Density Matrix

$$\Psi(x, q, t)$$

$$\bar{f} = \iint dx\, dq\, \Psi^* \hat{f} \Psi$$

$$\rho(q, q', t) = \int dx\, \Psi(x, q, t)\, \Psi^*(x, q', t)$$

$$\bar{f} = \int dq \left[\hat{f} \rho(q, q', t) \right]_{q'=q}$$

$$\rho(q, q, t) = \int dx\, |\Psi|^2 \geq 0 \text{ : prob. density}$$

"Pure" state: $\rho = \Psi(q, t)\, \Psi^*(q', t)$

Spectral representation

(assuming negligeable interaction bedween q & x over sufficiently long period of time)

$\Psi_n(q, t)$: stationary states, $= \Psi_n(q)\, e^{-\frac{i}{\hbar} E_n t}$

$$\rho(q, q', t) = \sum_{mn} \Psi_n^*(q', t)\, \Psi_m(q, t)\, c_{mn}$$

$$= \sum_{mn} W_{mn}\, \Psi_n^*(q')\, \Psi_m(q)$$

* $$= \sum_n \Psi_n^*(q')\, \hat{W}\, \Psi_n(q)$$

$$w_{mn} = C_{mn}\, e^{\frac{i}{\hbar}(E_n - E_m)t}$$

"Pure" state: $C_{mn} = C_m^* C_n$, $\Psi = \sum_n c_n \Psi_n(q,t)$

$$\left(= \sum_n \psi_n^*(q)\, \hat{w}\, \psi_n(q) \right)$$

$$\rho(q,q,t) = \sum_{mn} w_{mn}\, \psi_n^*(q)\, \psi_m(q) \geq 0$$

a) $w_n \equiv w_{nn} \geq 0$

b) $w_n w_m \geq |w_{mn}|^2$

c) $(w^2)_{mn} = w_{mn}$ in a "pure" state

$$\left[\begin{array}{l} \bar{f} = \sum_{mn} w_{mn} f_{mn} = \mathrm{Tr}(\hat{w}\hat{f}) \\ f_{mn} = \int dq\, \psi_n^*(q)\, \hat{f}\, \psi_m(q) \end{array}\right.$$

$$\mathrm{Tr}\,\hat{w} = \sum_n w_n = 1 \qquad (f = 1)$$

$$\left[\begin{array}{l} \dfrac{\partial w_{mn}}{\partial t} = \dfrac{i}{\hbar}(E_n - E_m)\, w_{mn} \\ \dot{\hat{w}} = \dfrac{i}{\hbar}[\hat{w}, \hat{H}] \end{array}\right.$$

Stationary case (required for stat. equil.)

$w_{mn} = 0$ - diagonal! $\bar{f} = \sum_n w_n f_{nn}$

$$\rho = \sum_i \hat{w} |i\rangle\langle i| \leftarrow \text{compare with } (*)$$

In the basis where $\hat{w}$ diagonalizes,

$$\rho = \sum_i w_i |i\rangle\langle i| \leftarrow \text{compare (3.4.8) Sakurai}$$

Examples 1 & 2 in Sakurai

$$\rho^2 = \rho$$

as ought do be in "pure" state

Example 3

ρ - diagonal, corresponds do equil.

$$w_{mn} = \iint dq\,dq'\,\rho(q,q')\,\psi_n(q')\,\psi_m^*(q)$$

$$i\hbar \frac{\partial \rho}{\partial t} = \left(\hat{H} - \hat{H}^{*\prime}\right)\rho(q,q',t)$$

$$dw_q = \rho(q,q,t)\,dq = \sum_n \psi_n^*(q)\,\hat{w}\,\psi_n(q)\,dq$$