# Lecture Density Matrix

Consider statistical ensemble of identically prepared Quantum systems:

prob $w_i$ to be in state $|\psi_i\rangle$

$$\sum_{i=1}^{m} w_i = 1 \qquad m = \# \text{ incoherent mixtures}$$

Expectation value of observable $\hat{A}$

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

notation denotes 2 kinds of averages - classical and Quantum.

Consider basis $|b_\alpha\rangle$ for $|\psi_i\rangle$ of dimension $N$.

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

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

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

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

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

or matricies

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

trace

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

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

<u>Properties of $\hat{\rho}$</u>

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

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

$$= \sum_{i=1}^{M} w_i \sum_{\alpha=1}^{N} |\psi_i^\alpha|^2 = 1$$

<u>Normalization</u>

## Eigenvalues of $\hat{\rho}$

define $\lambda_\alpha$ by $\hat{\rho} = \sum_{\alpha=1}^{N} \lambda_\alpha |b_\alpha\rangle\langle b_\alpha|$

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

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

$$= \sum_{\alpha=1}^{N} \lambda_\alpha \underbrace{\langle b_\beta | b_\alpha\rangle}_{\delta_{\alpha\beta}} \underbrace{\langle b_\alpha | b_\beta\rangle}_{\delta_{\alpha\beta}}$$

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

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

components in basis

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

$$\lambda_\beta \geq 0$$

and

$$\mathrm{tr}(\rho) = \sum_\beta \lambda_\beta = 1$$

$$\lambda_\beta \leq 1$$

A *pure* state has $w_j = 1$, $w_{i \neq j} = 0$

$$\hat{\rho} = |\psi_j\rangle\langle\psi_j|$$

$$[\hat{\rho}]_{\alpha\beta} = \sum \langle b_\alpha|\psi_j\rangle\langle\psi_j|b_\beta\rangle$$

and
$$[\hat{\rho}]_{\alpha\beta} = \sum_\gamma \lambda_\gamma \underbrace{\langle b_\alpha|b_\gamma\rangle}_{\delta_{\alpha\gamma}}\underbrace{\langle b_\gamma|b_\beta\rangle}_{\delta_{\gamma\beta}}$$
$$= \lambda_\alpha \delta_{\alpha\beta}$$

In basis $|b'_\alpha\rangle$ that diagonalizes $|\psi_i\rangle$

$$[\hat{\rho}]' = \mathrm{diag}[0, \ldots, 0, 1, 0, \ldots 0] \quad \text{(diagonal form)}$$

$\beta$ component: $\lambda_\beta = 1$, $\lambda_{\alpha\neq\beta} = 0$

For *pure* state only

$$\mathrm{tr}(\rho^2) = 1$$

Spin-1/2 example   $N=2$

$$\hat{\vec{S}} = \frac{\hbar}{2}\vec{\sigma} \qquad \sigma_x \doteq \begin{pmatrix}0&1\\1&0\end{pmatrix}$$

$$\sigma_y \doteq \begin{pmatrix}0&-i\\i&0\end{pmatrix}$$

$$\sigma_z \doteq \begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

traceless, Hermitian matrices / operator

rep. in $|\pm z\rangle$ basis

$$|+z\rangle \doteq \begin{pmatrix}1\\0\end{pmatrix}$$

$$|-z\rangle \doteq \begin{pmatrix}0\\1\end{pmatrix}$$

$$|\pm x\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\\pm 1\end{pmatrix}$$

Ex 1

let $|\psi\rangle = |+z\rangle$   pure

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

$$\doteq \begin{pmatrix}1\\0\end{pmatrix}(0,1) = \begin{pmatrix}1&0\\0&0\end{pmatrix}$$

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

$$= \mathrm{tr}\left[\begin{pmatrix}1&0\\0&0\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right] = 1$$

expectation values

$$\langle \hat{S}_x \rangle = \frac{\hbar}{2}\left(\frac{1}{4}\right)$$

$$\langle \hat{S}_y \rangle = 0$$

$$\langle \hat{S}_z \rangle = \frac{\hbar}{2}\left(\frac{3}{4}\right)$$

For spin-1/2 single particles

since $\hat{\rho}^{+} = \rho$ & $tr(\rho) = 1$

$[\rho]$ is 2x2 complex Hermitian (4)

parameters = 4 − 1 (norm) = $\underline{\underline{3}}$

We can write as

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

$\vec{a}$ 3 real number

You can prove

$$\langle \hat{S}_i \rangle = a_i\left(\frac{\hbar}{2}\right)$$

using $\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}$ identity

So Ex 1 $\quad \vec{a} = (0,0,1)$ $\quad \underline{|\vec{a}|^2 = 1}$

$$\hat{\rho} = \frac{1}{2}\left[\hat{I} + \sigma_z\right]$$

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

and Ex 3 $\quad \vec{a} = (\frac{1}{4}, 0, \frac{3}{4})$

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

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

In this case

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

pure $|\vec{a}|^2 = 1$, mixture $|\vec{a}|^2 < 1$

Ex 2 pure

$|\psi\rangle = |\pm x\rangle$ either

$$\hat{\rho} \doteq_{z\text{ basis}} \left(\frac{1}{\sqrt{2}}\right)^2 \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} (1, \pm 1)$$

$$= \frac{1}{2} \begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix}$$

this is a pure state, check $\hat{\rho}^2 = \hat{\rho}$

Ex 3

Silver atoms from are completely unpolarized, not pure, incoherent mixture.

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

$$\doteq \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \mathrm{tr}\, \rho = 1$$

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

Could equally well be written as equal sum of $|\pm x\rangle$ states

$$\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \frac{1}{2}, & \frac{1}{2} \\ \frac{1}{2}, & \frac{1}{2} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1/2, & -1/2 \\ -1/2, & 1/2 \end{pmatrix}$$

not unique ($\infty$ # ways to write)

<u>Expectation values</u>

$$\langle S_x \rangle = \mathrm{tr}\left[\begin{pmatrix} 1/2, & 0 \\ 0, & 1/2 \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\right] = 0$$

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

<u>Ex 3</u> incoherent mixture of pure states

$3/4$ of $|+z\rangle$ and $\frac{1}{4}|+x\rangle$

$$\hat{\rho} \doteq \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

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

Spin-½ system in quantum computing is Q-bit.

Bloch sphere representation

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)\underset{\overset{\shortparallel}{|+z\rangle}}{|0\rangle} + e^{+i\phi}\sin\left(\theta/2\right)\underbrace{|1\rangle}_{|-z\rangle}$$

$$[\rho] = \begin{pmatrix} \cos\theta/2 \\ e^{-i\phi}\sin\theta/2 \end{pmatrix}\left(\cos\theta/2,\ e^{+i\phi}\sin\theta/2\right)$$

$$= \begin{bmatrix} c^2 & e^{+i\phi}cs \\ e^{-i\phi}cs & s^2 \end{bmatrix}$$ half-angle

$$= \frac{1}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + a_x\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + a_y\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + a_z\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]$$

$$= \frac{1}{2}\begin{bmatrix} 1+a_z, & a_x + i a_y \\ a_x - i a_y, & 1-a_z \end{bmatrix}$$

so

$$\frac{1}{2}(1+a_z) = \cos^2\theta/2 = \frac{1}{2}(1+\cos\theta)$$

$$\frac{1}{2}(1-a_z) = \sin^2\theta/2 = \frac{1}{2}(1-\cos\theta)$$

$$a_z = \cos\theta$$

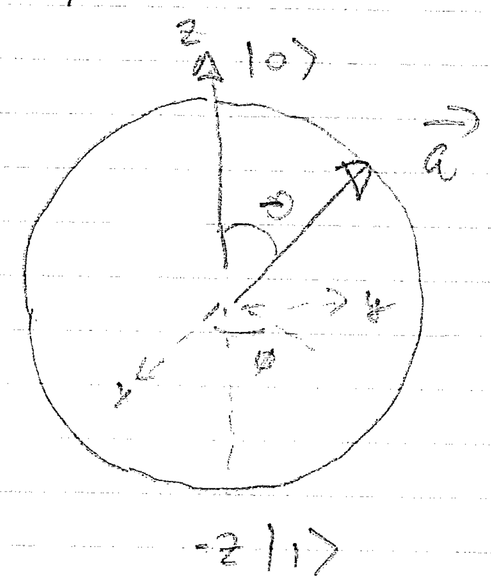
and

$$a_x \pm i a_y = \underbrace{2\cos\theta/2 \sin\theta/2}_{\sin\theta} (\cos\phi \pm i \sin\phi)$$

$$a_x = \sin\theta \cos\phi$$

$$a_y = \sin\theta \sin\phi$$

Bloch sphere:



time evolution of $\rho$

$w_i$ are constant in time

$$|\psi_i(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi_i(0)\rangle$$ Schrödinger representation

$$\rho(t) = \sum_{i=1}^{m} w_i \, e^{-i\hat{H}t/\hbar} |\psi_i(0)\rangle\langle\psi_i(0)| e^{+i\hat{H}t/\hbar}$$

$$\frac{\partial \rho}{\partial t} = \sum w_i \left(\frac{i}{\hbar}\right)\Big[ |\psi(t)\rangle\langle\psi(t)| \hat{H}$$

$$- \hat{H}|\psi(t)\rangle\langle\psi(t)| \Big]$$

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

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

time evolution of classical phase space density

given by Liouville's theorem (classical)

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

Hence name, density matrix.

## Entangled state

2 electron spin state $S=0$ in electrons a, b.

$$|0\rangle = \frac{1}{\sqrt{2}}\left( |+\rangle_a |-\rangle_b - |-\rangle_a |+\rangle_b \right)$$

rotational invariant

order from order

$[\rho]_{\alpha\beta}$ in basis

$|++\rangle$
$|+-\rangle$
$|-+\rangle$
$|--\rangle$

$$|0\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

$$[\rho]_{\alpha\beta} = \langle \alpha | 0 \rangle \langle 0 | \beta \rangle$$

$$= \left(\frac{1}{\sqrt{2}}\right)^2 \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & -1 & 0 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

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

$\rho^2 = \rho$ pure state