

## 4.4. Equilibrium Distribution. Correlation Functions

The operator point of view allows the use of methods of quantum mechanics. However, the Fokker-Planck (FP) hamiltonian [eq(4.22)] is not hermitian. Therefore, its left & right eigenvectors are not the same.

In the study of the equilibrium distribution, we shall assume ergodicity that can either be global or local in each connected component.

The equilibrium distribution, if exists, is defined as

$$P_0(\mathbf{q}) = \lim_{t \rightarrow \infty} P(\mathbf{q}, t) \quad (4.25)$$

$$= \lim_{t \rightarrow \infty} \langle \mathbf{q} | e^{-H(t-t_0)} | \mathbf{q}_0 \rangle \quad [ \text{ see eqs(4.7-8) } ]$$

From eq(4.23a or b), we get

$$\dot{P}_0(\mathbf{q}) = 0 = -\hat{H}(\mathbf{q}) P_0(\mathbf{q}) \quad (4.25a)$$

Thus, besides being, by definition, a time-independent solution of the FP equation,  $P_0(\mathbf{q})$  is also a right eigen-vector of  $H$  with eigenvalue 0.

Let  $| E \rangle$  &  $\langle E |$  be the right & left eigenstates of  $H$  associated with eigenvalue  $E$ . Then

$$H | E \rangle = E | E \rangle \quad \& \quad \langle E | H^\dagger = E^* \langle E | \quad (4.25b)$$

Using the completeness of eigenstates, eq(4.25) becomes

$$P_0(\mathbf{q}) = \lim_{t \rightarrow \infty} \sum_E \langle \mathbf{q} | e^{-H(t-t_0)} | E \rangle \langle E | \mathbf{q}_0 \rangle$$

$$= \lim_{t \rightarrow \infty} \sum_E e^{-E(t-t_0)} \langle \mathbf{q} | E \rangle \langle E | \mathbf{q}_0 \rangle$$

$$= \langle \mathbf{q} | 0 \rangle \langle 0 | \mathbf{q}_0 \rangle$$

$$= \psi_0(\mathbf{q}) \psi_0^*(\mathbf{q}_0) \quad (4.25c)$$

On the other hand, eq(4.25a) indicates

$$P_0(\mathbf{q}) = \langle \mathbf{q} | 0 \rangle = \psi_0(\mathbf{q})$$

$$\rightarrow \psi_0^*(\mathbf{q}_0) = 1 \quad \forall \mathbf{q}_0$$

$$\therefore \psi_0^*(\mathbf{q}) = 1 = \langle 0 | \mathbf{q} \rangle \quad (4.25d)$$

i.e., the left eigenfunction of  $H$  with eigenvalue 0 is the constant 1.

Using the completeness of  $| \mathbf{q} \rangle$ , we have

$$\langle 0 | 0 \rangle = \int d\mathbf{q} \langle 0 | \mathbf{q} \rangle \langle \mathbf{q} | 0 \rangle$$

$$= \int d\mathbf{q} P_0(\mathbf{q}) < \infty \quad (4.26)$$

where the final inequality assumes  $| 0 \rangle$  has a finite norm.

If all energy eigenstates are normalizable, i.e.,

$$\langle E | E \rangle = 1$$

then eq(4.25b) gives

$$\langle E | H | E \rangle = E \quad \& \quad \langle E | H^\dagger | E \rangle = E^*$$

$$\rightarrow \text{Re } E = \frac{1}{2} (E + E^*) = \frac{1}{2} \langle E | H + H^\dagger | E \rangle$$

Since  $\mathbf{q}$  &  $\hat{\mathbf{p}}$  are hermitian, eq(4.22a) gives

$$H = \frac{1}{2} \left[ \Omega \hat{\mathbf{p}}^2 - i \hat{\mathbf{p}} \cdot \mathbf{f}(\hat{\mathbf{q}}) \right] \quad H^* = \frac{1}{2} \left[ \Omega \hat{\mathbf{p}}^2 + i \mathbf{f}(\hat{\mathbf{q}}) \cdot \hat{\mathbf{p}} \right] \quad (4.26a)$$

$$\therefore H + H^* = \Omega \hat{\mathbf{p}}^2 + \frac{i}{2} \left[ \mathbf{f}(\hat{\mathbf{q}}) \cdot \hat{\mathbf{p}} - \hat{\mathbf{p}} \cdot \mathbf{f}(\hat{\mathbf{q}}) \right]$$

$$\begin{aligned} \langle E | [\mathbf{f}(\hat{\mathbf{q}}) \cdot \hat{\mathbf{p}} - \hat{\mathbf{p}} \cdot \mathbf{f}(\hat{\mathbf{q}})] | E \rangle &= \int d\mathbf{q} \int d\mathbf{q}' \langle E | \mathbf{q} \rangle \langle \mathbf{q} | [\mathbf{f}(\hat{\mathbf{q}}) \cdot \hat{\mathbf{p}} - \hat{\mathbf{p}} \cdot \mathbf{f}(\hat{\mathbf{q}})] | \mathbf{q}' \rangle \langle \mathbf{q}' | E \rangle \\ &= \int d\mathbf{q} \int d\mathbf{q}' \psi_E^*(\mathbf{q}) \langle \mathbf{q} | [\mathbf{f}(\mathbf{q}) \cdot \hat{\mathbf{p}} - \hat{\mathbf{p}} \cdot \mathbf{f}(\mathbf{q}')] | \mathbf{q}' \rangle \psi_E(\mathbf{q}') \\ &= \int d\mathbf{q} \int d\mathbf{q}' \psi_E^*(\mathbf{q}) [\mathbf{f}(\mathbf{q}) - \mathbf{f}(\mathbf{q}')] \cdot \langle \mathbf{q} | \hat{\mathbf{p}} | \mathbf{q}' \rangle \psi_E(\mathbf{q}') \\ &= \int d\mathbf{q} \int d\mathbf{q}' \psi_E^*(\mathbf{q}) \psi_E(\mathbf{q}') [\mathbf{f}(\mathbf{q}) - \mathbf{f}(\mathbf{q}')] \cdot \frac{1}{i} \nabla_{\mathbf{q}} \delta(\mathbf{q} - \mathbf{q}') \\ &= 0 \end{aligned}$$

$$\begin{aligned} \therefore \operatorname{Re} E &= \frac{1}{2} \langle E | \Omega \hat{\mathbf{p}}^2 | E \rangle \\ &= \frac{1}{2} \Omega \int d\mathbf{p} \langle E | \hat{\mathbf{p}}^2 | \mathbf{p} \rangle \langle \mathbf{p} | E \rangle \\ &= \frac{1}{2} \Omega \int d\mathbf{p} \mathbf{p}^2 \langle E | \mathbf{p} \rangle \langle \mathbf{p} | E \rangle \\ &= \frac{1}{2} \Omega \int d\mathbf{p} \mathbf{p}^2 |\psi_E(\mathbf{p})|^2 \end{aligned}$$

Since the integrand is everywhere real & non-negative, so is the integral. Hence

$$\operatorname{Re} E \geq 0 \quad (4.26b)$$

which means  $|0\rangle$  is the ground state of  $H$ .

If the state  $|0\rangle$  does not exist, then  $\operatorname{Re} E > 0$  and from eq(4.25),

$$\lim_{t \rightarrow \infty} P(\mathbf{q}, t) = 0$$

If the spectrum of  $H$  has a continuous part that extends down to, but not including, 0, then  $P(\mathbf{q}, t)$  decays algebraically, i.e.,  $P(\mathbf{q}, t) \propto t^n$ . One example is the brownian motion.

Otherwise,  $P(\mathbf{q}, t)$  decays exponentially, i.e.,

$$\dot{P}(\mathbf{q}, t) = -\frac{1}{\operatorname{Re} E} P$$

$$P(\mathbf{q}, t) \propto \exp(-t / \operatorname{Re} E)$$

where  $\tau = \operatorname{Re} E$  is called the relaxation time.

Note that given

$$P_0(\mathbf{q}) = e^{-E(\mathbf{q})} \quad (4.27)$$

does not determine  $\mathbf{f}(\mathbf{q})$  uniquely.

Putting eq(4.27) in eq(4.23) only gives

$$\nabla_{\mathbf{q}} \cdot \left[ (\Omega \nabla_{\mathbf{q}} + \mathbf{f}) e^{-E(\mathbf{q})} \right] = 0$$

$$\rightarrow \partial_i \left[ e^{-E(\mathbf{q})} (-\Omega \partial_i E + f_i) \right] = 0 \quad (4.28a)$$

$$\therefore [\partial_i - (\partial_i E)] (-\Omega \partial_i E + f_i) = 0 \quad (4.28)$$

Setting

$$-\Omega \partial_i E + f_i = V_i(\mathbf{q}) e^{E(\mathbf{q})} \quad (4.29)$$

turns eq(4.28a) into

$$\partial_i V_i(\mathbf{q}) = 0 = \nabla_{\mathbf{q}} \cdot \mathbf{V} \quad (4.30)$$

## Correlation Functions

Consider the general correlation functions

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \langle q(t_1) q(t_2) \dots q(t_n) \rangle_V \quad (4.31)$$

Assuming

$$q(t_0) = q_0 \quad \& \quad t_1 \leq t_2 \leq \dots \leq t_n$$

we can rewrite eq(4.31) as follows.

Using eq(4.5),

$$\langle O[q(t)] \rangle_V = \int d\mathbf{q} O(\mathbf{q}) P(\mathbf{q}, t; \mathbf{q}_0, t_0)$$

the average of  $q(t_n)$  for  $t_n \geq t > t_{n-1}$  can be written as

$$\langle q(t_n) \rangle_V = \int d q_n q_n P(q_n, t_n; q_{n-1}, t_{n-1})$$

so that

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \int d q_n q_n P(q_n, t_n; q_{n-1}, t_{n-1}) \langle q(t_1) q(t_2) \dots q(t_{n-1}) \rangle_V$$

Repeating the procedure for the other  $q(t_k)$ 's, we have

$$\begin{aligned} Z^{(n)}(t_1, t_2, \dots, t_n) &= \int d q_n d q_{n-1} \dots d q_1 q_n P(q_n, t_n; q_{n-1}, t_{n-1}) \\ &\quad \times q_{n-1} P(q_{n-1}, t_{n-1}; q_{n-2}, t_{n-2}) \dots q_1 P(q_1, t_1; q_0, t_0) \end{aligned}$$

Using eq(4.8), we have

$$\begin{aligned} Z^{(n)}(t_1, t_2, \dots, t_n) &= \int d q_n d q_{n-1} \dots d q_1 q_n \langle q_n | e^{-H(t_n - t_{n-1})} | q_{n-1} \rangle \\ &\quad \times q_{n-1} \langle q_{n-1} | e^{-H(t_{n-1} - t_{n-2})} | q_{n-2} \rangle \dots q_1 \langle q_1 | e^{-H(t_1 - t_0)} | q_0 \rangle \\ &= \int d q_n d q_{n-1} \dots d q_1 \langle q_n | \hat{q} e^{-H(t_n - t_{n-1})} | q_{n-1} \rangle \\ &\quad \times \langle q_{n-1} | \hat{q} e^{-H(t_{n-1} - t_{n-2})} | q_{n-2} \rangle \dots \langle q_1 | \hat{q} e^{-H(t_1 - t_0)} | q_0 \rangle \\ &= \int d q_n \langle q_n | \hat{q} e^{-H(t_n - t_{n-1})} \hat{q} e^{-H(t_{n-1} - t_{n-2})} \dots \hat{q} e^{-H(t_1 - t_0)} | q_0 \rangle \end{aligned}$$

Using

$$\begin{aligned} \langle 0 | &= \int d q \langle 0 | q \rangle \langle q | \\ &= \int d q \langle q | \quad [ \text{eq(4.25d) used} ] \end{aligned}$$

we have

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \langle 0 | \hat{q} e^{-H(t_n - t_{n-1})} \hat{q} e^{-H(t_{n-1} - t_{n-2})} \dots \hat{q} e^{-H(t_1 - t_0)} | q_0 \rangle \quad (4.32)$$

Introducing the ‘‘Heisenberg’’ picture operator

$$\hat{Q}(t) = e^{Ht} \hat{q} e^{-Ht} \quad (4.33a)$$

Using  $\langle 0 | H = 0$ , we have

$$\langle 0 | \hat{q} e^{-Ht_n} = \langle 0 | e^{Ht_n} \hat{q} e^{-Ht_n} = \langle 0 | \hat{Q}(t_n)$$

so that eq(4.32) becomes

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \langle 0 | \hat{Q}(t_n) \hat{Q}(t_{n-1}) \dots \hat{Q}(t_1) e^{Ht_0} | q_0 \rangle \quad (4.33)$$

If an equilibrium distribution already exists in the distant past at  $t_0 \rightarrow -\infty$ , we have

$$\begin{aligned} e^{Ht_0} | q_0 \rangle &= \sum_E e^{Et_0} | E \rangle \langle E | q_0 \rangle \\ &= | 0 \rangle \langle 0 | q_0 \rangle \quad \text{for } t_0 \rightarrow -\infty \\ &= | 0 \rangle \quad [\text{eq(4.25d) used}] \end{aligned}$$

$$\rightarrow Z^{(n)}(t_1, t_2, \dots, t_n) = \langle 0 | \hat{Q}(t_n) \hat{Q}(t_{n-1}) \dots \hat{Q}(t_1) | 0 \rangle \quad (4.34)$$

which is just the equilibrium correlation function [c.f. eq(2.40)].

## Time Evolution of Observables

The Heisenberg representation of a Schrodinger picture operator  $O(\hat{q})$  is defined as

$$\begin{aligned} O(\hat{q})(t) &= e^{Ht} O(\hat{q}) e^{-Ht} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k O(q)}{d q^k} \Big|_{q=0} e^{Ht} \hat{q}^k e^{-Ht} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k O(q)}{d q^k} \Big|_{q=0} \hat{Q}(t)^k \\ &= O[\hat{Q}(t)] \end{aligned}$$

$$\begin{aligned} \rightarrow \frac{d}{dt} O[\hat{Q}(t)] &= H e^{Ht} O(\hat{q}) e^{-Ht} - e^{Ht} O(\hat{q}) e^{-Ht} H \\ &= [H, O[\hat{Q}(t)]] \\ &= e^{Ht} H O(\hat{q}) e^{-Ht} - e^{Ht} O(\hat{q}) H e^{-Ht} \\ &= e^{Ht} (H O(\hat{q}) - O(\hat{q}) H) e^{-Ht} \\ &= e^{Ht} [H, O(\hat{q})] e^{-Ht} \quad (1) \end{aligned}$$

$$\therefore \frac{d}{dt} (O[\hat{Q}(t)] e^{Ht_0}) = [H, O[\hat{Q}(t)] e^{Ht_0}]$$

Eqs(4.5 & 4.33) then give

$$\begin{aligned} \langle O[q(t)] \rangle_{\nu} &= \langle 0 | O[\hat{Q}(t)] e^{Ht_0} | q_0 \rangle \quad (2) \\ &= \langle 0 | e^{Ht} O(\hat{q}) e^{-Ht} e^{Ht_0} | q_0 \rangle \\ &= \langle 0 | e^{H(t-t_0)} O(\hat{q}) e^{-H(t-t_0)} | q_0 \rangle \quad [\langle 0 | H = 0 \text{ used}] \\ &= \langle 0 | O[\hat{Q}(t-t_0)] | q_0 \rangle \end{aligned}$$

The matrix element of  $O[\hat{Q}(t-t_0)]$  between the states  $\langle 0 |$  &  $| q \rangle$  is defined as

$$\begin{aligned} O(q, t) &\equiv \langle 0 | O[\hat{Q}(t-t_0)] | q \rangle & (4.35a) \\ &= \langle 0 | O[\hat{Q}(t)] e^{Ht_0} | q \rangle \end{aligned}$$

$$\rightarrow \dot{O}(q, t) = \langle 0 | \dot{O}[\hat{Q}(t-t_0)] | q \rangle \quad (4.35b)$$

In the Schrodinger picture ( or at  $t = t_0$  )

$$[H, O(\hat{q})] = \left[ \frac{1}{2} \{ \Omega \hat{p}^2 - i \hat{p} f(\hat{q}) \}, O(\hat{q}) \right] \quad [\text{Eq(4.26a) used}] \quad (3)$$

Using

$$\begin{aligned} [\hat{p}, \hat{q}] &= -i \\ [\hat{p}, \hat{q}^k] &= [\hat{p}, \hat{q} \hat{q}^{k-1}] = [\hat{p}, \hat{q}] \hat{q}^{k-1} + \hat{q} [\hat{p}, \hat{q}^{k-1}] = -i \hat{q}^{k-1} + \hat{q} [\hat{p}, \hat{q}^{k-1}] \end{aligned} \quad (4)$$

Assuming

$$[\hat{p}, \hat{q}^n] = -i n \hat{q}^{n-1} \quad (5)$$

has been proved for  $n = k - 1$ , eq(1) becomes

$$[\hat{p}, \hat{q}^k] = -i \hat{q}^{k-1} - i(k-1) \hat{q}^{k-1} = -i k \hat{q}^{k-1}$$

thus proving eq(5) by the method of induction.

$$\begin{aligned} [\hat{p}, O(\hat{q})] &= \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k O(q)}{d q^k} \Big|_{q=0} [\hat{p}, \hat{q}^k] \\ &= -i \sum_{k=0}^{\infty} \frac{1}{(k-1)!} \frac{d^k O(q)}{d q^k} \Big|_{q=0} \hat{q}^{k-1} & [\text{Eq(5) used}] \\ &= -i \frac{\partial O(q)}{\partial q} \Big|_{q=\hat{q}} \\ &\equiv -i O'(\hat{q}) \end{aligned} \quad (6)$$

$$\begin{aligned} \langle 0 | [\hat{p}, O(\hat{q})] | q \rangle &= -i \langle 0 | O'(\hat{q}) | q \rangle \\ &= -i \frac{\partial O(q)}{\partial q} \langle 0 | q \rangle \\ &= -i \frac{\partial O(q)}{\partial q} & [\text{Eq(4.25d) used}] \end{aligned} \quad (7)$$

$$\begin{aligned} \rightarrow [\hat{p} f(\hat{q}), O(\hat{q})] &= [\hat{p}, O(\hat{q})] f(\hat{q}) \\ &= -i O'(\hat{q}) f(\hat{q}) & [\text{Eq(6) used}] \end{aligned}$$

$$\begin{aligned} \therefore \langle 0 | [\hat{p} f(\hat{q}), O(\hat{q})] | q \rangle &= -i \langle 0 | O'(\hat{q}) f(\hat{q}) | q \rangle \\ &= -i \frac{\partial O(q)}{\partial q} f(q) \\ &= -i f(q) \frac{\partial}{\partial q} \langle 0 | O(\hat{q}) | q \rangle \end{aligned} \quad (8)$$

Similarly

$$\begin{aligned} [\hat{p}^2, O(\hat{q})] &= [\hat{p}, O(\hat{q})] \hat{p} + \hat{p} [\hat{p}, O(\hat{q})] \\ &= -i \{ O'(\hat{q}) \hat{p} + \hat{p} O'(\hat{q}) \} \\ &= -i \{ [\hat{p}, O'(\hat{q})] + 2 O'(\hat{q}) \hat{p} \} \\ &= -i \{ -i O''(\hat{q}) + 2 O'(\hat{q}) \hat{p} \} \end{aligned}$$

where

$$O''(\hat{q}) = \left. \frac{\partial^2 O(q)}{\partial q^2} \right|_{q=\hat{q}}$$

$$\rightarrow \langle 0 | [\hat{p}^2, O(\hat{q})] | q \rangle = -\langle 0 | O''(\hat{q}) | q \rangle - 2i \langle 0 | O'(\hat{q}) \hat{p} | q \rangle \quad (9)$$

In the  $q$ -representation,

$$\langle q | \hat{p} | \psi \rangle = -i \partial_q \langle q | \psi \rangle$$

Using

$$\begin{aligned} \langle 0 | O'(\hat{q}) \hat{p} | q \rangle &= \langle q | \hat{p} O'(\hat{q}) | 0 \rangle^* \\ &= [-i \partial_q \langle q | O'(\hat{q}) | 0 \rangle]^* \\ &= i \partial_q \langle 0 | O'(\hat{q}) | q \rangle \\ &= i \partial_q^2 \langle 0 | O(\hat{q}) | q \rangle \end{aligned}$$

eq(9) becomes

$$\langle 0 | [\hat{p}^2, O(\hat{q})] | q \rangle = \partial_q^2 \langle 0 | O(\hat{q}) | q \rangle \quad (10)$$

Putting eqs(8 & 10) into eq(3) gives

$$\langle 0 | [H, O(\hat{q})] | q \rangle = \frac{1}{2} \left\{ \Omega \partial_q^2 - f(q) \frac{\partial}{\partial q} \right\} \langle 0 | O(\hat{q}) | q \rangle$$

In the Heisenberg picture at  $t - t_0$ , this becomes

$$\begin{aligned} \langle 0 | [H, O[\hat{Q}(t - t_0)]] | q \rangle &= \frac{1}{2} \left\{ \Omega \partial_q^2 - f(q) \frac{\partial}{\partial q} \right\} \langle 0 | O[\hat{Q}(t - t_0)] | q \rangle \\ &= \frac{1}{2} \left\{ \Omega \partial_q^2 - f(q) \frac{\partial}{\partial q} \right\} O(q, t) \end{aligned}$$

Eq(4.35b) thus becomes

$$\begin{aligned} \dot{O}(q, t) &= \frac{1}{2} \left\{ \Omega \partial_q^2 - f(q) \frac{\partial}{\partial q} \right\} O(q, t) \\ &= \frac{1}{2} \left\{ \Omega \partial_q - f(q) \right\} \frac{\partial}{\partial q} O(q, t) \end{aligned} \quad (4.35)$$

Using eq(4.35), we can write eq(2) as

$$\begin{aligned} \langle O[q(t)] \rangle_\nu &= \int dq \langle 0 | O[\hat{Q}(t)] e^{H t_0} | q \rangle \delta(q - q_0) \\ &= \int dq O(q, t) \delta(q - q_0) \end{aligned} \quad (4.36)$$