Density matrix

$$|\psi\rangle = \sum_n C_n |n\rangle$$

$$\{\hat{O}\} \qquad \hat{O}_i |n\rangle = O_{ni} |n\rangle$$

Let

$$\{|\psi\rangle\} \longrightarrow |\psi_1\rangle, |\psi_2\rangle, \ldots$$

$$\langle A\rangle_{est} = \sum_j \omega_j A_j = \sum_j \omega_j \langle\psi_j|\hat{A}|\psi_j\rangle$$

$$= \sum_j \omega_j \left(\sum_n C_{jn}^* \langle n|\right) \hat{A} \left(\sum_m C_{jm} |m\rangle\right)$$

$$= \sum_{m,n} \langle n|\hat{A}|m\rangle \sum_j \omega_j C_{jn}^* C_{jm}$$

but $\qquad C_{jm} = \langle m|\psi_j\rangle$

$$\sum_j \omega_j C_{jn}^* C_{jm} = \sum_j \omega_j \langle\psi_j|n\rangle\langle m|\psi_j\rangle$$

$$= \langle m| \left(\sum_j \omega_j |\psi_j\rangle\langle\psi_j|\right) |n\rangle$$

$$= \langle m|\hat{\rho}|n\rangle = \rho_{mn}$$ density matrix

$$\longrightarrow \qquad \langle A\rangle_{est} = \sum_{m,n} \langle n|\hat{A}|m\rangle\langle m|\hat{\rho}|n\rangle$$

$$= \sum_m \langle m|\hat{\rho}\hat{A}|m\rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$$

Properties:

$$\mathrm{Tr}(\hat{\rho}) = \langle \hat{1} \rangle = \langle\psi|\psi\rangle = 1$$

As

$$\mathrm{Tr}(\hat{\rho}) = \sum_j \langle i| \left(\sum_j \omega_j |j\rangle\langle j|\right) |i\rangle$$

$$= \sum_{ij} \omega_j \langle i|j\rangle\langle j|i\rangle = \sum_i \omega_i$$

Then,

$$\sum_i w_i = 1 \qquad \text{As it should be.}$$

where $w_i \geq 0$ and $w_i^* = w_i$, So

$$\hat{\rho}^+ = \left(\sum_j w_j |j\rangle\langle j|\right)^+ = \sum_j w_j |j\rangle\langle j| = \hat{\rho}$$

Keeping in mind that $\rho_{mn} = \sum_j w_j c_{jn}^* c_{jm}$, then

$$\hat{\rho} = \sum_{m,n} \rho_{mn} |m\rangle\langle n|$$

as

$$\rho(x', x) := \langle x'|\hat{\rho}|x\rangle = \sum_{m,n} \rho_{mn} \langle x'|m\rangle\langle n|x\rangle$$

$$= \sum_{m,n} \rho_{mn} \varphi_m(x') \varphi_n(x)$$

$$\langle A\rangle_{est} = tr(\hat{\rho}\hat{A}) = \int dx \langle x|\hat{\rho}\hat{A}|x\rangle$$

Also,

$$\langle x|\hat{\rho}\hat{A}|x\rangle = \int dx' \langle x|\hat{\rho}|x'\rangle\langle x'|\hat{A}|x\rangle$$

$$= \int dx' \rho(x,x')\langle x'|\hat{A}|x\rangle$$

$$\longrightarrow \langle\hat{A}\rangle_{est} = \iint dx\, dx'\, \rho(x,x')\langle x'|\hat{A}|x\rangle$$

If $w_j = \delta_{ij} \longrightarrow$ pure state

If $w_j \neq \delta_{ij} \longrightarrow$ mixed state

For pure states

$$\hat{\rho} = \sum_i |\psi_i\rangle\langle\psi_i| = \sum_i \delta_{pi} |\psi_i\rangle\langle\psi_i| = |\psi_p\rangle\langle\psi_p|$$

Projector $\hat{P}_p$

In the position representation.

$$\rho_p(x',x)=\langle x'|\psi_p\rangle\langle\psi_p|x\rangle=\psi_p(x')\psi_p^*(x)$$

Moreover,

$$\rho^2=|\psi_p\rangle\langle\psi_p|\psi_p\rangle\langle\psi_p|=|\psi_p\rangle\langle\psi_p|=\hat{\rho}$$

then

$$\hat{\rho}^2=\hat{\rho}\rightarrow \text{Eigenvalues } 0 \text{ and } 1$$

As a result

$\mathrm{Tr}(\hat{\rho})=1 \longrightarrow$ Just one eigenvalue is 1 and the others are 0

For pure states

$$\langle A\rangle_{est}=\mathrm{Tr}(\hat{\rho}\hat{A})=\mathrm{Tr}(|\psi_p\rangle\langle\psi_p|\hat{A}=\langle\psi_p|\hat{A}|\psi_p\rangle$$

Let $|\psi_p\rangle=\sum_n c_n|n\rangle$, then

$$\hat{\rho}=|\psi\rangle\langle\psi|=\sum_{n,m}c_n c_m^*|n\rangle\langle m|$$

$$=\sum_n|c_n|^2|n\rangle\langle n|+\sum_{n\neq m}c_n c_m^*|n\rangle\langle m|$$

interference

Example:

$$|+\rangle=\begin{pmatrix}1\\0\end{pmatrix}\quad,\quad|-\rangle=\begin{pmatrix}0\\1\end{pmatrix}$$

$$\begin{pmatrix}a\\b\end{pmatrix}=a|+\rangle+b|-\rangle \qquad \text{with } |a|^2+|b|^2=1$$

$$\hat{\rho}=\begin{pmatrix}a\\b\end{pmatrix}(a^*\ \ b^*)=\begin{pmatrix}a^*a & ab^*\\a^*b & bb^*\end{pmatrix}$$

$\hat{\rho}_\uparrow=\begin{pmatrix}1&0\\0&0\end{pmatrix}$ spin up $\qquad \hat{\rho}_\downarrow=\begin{pmatrix}0&0\\0&1\end{pmatrix}$ spin down

If $a=b=\frac{1}{\sqrt{2}} \longrightarrow \hat{P}_x = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

Let us think in

$$\hat{P} = p\,\hat{P}_\uparrow + (1-p)\,\hat{P}_\downarrow = \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix}$$

p in general $\neq 0, 1$.