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.

$$|\psi_i\rangle = \sum_{\alpha=1}^{N} |b_\alpha\rangle \underbrace{\langle b_\alpha | \psi_i \rangle}_{\text{amplitude } \psi_i^\alpha}$$

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

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

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

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

Or as matricies,

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

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

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

trace understood as referring to some basis

Properties of $\hat{\rho}$

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

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

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

Eigenvalue 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 eigenvalue $\lambda_\beta \leq 1$

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

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

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 $\hat{\rho}$,

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

one nonzero eigenvalue $= 1$

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

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

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 $\vec{a}$

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

previous example $\hat{\rho} = |+z\rangle\langle +z|$
has $\vec{a} = (0,0,1)$

$$\hat{\rho} = \frac{1}{2}[I + \sigma_z] = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

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

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

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

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

This is a mixture. In general

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

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

Mixture example: Silver atoms from oven are completely unpolarized, incoherent mixture

$$\hat{\rho} = \frac{1}{2}\left(|+\rangle\langle +| + |-\rangle\langle -|\right)$$

$$[\hat{\rho}] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad tr(\hat{\rho}) = 1$$

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

Note we could equally well have taken

$$\hat{\rho} = \frac{1}{2}\left(|+x\rangle\langle +x| + |-x\rangle\langle -x| \right)$$

giving same matrix

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

Easily compute $\langle S_x \rangle = \mathrm{tr}(\rho\, \sigma_x) = 0$

& $\langle S_y \rangle = \langle S_z \rangle = 0$

<u>Example</u> Incoherent mixture of
$\frac{3}{4}\,|+z\rangle$ & $\frac{1}{4}\,|+x\rangle$ $\quad \vec{a} = (1/4, 0, 3/4)$

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

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

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

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

<u>Note</u> Spin 1/2 system in quantum computing is called a Q-bit

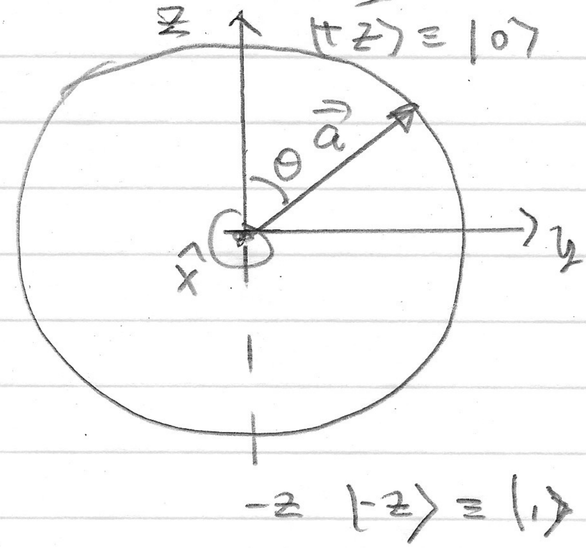
Block. Sphere :

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

<u>time evolution of $\hat{\rho}$</u>

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

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.