E7/1

Quantum system, 2 subsystems

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$$

Access to the 1st subsystem only.

Entangled state $|\psi\rangle = \sum_{\alpha, i} C_{\alpha i} |\alpha, i\rangle$

α: states $|\alpha\rangle \in \mathcal{H}_1$

i : states $|i\rangle$ in $\mathcal{H}_2$.

density matrix $\rho_{\alpha\beta} = \sum_i C^*_{\alpha i} C_{\beta i}$

density operator $\sum_{\alpha\beta} |\alpha\rangle \rho_{\alpha\beta} \langle\beta| = \hat{\rho}$

$\forall$ any operator acting only on the 1st subsystem

$$\langle\psi|\hat{A}|\psi\rangle = \mathrm{tr}(\hat{\rho}\hat{A}) = \sum_{\alpha\beta} \rho_{\alpha\beta} \langle\beta|\hat{A}|\alpha\rangle.$$

---

eigenvalues of ρ are ≥ 0, add up to 1

$$\hat{\rho} = \sum_{n} |n\rangle w_n \langle n|$$

then we have a mixed state:
with probability w_n the subsystem is in state $|n\rangle$.

---

if $|\psi\rangle = |\varphi\rangle \otimes |\chi\rangle$ no entanglement.

$\quad\quad\quad\quad \hat{\mathcal{H}}_1 \quad \hat{\mathcal{H}}_2$

then $\hat{\rho}_{\alpha\beta} = \langle\alpha|\varphi\rangle\langle\varphi|\beta\rangle$

$\hat{\rho} = |\varphi\rangle\langle\varphi|$: pure state

$w_1 = 1$, other $w_n = 0$.

(2)

pure state $|\varphi\rangle \Leftrightarrow \hat{\rho} = |\varphi\rangle\langle\varphi|$

$tr(\hat{\rho}\hat{A}) = \langle\varphi|\hat{A}|\varphi\rangle.$

OTOH, if $|\Psi\rangle$ is entangled.

then several $w_n \neq 0$, $\hat{\rho} \neq |\varphi\rangle\langle\varphi|$ for any $|\varphi\rangle$.

$\rightarrow$ mixed state

mixed state $\hat{\rho} = \sum_n |n\rangle w_n \langle n|$

is different from a pure state $|\varphi\rangle$ with similar probabilities $P(|\varphi\rangle \text{ is } |n\rangle) = w_n$,

$|\varphi\rangle = \sum_n \sqrt{w_n}\, |n\rangle \times e^{i\,phase}.$

$tr(\hat{\rho}\hat{A}) = \sum_n w_n \langle n|\hat{A}|n\rangle$ ← no off-diagonal terms

$\langle\varphi|\hat{A}|\varphi\rangle = \sum_{n,m} \sqrt{w_n w_m}\, \langle n|\hat{A}|m\rangle\, e^{i\,phase}$

Time evolution.

Suppose $\hat{H} = \hat{H}_1 + \hat{H}_2$ ← subsystem #2

↑ subsystem #1

no interaction between the subsystems

~~pure~~ un-entangled $|\Psi\rangle = |\varphi\rangle \otimes |\chi\rangle$

$|\varphi\rangle(t) \rightarrow e^{-i\hat{H}_1 t/\hbar}|\varphi\rangle_0$

$|\chi\rangle(t) \rightarrow e^{-i\hat{H}_2 t/\hbar}|\chi\rangle_0$

$\hat{\rho} = |\varphi\rangle\langle\varphi| \rightarrow e^{-i\hat{H}_1 t/\hbar}\,\hat{\rho}\,e^{+i\hat{H}_1 t/\hbar}$

13

Mixed state

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

each ρ $|\psi_n\rangle \to e^{-i\hat{H}_I t/\hbar}|\psi_n\rangle$

$$\boxed{\hat{\rho} = e^{-i\hat{H}_I t/\hbar}\hat{\rho}_S e^{+i\hat{H}_I t/\hbar}}$$

$$\boxed{i\hbar \frac{d}{dt}\hat{\rho} = -[\hat{\rho}, \hat{H}_I]}$$

In Schrödinger Picture.

In Heisenberg Picture $\hat{\rho}$ is time independent.

---

classical mechanics

particle motion in the phase space

$\vec{x}(t), \vec{p}(t)$

Ensemble : large # of similar systems.

in each system, particle in some pt in phase space $(\vec{x}, \vec{p})$.

$\Rightarrow$ density of particles in the phase space

$\rho(\vec{x}, \vec{p})$.

its time evolution is

$$\frac{\partial}{\partial t}\hat{\rho}(\vec{x}, \vec{p}; t) = -[\rho, H]_{\text{poisson}}.$$

$$i\hbar \frac{\partial}{\partial t} \hat{\rho} = -[\hat{\rho}, \hat{H}]$$

only when $\hat{H}_{int} = 0$.

Add interaction → ~~change~~
entanglement may change
with time

No ~~@~~ H_{int}

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

→ eigenvalues w_n of $\hat{\rho}$
stay unchanged.

Add $\hat{H}_{int}$ → w_n may change with
time.

In particular, a pure state
may evolve into a mixed state.

Extreme case: transient interaction
of a particle with an almost classical
detector.

un-entangled state before →
pure state of the particle.

After interaction → entanglement

$\hat{\rho} = \sum_n |\psi_n\rangle w_n \langle \psi_n|$ → mixed state of the particle

→ its wave function collapses
to $|\psi_n\rangle$ with probability w_n

5]

Mixed states $\hat{\rho}$ have entropy

in units of $k_{Boltzmann}$

$$S = \sum_n w_n \log \frac{1}{w_n} = -\sum_n w_n \log w_n$$

$$S = -\operatorname{tr}(\hat{\rho} \log \hat{\rho})$$

For a pure state $S = 0$

mixed state: $S > 0$

~~Max~~

Coherent evolution $\hat{\rho}(t) = \hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t,t_0)$

w_n are time-independent

$S = \text{const.}$

Interactions with the environment

→ ~~lose~~ loose some entanglement information → S grows.

For a large system, coarse graining

→ loose entanglement info

→ S grows.

In Equilibrium expect to maximize S.

For a system with finite $\dim(\mathcal{H}) = \nu < \infty$

~~the~~ maximal S is for $w_1 = \dots = w_\nu = \frac{1}{\nu}$

$$\hat{\rho} = \frac{1}{\nu} \cdot \mathbb{1} \qquad S_{max} = \log \nu$$

6

Infinite dim $(\mathcal{H}_1)$ → no upper bound on entropy.

Instead, maximize $\hat{\rho}$ under constraint of a given avg. energy $E = tr(\hat{\rho}\cdot\hat{H})$.

$\hat{\rho}$: Infinitesimal variations

$\hat{\rho} \to \hat{\rho} + \delta\hat{\rho}$

we seek $\delta S = -\delta\, tr(\hat{\rho}\log\rho) = 0$

constraints: $tr(\hat{\rho}) \equiv 1 \to tr(\delta\hat{\rho}) = 0.$

$\delta E = tr(\delta\hat{\rho}\cdot\hat{H}) = 0.$

Lemma: ∀ analytic function

$$f(x) = \sum_n c_n x^n$$

$$\delta\, tr(f(\hat{\rho})) = tr(f'(\hat{\rho})\delta\hat{\rho})$$

even if $[\delta\hat{\rho}, \hat{\rho}] \neq 0.$

$$\delta\, tr(\hat{\rho}) = tr(\delta\hat{\rho}\cdot 1)$$

$$\delta\, tr(\hat{\rho}^2) = tr(\hat{\rho}\delta\hat{\rho} + \delta\rho\hat{\rho}) = tr(2\hat{\rho}\delta\hat{\rho}).$$

$$\delta\, tr(\hat{\rho}^3) = tr(\hat{\rho}^2\delta\hat{\rho} + \hat{\rho}\delta\hat{\rho}\hat{\rho} + \delta\hat{\rho}\hat{\rho}^2)$$
$$= tr(3\hat{\rho}^2\delta\hat{\rho})$$

$$\delta\, tr(\hat{\rho}^n) = tr(n\hat{\rho}^{n-1}\delta\hat{\rho}).$$

$$\to \delta\, tr(f(\hat{\rho})) = tr(f'(\hat{\rho})\delta\hat{\rho})$$

7/7

$S = -\mathrm{tr}(\rho \log \rho)$

$f(x) = -x \log x$ is not analytic @ $x = 0$.

$$f(x) = \int_0^\infty \frac{dt}{t} \left(e^{-tx} - e^{-t}\right) \cdot x$$

$$S = \int_0^\infty \frac{dt}{t} \underbrace{\mathrm{tr}\left(\hat{\rho}\left(e^{-t\hat{\rho}} - e^{-t}\right)\right)}_{\text{analytic in } \hat{\rho}.}$$

$f'(x) = -\log x - 1$

$\delta S = -\mathrm{tr}\left((1 + \log \rho)\, \delta\hat{\rho}\right)$

$= -\mathrm{tr}\left(\log \hat{\rho}\, \delta\hat{\rho}\right)$

$\rightarrow$ want $\mathrm{tr}(\log \hat{\rho} \cdot \delta\hat{\rho}) = 0$

whenever $\mathrm{tr}(\delta\hat{\rho}) = 0$ and $\mathrm{tr}(\hat{H}\,\delta\hat{\rho}) = 0$

$\rightarrow -\log \hat{\rho} = \alpha + \beta \hat{H}$

for some constants $\alpha, \hat{\beta}$

$\hat{\rho} = e^{-\alpha} e^{-\beta \hat{H}}$ $\quad \mathrm{tr}\,\hat{\rho} = 1$

$$\boxed{\begin{aligned} \hat{\rho} &= \frac{1}{Z} e^{-\beta \hat{H}} \\ Z &= \mathrm{tr}\left(e^{-\beta \hat{H}}\right) \end{aligned}}$$

2

18

$Z \equiv$ partition function,

in terms of spectrum of $\hat{H}$

$$Z = \sum_n e^{-\beta E_n} \times \text{degeneracy}(E_n).$$

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}$$

eigenstates: definite energy states $|n\rangle$, $\hat{H}|n\rangle = E_n|n\rangle$.

probabilities $w_n = \frac{1}{Z} e^{-\beta E_n}$.

Boltzmann factor.

$$\beta = \frac{1}{\text{Temperature}}$$