Density matrix or Density operator

Pure state : $\rho = |\psi\rangle\langle\psi|$

$$\boxed{\langle A\rangle = \mathrm{Tr}(\rho A)}$$

General definition

$$\rho = \sum_i p_i \, |\psi_i\rangle\langle\psi_i|$$

$|\psi_1\rangle$, $|\psi_2\rangle$

$$\rho = p_1 |\psi_1\rangle\langle\psi_1| + p_2 |\psi_2\rangle\langle\psi_2|$$

$$p_1 + p_2 = 1$$

Matrix representation of ρ

$$\rho_{mn} = \langle \underline{m} | \rho | \underline{n} \rangle$$

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}$$

$$\rho_{12} = \langle 1|\rho|2\rangle$$

$$\rho = |\psi\rangle\langle\psi|$$

$$\boxed{\rho_{mn} = \langle m|\psi\rangle\langle\psi|n\rangle}$$

$$\rho_{mm} = \langle m|\psi\rangle\langle\psi|m\rangle$$
$$= \underline{\underline{|\langle m|\psi\rangle|^2}}$$

$\langle m|\psi\rangle$ and $\langle\psi|m\rangle$ are complex conjugates

$\{|m\rangle\}$ basis states

$$|\psi\rangle = \sum c_m |m\rangle$$

$$\langle m|\psi\rangle = c_m$$

$$\boxed{\rho_{mm} = |c_m|^2}$$

probability of find $|\psi\rangle$ in the state $|$

Diagonal elements in the density matrix gives the probability of finding the state $|\psi\rangle$ in one the eigen states. $|m\rangle$

Off-diagonal elements $m \neq n$

$$\rho_{mn} = \langle m|\rho|n\rangle = \langle m|\psi\rangle\langle\psi|n\rangle$$
$$= c_m c_n^*$$

$$c_m = |c_m| e^{i\phi_m}$$
$$c_n = |c_n| e^{i\phi_n}$$

$$\rho_{mn} = |c_m||c_n| e^{i(\underline{\phi_m - \phi_n})}$$

$\Rightarrow$ off diagonal elements depend on the relative phases between the states $|m\rangle$ and $|n\rangle$

responsible for the phenomena of quantum interference

coherence terms

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{i}{\sqrt{2}}|1\rangle \quad \text{(pure state)}$$
$$= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$$

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\end{pmatrix}$$
$$= \frac{1}{2}\begin{pmatrix}1 & i\\-i & 1\end{pmatrix}$$

- $\mathrm{Tr}(\rho) = \frac{1}{2} + \frac{1}{2} = \underline{\underline{1}}$

- $\boxed{\rho = \rho^{\dagger}}$

$$\rho^{\dagger} = \left[\left\{\frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}\right\}^{T}\right]^{c}$$

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

$$= \rho$$

- Density operator satisfies Liouville equation

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

Mixed states

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

$$\underline{\underline{\mathrm{Tr}(\rho) = 1}}$$

Prove that

1. $\mathrm{Tr}(\rho) = 1$ (Both for pure and mixed states)

2. $\mathrm{Tr}(\rho^2) < 1$ for mixed state

Proof

1. (a) Pure state:

$$\rho = |\psi\rangle\langle\psi|$$

$$|\psi\rangle = \sum c_m |m\rangle$$

$$
\begin{aligned}
Tr(\rho) &= \sum_n \langle n|\rho|n\rangle \\
&= \sum_n \langle n|\psi\rangle\langle\psi|n\rangle \\
&= \sum_n |\langle n|\psi\rangle|^2 \\
&= \sum_n |\overset{=\delta_{nm}}{\langle n|m\rangle}|^2 \, |c_m|^2 \\
&= \sum_n |c_n|^2 \\
&= 1
\end{aligned}
$$

(b) <u>Mixed state</u>

$$\rho = \sum_i p_i \, |\psi_i\rangle\langle\psi_i|$$

$$
\begin{aligned}
Tr(\rho) &= \sum_i \sum_m p_i \, \langle m|\psi_i\rangle\langle\psi_i|m\rangle \\
&= \sum_i \sum_m p_i \, |\langle m|\psi_i\rangle|^2 \qquad \boxed{|\psi_i\rangle = \sum_n c_n|n\rangle} \\
&= \sum_i \sum_m \sum_n p_i \, |\overset{=\delta_{mn}}{\langle m|n\rangle}|^2 \, |c_m|^2 \\
&= \sum_i \sum_n p_i |c_n|^2 \\
&= \sum_i p_i \sum_n |c_n|^2 \\
&= \sum_i p_i \qquad \because \sum_n |c_n|^2 = 1 \\
&= 1
\end{aligned}
$$

2.
$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

$$\rho^2 = \sum_i \sum_j p_i p_j \; |\psi_i\rangle \langle\psi_i|\psi_j\rangle \langle\psi_j|$$

$$Tr(\rho^2) = \sum_n \langle n|\rho^2|n\rangle$$

$$= \sum_n \sum_i \sum_j p_i p_j \; \langle n|\psi_i\rangle \langle\psi_i|\psi_j\rangle \langle\psi_j|n\rangle$$

$$= \sum_n \sum_i \sum_j p_i p_j \; \langle\psi_i|\psi_j\rangle \langle\psi_j|n\rangle \langle n|\psi_i\rangle$$

$$= \sum_i \sum_j p_i p_j \; \langle\psi_i|\psi_j\rangle \langle\psi_j| \underbrace{\left(\sum_n |n\rangle\langle n|\right)}_{I} |\psi_i\rangle$$

$$= \sum_i \sum_j p_i p_j \; \langle\psi_i|\psi_j\rangle \langle\psi_j|\psi_i\rangle$$

$$= \sum_i \sum_j p_i p_j \; |\langle\psi_i|\psi_j\rangle|^2$$

$$\leq \left[\sum_i p_i\right]^2$$

$$\leq 1$$

The equality holds only if $|\langle\psi_i|\psi_j\rangle|^2 = 1$ for every pair of states $|\psi_i\rangle$ and $|\psi_j\rangle$.

<u>Thus</u> $\quad Tr\,\rho^2 = 1$ for pure state

$\quad Tr\,\rho^2 < 1$ for mixed state

$\boxed{\text{A mixed state cannot be represented by a state vector but it is described by density operator}}$

(1) consider an ensemble 50% is in state $|0\rangle$

and 50% is in state $\frac{|0\rangle + |1\rangle}{\sqrt{2}}$

$$\boxed{\rho = \sum p_i |\psi_i\rangle\langle\psi_i|}$$

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}\left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \otimes \left(\frac{\langle 0| + \langle 1|}{\sqrt{2}}\right)$$

$$= \frac{1}{2}|0\rangle\langle 0| + \frac{1}{4}\Big[|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|\Big]$$

$$= \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| + \frac{1}{4}\Big[|0\rangle\langle 1| + |1\rangle\langle 0|\Big]$$

$$\rho = \begin{pmatrix} 3/4 & 1/4 \\ 1/4 & 1/4 \end{pmatrix}$$

(Partially mixed)

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