}(t)) = -\sum_n p_n \ln p_n = S(\hat{\rho}(0))}$$

von Neumann entropy is const. in time for closed qu. system!