3.10. Correlation Functions, Generating Functional, and Wick Expansion

The thermal correlation functions of n-variables $x(\tau_j)$ are defined as

$$G^{(n)}_{\omega^2}(\tau_1,\ \ldots,\ \tau_n) \equiv \frac{1}{Z}\oint \mathcal{D}\,x\,x(\tau_1)\ldots x(\tau_n)\exp\left(-\frac{1}{\hbar}\mathcal{A}_e\right) \tag{3.295a}$$

$$= \frac{1}{Z}\mathrm{Tr}\left\{\hat{T}_\tau\left[\hat{x}_H(\tau_1)\ldots\hat{x}_H(\tau_n)\,e^{-\beta\hat{H}}\right]\right\} \tag{3.296}$$

$$\equiv \langle\, x(\tau_1)\ldots x(\tau_n)\,\rangle \tag{3.295}$$

where $\hat{T}_\tau$ is the imaginary-time-ordering operator, $\hat{x}_H(\tau)$ an operator in the Heisenberg picture, and

$$Z = e^{-\beta F} = \mathrm{Tr}\,e^{-\beta\hat{H}} \tag{3.297}$$

$$= \oint \mathcal{D}\,x\,\exp\left(-\frac{1}{\hbar}\mathcal{A}_e\right)$$

is the partition function with Helmholtz free energy F.

Equivalence of (3.296) & (3.296a) can be demonstrated by the familiar time-slice technique. Obviously, one should work with lattices that include the n-points τ_j.

Let the result of time-ordering be

$$\hat{T}_\tau[\,\tau_1,\ \ldots,\ \tau_j,\ \ldots,\ \tau_n\,] = \left\{\,\tau_{t(n)},\ \ldots,\ \tau_{t(j)},\ \ldots,\ \tau_{t(1)}\,\right\} \tag{3.297a}$$

For convenience, we denote the end-points of the time interval as

$$\tau_{t(n+1)} = \beta\hbar \qquad\qquad \tau_{t(0)} = 0$$

so that the time-axis is divided into $n+1$ sections marked by $n+2$ points:

$$\beta\hbar \_\_\_ \tau_{t(n)} \_\_\_ \tau_{t(n-1)} \ldots\ldots \tau_{t(j)} \ldots\ldots \tau_{t(1)} \_\_\_ 0$$

The positions at these points are denoted as

$$x(\tau_{t(j)}) \equiv x_{t(j)}$$

with the the periodic B.C.

$$x(\beta\hbar) = x_{t(n+1)} = x(0) = x_{t(0)} \tag{3.297b}$$

Using

$$\left(x_{t(j)}\ \tau_{t(j)}\,\middle|\,x_{t(j-1)}\ \tau_{t(j-1)}\right) = \int_{x_{t(j-1)}}^{x_{t(j)}} \mathcal{D}\,x\exp\left(-\frac{1}{\hbar}\mathcal{A}_e\right)$$

(3.295) becomes

$$G^{(n)}_{\omega^2}(\tau_1,\ \ldots,\ \tau_n) = \frac{1}{Z}\left(\prod_{j=1}^{n+1}\int_{-\infty}^{\infty} d\,x_{t(j)}\right)\left(x_{t(n+1)},\ \beta\hbar\,\middle|\,x_{t(n)}\ \tau_{t(n)}\right)x_{t(n)} \tag{3.298}$$

$$\cdot\ \ldots\cdot x_{t(j)}\left(x_{t(j)}\ \tau_{t(j)}\,\middle|\,x_{t(j-1)}\ \tau_{t(j-1)}\right)x_{t(j-1)}$$

$$\cdot\ \ldots\cdot x_{t(1)}\left(x_{t(1)}\ \tau_{t(1)}\,\middle|\,x_{t(n+1)},\ 0\right)$$

Using [c.f. (3.233-4)]

$$Z[j] = \oint \mathcal{D}\,x\,\exp\left(-\frac{1}{\hbar}\mathcal{A}_e[j]\right)$$

$$= \oint \mathcal{D}\,x\,\exp\left\{-\frac{1}{\hbar}\left[\mathcal{A}_e + \mathcal{A}^j_e\right]\right\} \tag{3.298a}$$

where

$$\mathcal{A}_e^j = -\int_0^{\beta\hbar} d\tau\, j(\tau)\, x(\tau) \tag{3.298b}$$

we get

$$\frac{\delta}{\delta j(\tau_1)} Z[j] = \frac{1}{\hbar} \oint \mathcal{D}x\, x(\tau_1) \exp\left(-\frac{1}{\hbar}\mathcal{A}_e[j]\right)$$

so that (3.295) becomes

$$G_{\omega^2}^{(n)}(\tau_1, \ldots, \tau_n) = \left\{ \frac{1}{Z[j]} \hbar \frac{\delta}{\delta j(\tau_1)} \ldots \hbar \frac{\delta}{\delta j(\tau_n)} Z[j] \right\}_{j=0} \tag{3.299}$$

In the case of a harmonic action, $Z[j]$ takes the separable form [see (3.243-4)]

$$Z[j] = Z_\omega \exp\left(-\frac{1}{\hbar}\mathcal{A}_e^j\right) \tag{3.299a}$$

where

$$-\mathcal{A}_e^j = \frac{1}{2M} \int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, j(\tau)\, G_{\omega^2,e}^p(\tau - \tau')\, j(\tau') \tag{3.299b}$$

Hence,

$$G_{\omega^2}^{(n)}(\tau_1, \ldots, \tau_n) = \left\{ \hbar \frac{\delta}{\delta j(\tau_1)} \ldots \hbar \frac{\delta}{\delta j(\tau_n)} \exp\left(-\frac{1}{\hbar}\mathcal{A}_e^j\right) \right\}_{j=0} \tag{3.300}$$

which no longer depends on Z_ω.

The functional derivatives are easily performed by 1st expanding the exponential as a Taylor series. The condition $j = 0$ means that all odd power terms must vanish.

For $n = 2$, we have

$$\hbar \frac{\delta}{\delta j(\tau)} \exp\left\{-\frac{1}{\hbar}\mathcal{A}_e^j\right\}$$
$$= \hbar \frac{\delta}{\delta j(\tau)} \left\{ 1 + \frac{1}{2M\hbar} \int_0^{\beta\hbar} d\tau_1 \int_0^{\beta\hbar} d\tau_2\, j(\tau_1)\, G_{\omega^2,e}^p(\tau_1 - \tau_2)\, j(\tau_2) + O[j^4] \right\}$$
$$= \frac{1}{2M} \left\{ \int_0^{\beta\hbar} d\tau_2\, G_{\omega^2,e}^p(\tau - \tau_2)\, j(\tau_2) + \int_0^{\beta\hbar} d\tau_1\, j(\tau_1)\, G_{\omega^2,e}^p(\tau_1 - \tau) \right\} + O[j^3]$$
$$= \frac{1}{M} \int_0^{\beta\hbar} d\tau_1\, G_{\omega^2,e}^p(\tau - \tau_1)\, j(\tau_1) + O[j^3]$$

where we've used the symmetric property of all Green functions

$$G(\tau, \tau') = G(\tau', \tau) \tag{3.300a}$$

which inherent to their defining differential equations.

Hence,

$$\hbar \frac{\delta}{\delta j(\tau')} \hbar \frac{\delta}{\delta j(\tau)} \exp\left(-\frac{1}{\hbar}\mathcal{A}_e^j\right) = \frac{\hbar}{M} G_{\omega^2,e}^p(\tau - \tau') + O[j^2]$$

Therefore,

$$G_{\omega^2}^{(2)}(\tau_1, \tau_2) = \frac{\hbar}{M} G_{\omega^2,e}^p(\tau_1 - \tau_2) \tag{3.301}$$

For a general even n, we see that the only surviving terms in (3.300) are products of $\frac{n}{2}$ factors of $G_{\omega^2}^{(2)}(\tau_j, \tau_k)$ that come from the $\frac{n}{2}$-order of the Taylor expansion of $\exp\left(-\frac{1}{\hbar}\mathcal{A}_e^j\right)$. Hence, (3.300) becomes

$$G_{\omega^2}^{(n)}(\tau_1, \ldots, \tau_n) = \frac{\hbar^{n/2}}{(n/2)!} \left\{ \frac{\delta}{\delta j(\tau_1)} \cdots \frac{\delta}{\delta j(\tau_n)} \left(\mathcal{A}_e^j\right)^{n/2} \right\}_{j=0} \tag{3.301a}$$

Owing to the symmetry (3.300a), the functional derivatives in (3.301a) produce $\frac{n!}{2^n}$ terms, each of which is a product of $\frac{n}{2}$ factors of $G_{\omega^2}^{(2)}(\tau_j, \tau_k)$. On the other hand, the number of distinct terms in (3.301a) is

$$\frac{n!}{2^{n/2}\left(\frac{n}{2}\right)!} = \frac{n(n-1)\ldots 2\cdot 1}{2^{n/2}\left(\frac{n}{2}\right)\left(\frac{n}{2}-1\right)\ldots 2\cdot 1} = \frac{n(n-1)\ldots 2\cdot 1}{n\,(n-2)\ldots 4\cdot 2} = (n-1)!!$$

which is just the number of distinct ways to pair up n objects with both orders within each pair and among the $\frac{n}{2}$ pairs being immaterial. Hence, there are

$$\frac{n!}{2^n} \Big/ \left(\frac{n!}{2^{n/2}\left(\frac{n}{2}\right)!}\right) = \left(\frac{n}{2}\right)!$$

copies of each distinct term in (3.301a). Therefore, (3.301a) can be written as

$$G_{\omega^2}^{(n)}(\tau_1, \ldots, \tau_n) = \sum_P G_{\omega^2}^{(2)}(\tau_{P(1)}, \tau_{P(2)}) \ldots G_{\omega^2}^{(2)}(\tau_{P(n-1)}, \tau_{P(n)}) \tag{3.302}$$

where P is the set of index permutations that produce all distinct product terms.

(3.302) is known as Wick's rule or Wick's expansion.

As an example, consider the case $n = 4$. The $(4-1)!! = 3$ distinct terms can be read from the following "pairing" graphs

$$\dot{1}\,\dot{2}\,\overset{\times}{3}\,\overset{\times}{4} \qquad \dot{1}\,\overset{\times}{2}\,\dot{3}\,\overset{\times}{4} \qquad \dot{1}\,\overset{\times}{2}\,\overset{\times}{3}\,\dot{4} \tag{3.303}$$

→ $G(1,2)\,G(3,4)\;\; G(1,3)\,G(2,4)\;\; G(1,4)\,G(2,3)$

or $\langle 1, 2\rangle\langle 3, 4\rangle \qquad \langle 1, 3\rangle\langle 2, 4\rangle \qquad \langle 1, 4\rangle\langle 2, 3\rangle$

where

$$G(i, j) \equiv \langle i, j\rangle \equiv G_{\omega^2}^{(2)}(\tau_i, \tau_j) \equiv \langle x(\tau_i)\, x(\tau_j)\rangle$$

Note: In hand-writtings, it's more vivid to use $\overset{\frown}{j\,k}$ instead of $\dot{j}\,\dot{k}$ to denote a pairing.

Another form of the Wick's rule is

$$\left\langle e^{K x}\right\rangle = e^{K^2 \langle x^2\rangle/2} \tag{3.304}$$

To prove this, we begin by writing (3.233) as

$$Z_\omega[j] = Z_\omega \left\langle \exp\left\{ \frac{1}{\hbar} \int_0^{\beta\hbar} d\tau\, j(\tau)\, x(\tau) \right\} \right\rangle \tag{3.305}$$

so that (3.243) implies

$$\left\langle \exp\left\{ \frac{1}{\hbar} \int_0^{\beta\hbar} d\tau\, j(\tau)\, x(\tau) \right\} \right\rangle$$
$$= \exp\left\{ \frac{1}{2M\hbar} \int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, j(\tau)\, G_{\omega^2,e}^{p}(\tau-\tau')\, j(\tau') \right\} \tag{3.306}$$

For

$$j(\tau) = \hbar K\, \delta(\tau - \tau_1)$$

(3.306) becomes

$$\left\langle \exp\left[K x(\tau_1) \right] \right\rangle_T = \exp\left\{ \frac{\hbar}{2M} K^2\, G_{\omega^2,e}^{p}(\tau_1) \right\}$$
$$= \exp\left\{ \frac{1}{2} K^2 \langle x(\tau_1)\, x(\tau_1)\rangle \right\} \quad \text{[(3.301) used.]} \tag{3.306a}$$

thus proving (3.304).

Let

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{\boldsymbol{k}} e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}}\,\boldsymbol{u}(\boldsymbol{k})$$

we have

$$-\nabla\cdot\boldsymbol{u}(\boldsymbol{x}) = \sum_{\boldsymbol{k}} e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}}\,\boldsymbol{k}\cdot\boldsymbol{u}(\boldsymbol{k})$$

Using (3.304), the Gaussian approximation of the Debye-Waller factor can be written as

$$\begin{aligned} e^{-W} &\equiv \left\langle e^{-\nabla\cdot\boldsymbol{u}(\boldsymbol{x})}\right\rangle \\ &= \exp\left\{\frac{1}{2}\sum_{\boldsymbol{k},\boldsymbol{k}'}\left\langle e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}}\,e^{i\,\boldsymbol{k}'\cdot\boldsymbol{x}}\right\rangle \boldsymbol{k}\cdot\boldsymbol{u}(\boldsymbol{k})\,\boldsymbol{k}'\cdot\boldsymbol{u}(\boldsymbol{k}')\right\} \\ &= \exp\left\{\frac{1}{2}\sum_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\boldsymbol{k},-\boldsymbol{k}'}\,\boldsymbol{k}\cdot\boldsymbol{u}(\boldsymbol{k})\,\boldsymbol{k}'\cdot\boldsymbol{u}(\boldsymbol{k}')\right\} \\ &= \exp\left\{-\frac{1}{2}\sum_{\boldsymbol{k}}\boldsymbol{k}\cdot\boldsymbol{u}(\boldsymbol{k})\,\boldsymbol{k}\cdot\boldsymbol{u}(-\boldsymbol{k})\right\} \\ &= \exp\left\{-\frac{1}{2}\sum_{\boldsymbol{k}}\left|\boldsymbol{k}\cdot\boldsymbol{u}(\boldsymbol{k})\right|^2\right\} \end{aligned} \qquad (3.308)$$

The Wick's rule implies

$$\langle x(\tau)\rangle = \left\{\hbar\frac{\delta}{\delta j(\tau)}\exp\left(-\frac{1}{\hbar}\mathcal{A}_e^j[j]\right)\right\}_{j=0} = 0$$

In case $\langle x(\tau)\rangle \neq 0$, (3.299a) should be replaced with

$$\begin{aligned} -\mathcal{A}_e^j[j] &= \int_0^{\beta\hbar} d\tau\, j(\tau)\,[\,x(\tau) - \langle x\rangle\,] \\ &= \frac{1}{2M}\int_0^{\beta\hbar} d\tau\int_0^{\beta\hbar} d\tau'\, j(\tau)\,G^p_{\omega^2,e}(\tau-\tau')\,j(\tau') \end{aligned}$$

so that (3.301a) gives

$$G^{(1)}_{\omega^2}(\tau_i,\ \tau_j) = \langle x\rangle$$

$$G^{(2)}_{\omega^2}(\tau_i,\ \tau_j) = \left\langle\left[x(\tau_i) - \langle x\rangle\right]\left[x(\tau_j) - \langle x\rangle\right]\right\rangle$$

(3.306a) is thus revised as

$$\begin{aligned} \left\langle\exp\left\{K\left[x(\tau_1) - \langle x\rangle\right]\right\}\right\rangle &= \exp\left\{\frac{\hbar}{2M}K^2\,G^p_{\omega^2,e}(\tau_1)\right\} \\ &= \exp\left\{\frac{1}{2}K^2\left\langle\left[x(\tau_1) - \langle x\rangle\right]\left[x(\tau_1) - \langle x\rangle\right]\right\rangle\right\} \end{aligned}$$

$$\to \quad \left\langle\exp\left\{K\,x(\tau_1)\right\}\right\rangle = \exp\left\{\frac{1}{2}K^2\left\langle\left[x(\tau_1) - \langle x\rangle\right]\left[x(\tau_1) - \langle x\rangle\right]\right\rangle + K\langle x\rangle\right\} \qquad (3.309)$$

3.10.1. Real-Time Correlation Functions

The correlation functions for the real-time fluctuations $\delta x(t)$ are similarly defined. Dropping the δ for the sake of simplicity, we have

$$\begin{aligned} G^{(n)}_{\omega^2}(t_1,\ \ldots,\ t_n) &\equiv \frac{1}{Z}\int_{x_b=x_a=0}\mathcal{D}x\, x(t_1)\ldots x(t_n)\exp\left(\frac{i}{\hbar}\mathcal{A}\right) \\ &\equiv \langle x(t_1)\ldots x(t_n)\rangle \end{aligned} \qquad (3.310a)$$

where

$$Z = \int_{x_b=x_a=0} \mathcal{D}\, x \, \exp\left(\frac{i}{\hbar}\mathcal{A}\right) = (\,0\ t_b \mid 0\ t_a)_\omega \qquad (3.310b)$$

(3.298-9) now become [see §3.1]

$$\begin{aligned} Z[j] &= \int \mathcal{D}\, x \, \exp\left(\frac{i}{\hbar}\mathcal{A}[j]\right) \\ &= \int \mathcal{D}\, x \, \exp\left\{\frac{i}{\hbar}[\mathcal{A} + \mathcal{A}_j]\right\} \qquad (3.310c) \\ &= (\,0\ t_b \mid 0\ t_a)^j_\omega \end{aligned}$$

where

$$\mathcal{A}_j = \int_{t_a}^{t_b} d\,t\, j(t)\, x(t) \qquad (3.310d)$$

we get

$$\frac{\delta}{\delta\, j(t_1)} Z[j] = \frac{i}{\hbar} \int \mathcal{D}\, x\, x(t_1) \exp\left(\frac{i}{\hbar}\mathcal{A}[j]\right)$$

$$G^{(n)}_{\omega^2}(t_1,\ \ldots,\ t_n) = \left\{\frac{1}{Z[j]}\frac{\hbar}{i}\frac{\delta}{\delta\, j(t_1)} \ldots \frac{\hbar}{i}\frac{\delta}{\delta\, j(t_n)} Z[j]\right\}_{j=0} \qquad (3.310e)$$

In the case of a harmonic action, $Z[j]$ takes the separable form

$$Z[j] = Z_\omega \exp\left(\frac{i}{\hbar}\tilde{\mathcal{A}}_{j,\text{fl}}\right) \qquad (3.310f)$$

where [see (3.22)]

$$\tilde{\mathcal{A}}_{j,\,\text{fl}} = \frac{1}{2\,M}\int_{t_a}^{t_b} d\,t \int_{t_a}^{t_b} d\,t'\ j(t)\, G_{\omega^2}(t,\,t')\, j(t') \qquad (3.310g)$$

with [see (3.36)]

$$G_{\omega^2}(t,\,t') = \frac{1}{\omega \sin\omega\,(t_b - t_a)} \sin\omega\,(t_b - t_>) \sin\omega\,(t_< - t_a) \qquad (3.310h)$$

Hence, (3.310e) simplifies to

$$G^{(n)}_{\omega^2}(t_1,\ \ldots,\ t_n) = \left\{\frac{\hbar}{i}\frac{\delta}{\delta\, j(t_1)} \ldots \frac{\hbar}{i}\frac{\delta}{\delta\, j(t_n)} \exp\left(\frac{i}{\hbar}\tilde{\mathcal{A}}_{j,\text{fl}}\right)\right\}_{j=0} \qquad (3.310i)$$

which no longer depends on Z_ω.

For $n = 2$, we have

$$\begin{aligned} &\frac{\hbar}{i}\frac{\delta}{\delta\, j(t)} \exp\left(\frac{i}{\hbar}\tilde{\mathcal{A}}_{j,\text{fl}}\right) \\ &= \frac{\hbar}{i}\frac{\delta}{\delta\, j(t)}\left\{1 + \frac{i}{2\,M\,\hbar}\int_{t_a}^{t_b} d\,t_1 \int_{t_a}^{t_b} d\,t_2\, j(t_1)\, G_{\omega^2}(t_1 - t_2)\, j(t_2) + O\left[j^4\right]\right\} \\ &= \frac{1}{2\,M}\left\{\int_{t_a}^{t_b} d\,t_2\, G_{\omega^2}(t - t_2)\, j(t_2) + \int_{t_a}^{t_b} d\,t_1\ j(t_1)\, G_{\omega^2}(t_1 - t)\right\} + O\left[j^3\right] \\ &= \frac{1}{M}\int_{t_a}^{t_b} d\,t_1\, G_{\omega^2}(t - t_1)\, j(t_1) + O\left[j^3\right] \end{aligned}$$

where we’ve used the symmetric property of all Green functions

$$G(t,\,t') = G(t',\,t)$$

which inherent to their defining differential equations.

Hence,

$$\frac{\hbar}{i}\frac{\delta}{\delta\, j(t')}\frac{\hbar}{i}\frac{\delta}{\delta\, j(t)} \exp\left(\frac{i}{\hbar}\tilde{\mathcal{A}}_{j,\text{fl}}\right) = \frac{\hbar}{i\,M} G_{\omega^2}(t - t') + O\left[j^2\right]$$

Therefore,

$$G^{(2)}_{\omega^2}(t,\, t') = \frac{\hbar}{i\, M}\, G_{\omega^2}(t - t') \tag{3.310}$$

The velocity correlation functions can be calculated by replacing the source term (3.310d) with

$$\mathcal{A}_k = \int_{t_a}^{t_b} d\,t\, k(t)\, \dot{x}\,(t) \tag{3.311a}$$

so that

$$\langle\, \dot{x}\,(t_1) \ldots \dot{x}(t_n)\, \rangle\ = \left\{ \frac{\hbar}{i}\, \frac{\delta}{\delta\, k(t_1)} \ldots \frac{\hbar}{i}\, \frac{\delta}{\delta\, k(t_n)}\, \exp\!\left(\frac{i}{\hbar}\, \tilde{\mathcal{A}}_{j,v} \right) \right\}_{k=0} \tag{3.311b}$$

The Lagrangian thus becomes

$$L = \frac{1}{2}\, m\, \dot{x}^2 - \frac{1}{2}\, m\, \omega^2\, x^2 + k(t)\, \dot{x}$$

which gives the classical eq. of motion as

$$\ddot{x} + \omega^2\, x = -\frac{\dot{k}}{M}$$

$$\to \qquad x(t) = \frac{1}{M} \int_{t_a}^{t_b} d\, t'\, G_{\omega^2}(t,\, t')\, \dot{k}(t')$$

$$\therefore \qquad \dot{x}(t) = \frac{1}{M} \int_{t_a}^{t_b} d\, t'\, \partial_t\, G_{\omega^2}(t,\, t')\, \dot{k}(t')$$

Using the trick (3.22a), we have

$$\begin{aligned} \tilde{\mathcal{A}}_{k,\,\text{fl}} &= \frac{1}{2\, M} \int_{t_a}^{t_b} d\, t \int_{t_a}^{t_b} d\, t'\;\, k(t\,)\, \partial_t\, G_{\omega^2}(t,\, t')\, \dot{k}(t') \\ &= -\frac{1}{2\, M} \int_{t_a}^{t_b} d\, t \int_{t_a}^{t_b} d\, t'\;\, k(t\,)\, \partial_t \partial_{t'}\, G_{\omega^2}(t,\, t')\, k(t') \end{aligned} \tag{3.311c}$$

For $n = 2$, we have

$$\langle\, \dot{x}(t)\, \dot{x}(t')\, \rangle = i\, \frac{\hbar}{M}\, \partial_t \partial_{t'}\, G_{\omega^2}(t - t') \tag{3.311d}$$

(3.311d) thus becomes

$$\langle\, \dot{x}(t)\, \dot{x}(t')\, \rangle = i\, \frac{\hbar\, \omega}{M}\, \frac{1}{\sin\, \omega(t_b - t_a)}\, \cos\, \omega(t_b - t_>)\, \cos\, \omega(t_< - t_a) \tag{3.311}$$

$$\to \qquad \langle\, \dot{x}(t_b)\, \dot{x}(t_b)\, \rangle = i\, \frac{\hbar\, \omega}{M}\, \frac{\cos\, \omega(t_b - t_a)}{\sin\, \omega\, (t_b - t_a)} = i\, \frac{\hbar\, \omega}{M}\, \cot\omega(t_b - t_a) \tag{3.312}$$

For a D-D system,

$$(\, \boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) = \int \mathcal{D}\, \boldsymbol{x}\, \exp\!\left[\frac{i}{\hbar} \int_{t_a}^{t_b} d\, t\, L(\boldsymbol{x},\, \dot{\boldsymbol{x}}) \right] \tag{3.313a}$$

we have

$$\begin{aligned} i\, \hbar\, \partial_{t_b} (\, \boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) &= -\int \mathcal{D}\, \boldsymbol{x}\, L\, (\boldsymbol{x}_b,\, \dot{\boldsymbol{x}}_b)\, \exp\!\left[\frac{i}{\hbar} \int_{t_a}^{t_b} d\, t\, L(\boldsymbol{x},\, \dot{\boldsymbol{x}}) \right] \\ &= -\left\langle L(\boldsymbol{x}_b,\, \dot{\boldsymbol{x}}_b) \right\rangle (\, \boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) \end{aligned} \tag{3.313}$$

Now,

$$\begin{aligned} \left\langle L(\boldsymbol{x}_b,\, \dot{\boldsymbol{x}}_b) \right\rangle &= \left\langle L\left[\boldsymbol{x}_{\text{cl}}(t_b),\, \dot{\boldsymbol{x}}_{\text{cl}}(t_b) \right] + L(\boldsymbol{x}_b,\, \dot{\boldsymbol{x}}_b) - L\left[\boldsymbol{x}_{\text{cl}}(t_b),\, \dot{\boldsymbol{x}}_{\text{cl}}(t_b) \right] \right\rangle \\ &= \left\langle L\left[\boldsymbol{x}_{\text{cl}}(t_b),\, \dot{\boldsymbol{x}}_{\text{cl}}(t_b) \right] \right\rangle + \left\langle L_{\text{fl}}(\boldsymbol{x}_b,\, \dot{\boldsymbol{x}}_b) \right\rangle \end{aligned} \tag{3.314a}$$

where

$$L_{\text{fl}}(\boldsymbol{x}_b, \dot{\boldsymbol{x}}_b) = L(\boldsymbol{x}_b, \dot{\boldsymbol{x}}_b) - L\left[\boldsymbol{x}_{\text{cl}}(t_b), \dot{\boldsymbol{x}}_{\text{cl}}(t_b)\right] \tag{3.314b}$$

Let

$$L = \frac{1}{2} M \dot{\boldsymbol{x}}^2 - V(\boldsymbol{x}) \tag{3.314c}$$

and

$$\boldsymbol{x}(t) = \boldsymbol{x}_{\text{cl}}(t) + \delta \boldsymbol{x}(t)$$

then

$$\left\langle L_{\text{fl}}(\boldsymbol{x}_b, \dot{\boldsymbol{x}}_b) \right\rangle = \frac{1}{2} M \left\langle \delta \dot{\boldsymbol{x}}_b^2 \right\rangle \tag{3.314}$$

since

$$\delta \boldsymbol{x}_b = \delta \boldsymbol{x}_{\boldsymbol{a}} = 0 \tag{3.314d}$$

The solution of (3.313) is

$$\begin{aligned}(\boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) &= C \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} d\,t \left\langle L(\boldsymbol{x}, \dot{\boldsymbol{x}}) \right\rangle\right] \\ &= C \exp\left\{\frac{i}{\hbar} \int_{t_a}^{t_b} d\,t\, L\left[\boldsymbol{x}_{\text{cl}}(t), \dot{\boldsymbol{x}}_{\text{cl}}(t)\right]\right\} \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} d\,t \left\langle L_{\text{fl}}(\boldsymbol{x}, \dot{\boldsymbol{x}}) \right\rangle\right] \\ &= C \exp\left\{\frac{i}{\hbar} A_{\text{cl}}\right\} \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} d\,t\, \frac{1}{2} M \left\langle \delta \dot{\boldsymbol{x}}^2 \right\rangle\right]\end{aligned} \tag{3.315}$$

where C is the integration “constant” that can be a function of $\boldsymbol{x}_b$ & $\boldsymbol{x}_a$ and

$$A_{\text{cl}} = \int_{t_a}^{t_b} d\,t\, L\left[\boldsymbol{x}_{\text{cl}}(t), \dot{\boldsymbol{x}}_{\text{cl}}(t)\right] \tag{3.315a}$$

is the classical action.

Using (2.27), we have

$$(\boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) = \int_{\boldsymbol{x}(t_a) = \boldsymbol{x}_a}^{\boldsymbol{x}(t_b) = \boldsymbol{x}_b} \mathcal{D}' \boldsymbol{x} \int \frac{\mathcal{D} \boldsymbol{p}}{(2 \pi \hbar)^3} \exp\left(\frac{i}{\hbar} \mathcal{A}'\right)$$

where

$$\begin{aligned}\mathcal{A}' &= \int_{t_a}^{t_b} d\,t \left\{\boldsymbol{p}(t) \cdot \dot{\boldsymbol{x}}(t) - H[\boldsymbol{x}(t), \boldsymbol{p}(t), t]\right\} \\ &= \boldsymbol{p}(t) \cdot \boldsymbol{x}(t) \Big|_{t_a}^{t_b} + \int_{t_a}^{t_b} d\,t \left\{-\dot{\boldsymbol{p}}(t) \cdot \boldsymbol{x}(t) - H[\boldsymbol{x}(t), \boldsymbol{p}(t), t]\right\}\end{aligned}$$

$$\begin{aligned}\to \qquad \frac{\hbar}{i} \nabla_b (\boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) &= \int \mathcal{D}' \boldsymbol{x} \int \frac{\mathcal{D} \boldsymbol{p}}{(2 \pi \hbar)^3}\, \boldsymbol{p}_b \exp\left(\frac{i}{\hbar} \mathcal{A}'\right) \\ &= \langle \boldsymbol{p}_b \rangle (\boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) \\ &= \boldsymbol{p}_{\text{cl}}(t_b) (\boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) \qquad \text{[Due to (3.314d).]}\end{aligned} \tag{3.316}$$

From (3.315), we have

$$\frac{\hbar}{i} \nabla_b (\boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) = \left[\nabla_b A_{\text{cl}} + \frac{\hbar}{i} \frac{\nabla_b C}{C}\right] (\boldsymbol{x}_b\, t_b \mid \boldsymbol{x}_a\, t_a) \tag{3.316a}$$

Comparing with (3.316), we have

$$\frac{\hbar}{i} \frac{\nabla_b C}{C} = 0$$

so that C is indeed a constant. (3.315) is thus just the familiar expression (2.151).

Using (3.312) on each spatial dimension of (3.314), we have

$$\left\langle L_{\text{fl}}(\boldsymbol{x}_b, \dot{\boldsymbol{x}}_b) \right\rangle = \frac{1}{2} M \left\langle \delta \dot{\boldsymbol{x}}_b^2 \right\rangle = i \frac{\hbar \omega}{2} D \cot \omega (t_b - t_a) \tag{3.317}$$

where D is the dimension of the system.