Phys 521 Fall 2023

Lecture: Density Matrix

If we do not have enough information to know system is in a specific state, we can consider a statistical ensemble of identically prepared quantum systems.

Form incoherent mixture of M states $|\psi_i\rangle$ with probability w_i,

$$\sum_{i=1}^{M} w_i = 1$$

Expectation value of some observable $\hat{A}$

$$\langle \bar{A} \rangle = \sum_{i=1}^{M} w_i \langle \psi_i | \hat{A} | \psi_i \rangle$$

where notation denotes two kinds of average - classical and quantum.

Introduce basis $|b_\alpha\rangle$ for $|\psi_i\rangle$ of dimention N.

$$|\psi_i\rangle = \sum_{\alpha=1}^{N} |b_\alpha\rangle \langle b_\alpha | \psi_i \rangle$$

amplitude ψ_i^α

$$\langle \bar{A} \rangle = \sum_{\alpha=1}^{N} \sum_{i=1}^{M} w_i \langle \psi_i | \hat{A} | b_\alpha \rangle \langle b_\alpha | \psi_i \rangle$$

note: cannot write a mixed state as a wave function.

$$\langle\hat{A}\rangle = \sum_{\alpha}\sum_{i} w_i \langle b_\alpha|\psi_i\rangle\langle\psi_i|\hat{A}|b_\alpha\rangle$$

$$= \sum_{\alpha} \langle b_\alpha| \underbrace{\left\{\sum_{i=1}^{M} w_i |\psi_i\rangle\langle\psi_i|\right\}}_{\equiv\ \hat{\rho}\ \underline{\text{density operator}}} \hat{A}|b_\alpha\rangle$$

$$\equiv \sum_{\alpha} \langle b_\alpha|\hat{\rho}\hat{A}|b_\alpha\rangle$$

Or as matricies,

$$\langle\hat{A}\rangle = \sum_{\alpha,\beta} \langle b_\alpha|\hat{\rho}|b_\beta\rangle\langle b_\beta|\hat{A}|b_\alpha\rangle$$

trace

$$= \sum_{\alpha,\beta} [\rho]_{\alpha\beta}[\hat{A}]_{\beta\alpha} = \mathrm{tr}(\rho A)$$

$$= \mathrm{tr}(A\rho) \equiv \mathrm{tr}(\hat{\rho}\hat{A})$$

trace understood as referring to some basis

Properties of $\hat{\rho}$

$$tr(\hat{\rho}) = \sum_\alpha \langle b_\alpha | \hat{\rho} | b_\alpha \rangle$$

$$= \sum_{i=1}^{m} w_i \sum_\alpha \langle b_\alpha | \psi_i \rangle \langle \psi_i | \beta_\alpha \rangle$$

$$= \sum_{i=1}^{M} w_i \underbrace{\langle \psi_i | \psi_i \rangle}_{\text{normalized to } 1} = \sum_i^{M} w_i = 1$$

Eigenvalues of $\hat{\rho}$

$$\lambda_\beta \equiv \langle b_\beta | \hat{\rho} | b_\beta \rangle$$

$$= \sum_{i=1}^{m} w_i \langle b_\beta | \psi_i \rangle \langle \psi_i | b_\beta \rangle$$

$$= \sum_{i=1}^{m} w_i \, |\psi_i^\beta|^2$$

since $|\psi_i^\beta| \geq 0$ & $w_i \geq 0$, $\lambda_\beta \geq 0$

$$tr(\hat{\rho}) = \sum \langle b_\beta | \hat{\rho} | b_\beta \rangle = \sum \lambda_\beta = 1$$

so eigenvalues $\lambda_\beta \leq 1$

We can express $\hat{\rho}$ in terms of eigenvalues,

$$\hat{\rho} = \sum_\alpha \lambda_\alpha |b_\alpha\rangle\langle b_\alpha|$$

since then $\langle b_\beta|\rho|b_\beta\rangle = \lambda_\beta$

A pure state has one $w_j = 1$, and all others $w_{i \neq j} = 0$. Then

$$\hat{\rho} = |\psi_i\rangle\langle\psi_i| \qquad \text{pure}$$

and therefore $\hat{\rho}^2 = |\psi_i\rangle\underbrace{\langle\psi_i|\psi_i\rangle}_{1}\langle\psi_i| = \hat{\rho}$

and $\mathrm{tr}\,\hat{\rho}^2 = \mathrm{tr}\,\hat{\rho} = 1$ pure only

$$\hat{\rho}^2 = \hat{\rho}$$

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

In basis that diagonalizes $\hat{\rho}$,

$$[\hat{\rho}] = \text{diag.}[0, 0, \ldots 0, 1, 0, \ldots 0]$$

One non zero eigenvalue $= 1$

Spin-1/2 Examples ($N=2$)

$\hat{S} = \frac{\hbar}{2}\vec{\sigma}$

Suppose $\hat{\rho} = |+z\rangle\langle +z|$ pure

$$\hat{\rho} \doteq \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$$

$$\langle \hat{S}_z \rangle = tr(\hat{\rho}\hat{S}_z) = \frac{\hbar}{2} tr\left[\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\right] = \frac{\hbar}{2}$$

$$\langle \hat{S}_y \rangle = tr(\hat{\rho}\hat{S}_y) = \frac{\hbar}{2} tr\left[\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix}\right]$$

$$= \frac{\hbar}{2} tr\begin{bmatrix}0 & -i\\0 & 0\end{bmatrix} = 0$$

similarly, $\langle \hat{S}_x \rangle = 0$

check: $tr(\hat{\rho}) = 1$ & $\hat{\rho}^2 = \hat{\rho}$

In general, for spin-1/2 ensemble,

$[\hat{\rho}]$ is 2×2 complex, hermitian, $tr(\hat{\rho})=1$

matrix parameterized by 3 real parameters a_1, a_2, a_3 and can be written as

$$\hat{\rho} = \frac{1}{2}\left[\hat{I} + \vec{a}\cdot\vec{\sigma}\right]$$

note: Commins uses $\vec{P}$ for polarization instead of $\vec{a}$

$$\hat{\rho}^2 = \frac{1}{4}\left[1 + 2\vec{a}\cdot\vec{\sigma} + (\vec{a}\cdot\vec{\sigma})^2\right]$$

$$(a\cdot\sigma)^2 = a_i a_j \sigma_i \sigma_j = a_i a_j (\delta_{ij} + i\varepsilon_{ijk}\sigma_k)$$

$$= |\vec{a}|^2 \qquad \qquad \vec{a}\times\vec{a} = 0$$

$$\rho^2 = \frac{1}{4}(1+|\vec{a}|^2) + \frac{1}{2}\vec{a}\cdot\vec{\sigma}$$

for pure state $\rho^2 = \rho \Rightarrow |\vec{a}|^2 = 1$

You can easily show $\langle \hat{S}_i \rangle = a_i \frac{\hbar}{2}$

previous example $\hat{\rho} = |+z\rangle\langle +z| \doteq_z \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

has $\vec{a} = (0,0,1)$ $\quad \rho = \frac{1}{2}[I + \sigma_z]$

consider $\vec{a} = \frac{1}{4}(1,0,3)$

$$\rho = \frac{1}{2}\left[I + \frac{1}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] = \frac{1}{8}\begin{pmatrix} 7 & 1 \\ 1 & 1 \end{pmatrix}$$

check $\mathrm{tr}(\rho) = 1$

In this case $|\vec{a}|^2 = \frac{1}{16}(1+3^2) = \frac{10}{16} < 1$

this is a mixture. In general

$|\vec{a}| = 1 \qquad$ pure

$|\vec{a}| < 1 \qquad$ mixture

mixture example: silver atoms from oven completely unpolarized incoherent mixture

$$\rho = \frac{1}{2}\left(|+z\rangle\langle +z| + |-z\rangle\langle -z| \right) \doteq \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$tr(\rho) = 1$ but $\rho^2 \neq \rho$ and $tr(\rho^2) = \frac{1}{2}$

Note, we could equally have written

$$\rho = \frac{1}{2}\left(|+x\rangle\langle +x| + |-x\rangle\langle -x| \right) \doteq \frac{1}{2}\left[\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \right]$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{same matrix}$$

easily compute $\langle S_x \rangle = tr(\rho\, \sigma_x) = 0 = \langle S_y \rangle = \langle S_z \rangle$

<u>Example</u> incoherent mixture:

$$\frac{3}{4}\, |+z\rangle + \frac{1}{4}\, |+x\rangle \qquad \vec{a} = \left(\frac{1}{4}, 0, \frac{3}{4}\right)$$

$$\rho = \frac{1}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right]$$

$$= \frac{1}{8}\begin{pmatrix} 7 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\langle S_x \rangle = \frac{\hbar}{8} \quad \langle S_y \rangle = 0 \quad \langle S_z \rangle = \frac{3\hbar}{8}$$

<u>Note</u>: Spin ½ system in quantum computing is called a <u>Q-bit</u>

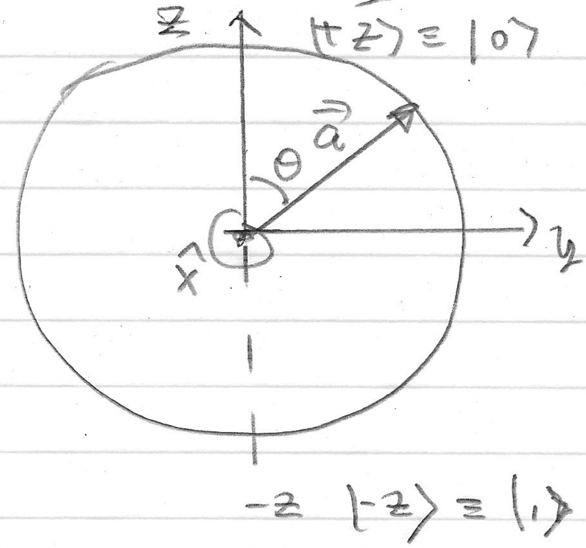
Block Sphere :

Arbitrary spin state written as a rotation of $|+z\rangle$

$$|\psi\rangle = \cos\theta/2 \; |+z\rangle + e^{i\phi} \sin\theta/2 \; |-z\rangle$$

polarization vector $\vec{a}$ of density matrix

$$\hat{\rho} = \frac{1}{2}\left[\vec{I} + \vec{a}\cdot\vec{\sigma}\right]$$



ϕ is azimuthal angle.

in Quantum information $|+z\rangle \equiv |0\rangle$ & $|-z\rangle \equiv |1\rangle$

$|\vec{a}| = 1$ pure

$|\vec{a}| < 1$ mixture

time evolution of $\hat{\rho}$

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

Schrodinger,

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

$$\hat{\rho}(t) = \sum_{i=1}^{m} w_i\,|\psi_i(t)\rangle\langle\psi_i(t)|$$

$$\frac{\partial\hat{\rho}}{\partial t} = \sum_{i=1}^{m} w_i\left[\frac{1}{i\hbar}\hat{H}|\psi(t)\rangle\langle\psi_i(t)| - \frac{1}{i\hbar}|\psi(t)\rangle\langle\psi(t)|\hat{H}\right]$$

$$= \frac{1}{i\hbar}\left[\hat{H},\hat{\rho}\right]$$

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

Which is like time evolution of classical phase space density which is given by Liouville's theorem

$$\frac{\partial\rho_c}{\partial t} = -\{\rho_c, H_c\}$$ classical Poisson bracket

Hence the name, density matrix.

Connection to Statistical mechanics (Commins)

Ensemble of particles in thermal equilibrium at temperature T.
Consider each particle to be in energy eigenstate $|E_n\rangle$, energy E_n.

probability $P_n = \frac{1}{Z}\exp(-E_n/kT)$

k Boltzmann constant. partition function

$$Z = \sum_n \exp(-E_n/kT)$$

mean energy $U = \sum_n P_n E_n$

Partition function is related to free energy F *

$$F \equiv U - TS = -kT\ln(Z) \quad \text{where } S = \text{entropy}$$

Then $S = k\ln(Z) + \frac{U}{T}$

with $\ln(P_n Z) = -\frac{E_n}{kT}$

$$\frac{U}{T} = \frac{1}{T}\sum E_n P_n = -k\sum_{P_n} P_n \ln(\underbrace{P_n Z}_{\ln(Z)+\ln(P_n)})$$

$$= -k\sum_n P_n\left[\ln(Z) + \ln(P_n)\right]$$

$$= -k\ln(Z) - k\sum_n P_n \ln P_n \quad (\Sigma P_n = 1)$$

giving $\boxed{S = -k\sum_n P_n \ln P_n}$

* recall: for system interacting with environment @T equilibrium is obtained by minimizing the thermodynamic potential F, the Helmholtz free energy

density matrix for system is:

$$\hat{\rho} = \sum p_n |E_n\rangle\langle E_n|$$

matrix $\rho = \mathrm{diag}(p_1, p_2, \ldots, p_n)$

$$\mathrm{tr}\,\rho = \sum p_n = 1$$

$$\ln \rho = \mathrm{diag}(\ln p_1, \ldots \ln p_n)$$

$$\rho \ln \rho = \mathrm{diag}(p_1 \ln p_1, \ldots p_n \ln p_n)$$

$$\mathrm{tr}(\rho \ln \rho) = \sum_n p_n \ln p_n$$

giving $S = -k\,\mathrm{tr}(\rho \ln \rho)$

Generalized to any system with density matrix ρ, this is the von Neumann entropy.