PHYS 414: 4-20-20

ensemble of quantum sys

fraction p_n of state $|\psi_n\rangle$ $\Rightarrow$ $\hat{\rho} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$

for $n = 1, \ldots$

i) $\hat{\rho}^\dagger = \hat{\rho}$ ii) $\mathrm{tr}(\hat{\rho}) = 1$

iii) any observ. w/ oper $\hat{O}$

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

- $\hat{\rho} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$ complete basis: $\{|m\rangle\}$

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

matrix repr. of $\hat{\rho}$:

$$\begin{pmatrix} \cdot & \cdots & & \cdot \\ \cdot & & & \cdot \\ \cdot & \cdots & & \cdot \\ \cdots & & \rho_{mn} & \cdots \\ \cdot & \cdots & & \cdot \end{pmatrix}$$

iv) diag. elements of $\hat{\rho}$ in any basis are always ≥ 0 (positive semi-definite matrix)

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

"population" of basis state m

$$= \sum_n \underbrace{p_n}_{\geq 0} \underbrace{|\langle m|\psi_n\rangle|^2}_{\geq 0} \geq 0$$

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

Imagine that we have Hamilt. $\hat{H}$

& $\{|i\rangle\}$ is the basis of e-states of $\hat{H}$:

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

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

$$= \sum_i \langle i|\hat{\rho}\hat{H}|i\rangle$$

$$= \sum_i E_i \langle i|\hat{\rho}|i\rangle$$

$$\boxed{\langle H\rangle = \sum_i E_i \rho_{ii}}$$

ρ_{ii} = prob. of actually measuring E_i in our ensemble

populations $\Leftrightarrow$ probs of getting certain outcomes upon measuring ensem.

$$\bar{E} = \sum_n p_n E_n$$

nice analogy b/t classical & quantum .... but it gets complicated

classical state n:

$E_n, x_n, \ldots$ definite characteristics that can be measured simultaneously

$\Rightarrow$ hence descr. by one prob. p_n

classical entropy: $S = -k_B \sum_n p_n \ln p_n$

How do we generalize to quantum?

Another complication:

Usually there are <u>many</u> (infinite) ensembles which give you the same $\hat{\rho}$:

An experimentalist can prepare the ensemble completely differently + still end up w/ ensembles which are completely indisting. w/ respect to measurements, i.e. $tr(\hat{\rho}\hat{O})$ will be the same for any $\hat{O}$ on both ensembles

example: ensemble 1:

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

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

ensemble 2:

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

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

$\Rightarrow$ end up w/ exactly same $\hat{\rho}$:

$$\hat{\rho} = \frac{1}{2}|u\rangle\langle u| + \frac{1}{2}|v\rangle\langle v| \quad \leftarrow \text{plug in def'ns of } |u\rangle + |v\rangle$$

$$= p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1|$$

If $\hat{\rho}$ is not a pure ensemble, there are usually an infinite # of <u>ways to prepare it</u>: called different <u>decompositions</u> of $\hat{\rho}$

However every $\hat{\rho}$ has one special decomposition called the <u>orthonormal decomposition</u>:

since $\hat{\rho}$ is Hermitian $\Rightarrow$ complete basis $|\phi_n\rangle$ of e-vecs of $\hat{\rho}$

$$\hat{\rho}\,|\phi_n\rangle = p_n\,|\phi_n\rangle \qquad \langle\phi_n|\phi_m\rangle = \delta_{nm}$$

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

$\Rightarrow$ $\hat{\rho}$ is diag. in that basis, +

hence $\hat{\rho} = \sum_n p_n |\phi_n\rangle\langle\phi_n|$ ON decomp.

b/c $\{|\phi_n\rangle\}$ are ON $\Rightarrow$ they are "distinguishable"

$\Rightarrow$ if we do measurement + find the sys in state $|\phi_n\rangle$ we can be sure that we were not in another state $|\phi_m\rangle$, $m \neq n$, before the measurement

$\Rightarrow$ von Neumann used this nice feature to argue that quantum entropy should be defined w/ respect to ON decomp.

quantum (von Neumann) entropy

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

trad. w/o k_B factor

where $\{p_n\}$ are e-vals of $\hat{\rho}$ [ON decomp.]

$$\equiv -\operatorname{tr}(\hat{\rho}\ln\hat{\rho})$$

In prev. example: $\{|0\rangle, |1\rangle\}$ is the ON basis

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

How does $S(\hat{\rho})$ change in time? $\rightsquigarrow$ 2nd law?

$\Rightarrow$ How does $\hat{\rho}$ change in time?

$t=0$: prepare our sys. in ON decomp

$$\hat{\rho}(0) = \sum_n p_n |\phi_n(0)\rangle\langle\phi_n(0)|$$

where

$$\langle\phi_n(0)|\phi_m(0)\rangle = \delta_{nm}$$

isolated sys (no inter. w/ rest of universe) described by Hamiltonian $\hat{H}(t)$

time evol. of $|\psi\rangle$ described by:

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

sol'n always of form: $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$

where $\hat{U}$ is a unitary oper.

$$\hat{U}^\dagger(t)\hat{U}(t) = \hat{\mathbb{1}} = \hat{U}(t)\hat{U}^\dagger(t)$$

special case where $\hat{H}(t) = \hat{H}$

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

in an ensemble, every state will evolve w/ unitary operator:

$t=0$		$\longrightarrow$	later time	
frac	state		frac	state
p_n	$\|\phi_n(0)\rangle$		p_n	$\hat{U}(t)\|\phi_n(0)\rangle = \|\phi_n(t)\rangle$

later time
$$\hat{\rho}(t) = \sum_n p_n |\phi_n(t)\rangle\langle\phi_n(t)|$$
$$= \sum_n p_n \hat{U}(t)|\phi_n(0)\rangle\langle\phi_n(0)|\hat{U}^\dagger(t)$$
$$= \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t)$$

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

is the ON decomp. of $\hat{\rho}(t)$

b/c $\langle\phi_n(t)|\phi_m(t)\rangle$

$$= \langle\phi_n(0)|\underbrace{\hat{U}^+(t)\,\hat{U}(t)}_{\hat{\mathbb{1}}}|\phi_m(0)\rangle$$

$$= \langle\phi_n(0)|\phi_m(0)\rangle = \delta_{nm}$$

prob. in ON decomp $\{p_n\}$ have stayed <u>exactly</u> the same for time 0 and t

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

quantum entropy for an isolated sys always stays the same!