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

ensemble: $|\psi_n\rangle$ appears w/ prob. p_n

observable $\hat{H}$: $\langle H\rangle = \mathrm{tr}(\hat{\rho}\hat{H})$

example:

$\hat{H}|0\rangle = E_0|0\rangle$

$\hat{H}|1\rangle = E_1|1\rangle$

ensemble A:

states	prob
$\|0\rangle$	p
$\|1\rangle$	$1-p$

ensemble B:

states	prob
$\|u\rangle$	$\frac{1}{2}$
$\|v\rangle$	$\frac{1}{2}$

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

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

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

turns out: $\hat{\rho}_A = \hat{\rho}_B = \hat{\rho}$

Because $\hat{\rho}$ is <u>same</u> for both ensembles

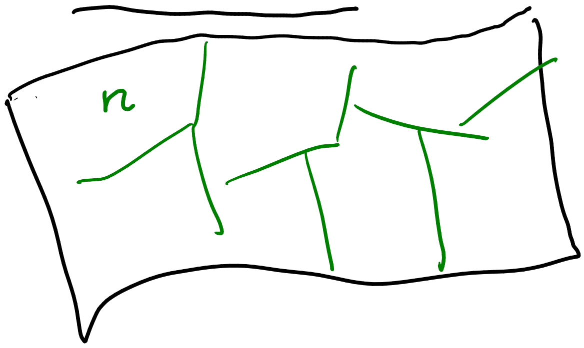
$\Rightarrow$ any observable avgs measured from ensembles will be <u>same</u>

idea that $\hat{\rho}$ can correspond to more than one ensemble $\Rightarrow$ decompositions of $\hat{\rho}$. In general: ∞ # of decomp. for any mixed ensemble

$\Rightarrow$ makes it problematic to use p_n for a given ensemble to define things like entropy takeaway: 1) have to focus on $\hat{\rho}$, not p_n for time evolution, etc.

2) have to be careful about entropy

<u>classical system</u>



phase space at const. E_{tot}

classical states are distinguishable: if we meas. we are in state n, definitely <u>not</u> in state $m \neq n$

p_n = frac. of ensemble in state n

$$S(\vec{p}) = -k_B \sum_n p_n \ln p_n$$

<u>quantum system</u>

von Neumann solution: choose the decomp. of $\hat{\rho}$ where states $|\phi_n\rangle$ are all orthog. to each other

$\Rightarrow$ guarantees <u>distinguishability</u>

why it works: $\hat{\rho}$ is Hermitian

real #'s

arbitrary decomp: $\hat{\rho} = \sum_n \tilde{p}_n |\psi_n\rangle\langle\psi_n|$

$$\hat{\rho}^\dagger = \sum_n \tilde{p}_n |\psi_n\rangle\langle\psi_n| = \hat{\rho}$$

there exists a basis of e-vecs : $\hat{\rho}|\phi_n\rangle = p_n|\phi_n\rangle$

$\hookrightarrow$ e-val

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

diagonalize $\hat{\rho}$: $\hat{\rho} = \sum_{n=1}^{N} p_n |\phi_n\rangle\langle\phi_n|$ orthonormal decomp. (OD)

$\{|\phi_n\rangle\}$ basis $\rho = \begin{pmatrix} p_1 & & 0 \\ & \ddots & \\ 0 & & p_N \end{pmatrix}$

N = dim. of Hilbert space

ensemble:

States	prob
$\|0\rangle$	$1/2$
$\frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)$	$1/2$

$$\hat{\rho} = \sum_{n=1}^{M} \tilde{p}_n |\psi_n\rangle\langle\psi_n| = \sum_{i,j=1}^{N} \rho_{ij} |i\rangle\langle j|$$

$M \neq N$

basis $\{|i\rangle,\ i=1,\dots,N\}$ $\rho_{ij} = \langle i|\hat{\rho}|j\rangle$

in general ρ_{ij} has comp's everywhere

but in special basis $\{|i\rangle = |\phi_i\rangle\}$

$\exists$ ρ_{ij} is 0 when $i \neq j$

von Neumann definition of entropy:

i) take $\hat{\rho}$

ii) calculate ON decomp. (diagonalize $\hat{\rho}$)

iii) e-vals p_n $\Longrightarrow$

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

$$S(\hat{\rho}) \equiv - \sum_n p_n \ln p_n$$

k_B usually left out

What is the problem?

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

simplest case: isolated system (no interactions w/ rest of universe)

closed quantum system

described by Hamilt. $\hat{H}(t)$

wavefunction $|\psi(t)\rangle$:

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

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

unitary operator: propagator

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

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

ensemble:

$\underline{t=0}$		$\rightsquigarrow$	$\underline{\text{later time } t}$	
prob.	state		prob.	state
p_1	$\lvert\phi_1(0)\rangle$		p_1	$\lvert\phi_1(t)\rangle = \hat{U}(t)\lvert\phi_1(0)\rangle$
p_2	$\lvert\phi_2(0)\rangle$		p_2	$\lvert\phi_2(t)\rangle = \hat{U}(t)\lvert\phi_2(0)\rangle$
$\vdots$	$\vdots$		$\vdots$	$\vdots$

$$\begin{aligned}
\hat{\rho}(t) &= \sum_n p_n \lvert\phi_n(t)\rangle\langle\phi_n(t)\rvert \\
&= \sum_n p_n \hat{U}(t)\lvert\phi_n(0)\rangle\langle\phi_n(0)\rvert\hat{U}^\dagger(t) \\
&= \hat{U}(t)\left[\sum_n p_n \lvert\phi_n(0)\rangle\langle\phi_n(0)\rvert\right]\hat{U}^\dagger(t) \\
&= \hat{U}(t)\,\hat{\rho}(0)\,\hat{U}^\dagger(t)
\end{aligned}$$

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

dynamics of $\hat{\rho}(t)$ for closed qu. sys.

let's say we start in OD at $t=0$

claim: we are still in OD at $t>0$

$$\langle \phi_n(t) | \phi_m(t) \rangle =$$

$$\langle \phi_n(0) | \hat{U}^\dagger(t) \hat{U}(t) | \phi_m(0) \rangle$$

$$= \langle \phi_n(0) | \phi_m(0) \rangle$$

$$= \delta_{nm}$$

$\hat{\rho}(t)$ stays diag. in $\{ |\phi_n(t)\rangle \}$

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

von Neumann entropy for closed sys, never increases!

$S(\hat{\rho})$ not same $S(t)$

a classical ergodic + mixing sys.

$$S(t) \xrightarrow[t\to\infty]{} S^{eq} = k_B \ln N \quad \text{maximum}$$

increases