2.5. Generating Functional of Correlation Functions. Perturbative Expansion

2.5.1. Harmonic Oscillator Coupled to an External Force

Consider the imaginary time Lagrangian

$$L = -\frac{1}{2} m \dot{q}^2 - \frac{1}{2} m \omega^2 q^2 + b(t)\, q \qquad (2.41a)$$

$$\rightarrow \qquad p \equiv -i \frac{\partial L}{\partial \dot{q}} = i m \dot{q}$$

$$\begin{aligned} H &= \frac{\partial L}{\partial \dot{q}} \dot{q} - L \\ &= -\frac{1}{2} m \dot{q}^2 + \frac{1}{2} m \omega^2 q^2 - b(t)\, q \\ &= \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 q^2 - b(t)\, q \end{aligned} \qquad (2.41)$$

$$\begin{aligned} S_G(q, b) &= -\int_{-\tau/2}^{\tau/2} dt\, L \\ &= \int_{-\tau/2}^{\tau/2} dt \left[\frac{1}{2} m \dot{q}^2 + \frac{1}{2} m \omega^2 q^2 - b(t)\, q \right] \end{aligned} \qquad (2.42)$$

$$\operatorname{tr} U_G\left(\frac{\tau}{2}, -\frac{\tau}{2} \right) = \int_{q(\frac{\tau}{2}) = q(-\frac{\tau}{2})} [d\, q(t)] \exp\left[-\frac{S_G(q, b)}{\hbar} \right] \qquad (2.43)$$

As in §1.1, set

$$q(t) = q_c(t) + r(t) \qquad (2.44)$$

with periodic boundary conditions (B.C.)

$$q_c\left(\frac{\tau}{2} \right) = q_c\left(-\frac{\tau}{2} \right) \qquad \rightarrow \qquad r\left(\frac{\tau}{2} \right) = r\left(-\frac{\tau}{2} \right) \qquad (2.44a)$$

$$\dot{q}_c\left(\frac{\tau}{2} \right) = \dot{q}_c\left(-\frac{\tau}{2} \right)$$

Hence,

$$S_G(q, b) = S_0(r) + S_G(q_c, b) + S_L(q_c) \qquad (2.44b)$$

where

$$S_0(r) = \int_{-\tau/2}^{\tau/2} dt \left(\frac{1}{2} m \dot{r}^2 + \frac{1}{2} m \omega^2 r^2 \right)$$

$$S_G(q_c, b) = \int_{-\tau/2}^{\tau/2} dt \left[\frac{1}{2} m \dot{q}_c^2 + \frac{1}{2} m \omega^2 q_c^2 - b(t)\, q_c \right]$$

$$S_L(q_c) = \int_{-\tau/2}^{\tau/2} dt \left(m \dot{r} \dot{q}_c + m \omega^2 r\, q_c - b\, r \right)$$

Integrate by part gives

$$\begin{aligned} \int_{-\tau/2}^{\tau/2} dt\, \dot{r} \dot{q}_c &= \int_{-r(\tau/2)}^{r(\tau/2)} dr\, r\, \dot{q}_c \\ &= r\left(\frac{\tau}{2} \right) \dot{q}_c\left(\frac{\tau}{2} \right) - r\left(-\frac{\tau}{2} \right) \dot{q}_c\left(-\frac{\tau}{2} \right) - \int_{-\tau/2}^{\tau/2} dt\, r\, \ddot{q}_c \end{aligned}$$

$$= -\int_{-\tau/2}^{\tau/2} d\,t\; r\, \ddot{q}_c \qquad \text{[see (2.44a)]}$$

The imaginary time Euler-Lagrange eq. for the Lagrangian in eq(2.41a) is (see §2.1)

$$m\, \ddot{q}_c = m\, \omega^2\, q_c - b \qquad (2.45a)$$

$\rightarrow$ $\quad S_L(q_c) = 0$

$$S_G(q,\, b) = S_0(r) + S_G(q_c,\, b)$$

$\Delta\,(t)$

Solution to eq(2.45a)

$$m\, \ddot{q}_c = m\, \omega^2\, q_c - b$$

is

$$q_c(t) = \frac{1}{m} \int_{-\tau/2}^{\tau/2} \Delta(t-u)\, b(u)\, d\,u \qquad (2.45b)$$

where the green function Δ satisfies

$$\ddot{\Delta} - \omega^2\, \Delta = -\delta(t) \qquad (2.45c)$$

Thus,

$$m\, \ddot{q}_c(t) - \omega^2\, q_c = \int_{-\tau/2}^{\tau/2} \left[\ddot{\Delta}(t-u) - \omega^2\, \Delta(t-u) \right] b(u)\, d\,u$$

$$= -\int_{-\tau/2}^{\tau/2} \delta(t-u)\, b(u)\, d\,u$$

$$= -b(t)$$

as claimed.

Consider eq(2.45c) with periodic B.C.

$$\Delta\left(\frac{\tau}{2}\right) = \Delta\left(-\frac{\tau}{2}\right) \qquad \dot{\Delta}\left(\frac{\tau}{2}\right) = \dot{\Delta}\left(-\frac{\tau}{2}\right)$$

The independent solutions to the homogeneous eq.

$$\ddot{\psi} - \omega^2\, \psi = 0$$

are

$$\psi_1 = \cosh \omega\, t \qquad \& \qquad \psi_2 = \sinh \omega\, t$$

Integrating eq(2.45c) gives the discontinuity of $\dot{\Delta}$ at $t = 0$:

$$\lim_{\epsilon \to 0} \left[\dot{\Delta}(\epsilon) - \dot{\Delta}(-\epsilon) \right] = -1$$

In order to satisfy the B.C. on Δ, we use ψ_1 & set

$$\Delta(t) = \begin{cases} A \cosh\left[\omega\left(\frac{\tau}{2} - t\right) \right] & \text{for } t > 0 \\ A \cosh\left[\omega\left(t + \frac{\tau}{2}\right) \right] & \text{for } t < 0 \end{cases} \qquad (\, A = \text{const}\,)$$

$$= A \cosh\left[\omega\left(\frac{\tau}{2} - |\,t\,| \right) \right]$$

so that

$$\Delta\left(\frac{\tau}{2}\right) = \Delta\left(-\frac{\tau}{2}\right) = A$$

Note that by construction, $\Delta(t)$ satisfies eq(2.45c) for $t \neq 0$ automatically.

The singularity at $t = 0$ is handled as follows,

$$\dot{\Delta}\,(t) = \begin{cases} -A\, \omega \sinh\left[\omega\left(\frac{\tau}{2} - t\right) \right] & \text{for } t > 0 \\ A\, \omega \sinh\left[\omega\left(t + \frac{\tau}{2}\right) \right] & \text{for } t < 0 \end{cases}$$

$$= \mp A\,\omega \sinh\left[\omega\left(\frac{\tau}{2} - |t|\right)\right]$$

$$\therefore \qquad \lim_{\epsilon\to 0}\left[\dot{\Delta}(\epsilon) - \dot{\Delta}(-\epsilon)\right] = -2\,A\,\omega \sinh\frac{\omega\,\tau}{2} = -1$$

$$\rightarrow \qquad A = \frac{1}{2\,\omega \sinh\frac{\omega\,\tau}{2}}$$

Hence,

$$\Delta(t) = \frac{1}{2\,\omega \sinh\frac{\omega\,\tau}{2}} \cosh\left[\omega\left(\frac{\tau}{2} - |t|\right)\right] \qquad (2.45)$$

$$= \frac{1}{2\,\omega \sinh\frac{\omega\,\tau}{2}}\left(\cosh\frac{\omega\,\tau}{2}\cosh\omega\,|t| - \sinh\frac{\omega\,\tau}{2}\sinh\omega\,|t|\right)$$

$$= \frac{1}{2\,\omega}\left(\coth\frac{\omega\,\tau}{2}\cosh\omega\,|t| - \sinh\omega\,|t|\right)$$

For $\tau\to\infty$, we have

$$\coth\frac{\omega\,\tau}{2} = 1$$

$$\Delta(t) = \frac{1}{2\,\omega}(\cosh\omega\,|t| - \sinh\omega\,|t|)$$

$$= \frac{1}{2\,\omega} e^{-\omega|t|} \qquad (2.46)$$

$\mathcal{Z}_G(b, \beta)$

Using

$$\int_{-\tau/2}^{\tau/2} d\,t\,\dot{q}_c^2 = \int_{-q_c(\tau/2)}^{q_c(\tau/2)} d\,q_c\,\dot{q}_c$$

$$= q_c\left(\frac{\tau}{2}\right)\dot{q}_c\left(\frac{\tau}{2}\right) - q_c\left(-\frac{\tau}{2}\right)\dot{q}_c\left(-\frac{\tau}{2}\right) - \int_{-\tau/2}^{\tau/2} d\,t\;q_c\,\ddot{q}_c$$

$$= -\int_{-\tau/2}^{\tau/2} d\,t\;q_c\,\ddot{q}_c \qquad \text{[see eq(2.44a)]}$$

we have, from eq(2.42),

$$S_G(q_c, b) = \int_{-\tau/2}^{\tau/2} d\,t\left[\frac{1}{2}\,m\,\dot{q}_c^2 + \frac{1}{2}\,m\,\omega^2\,q_c^2 - b(t)\,q_c\right]$$

$$= \int_{-\tau/2}^{\tau/2} d\,t\,q_c\left[-\frac{1}{2}\,m\,\ddot{q}_c^2 + \frac{1}{2}\,m\,\omega^2\,q_c - b\,(t)\right]$$

$$= -\frac{1}{2}\int_{-\tau/2}^{\tau/2} d\,t\,q_c\,b(t) \qquad \text{[see eq(2.45a)]}$$

Using eq(2.45b), we have

$$S_G(q_c, b) = -\frac{1}{2\,m}\int_{-\tau/2}^{\tau/2} d\,t\int_{-\tau/2}^{\tau/2} d\,u\;b(t)\,\Delta(t-u)\,b(u)$$

With

$$S_G(q, b) = S_0(r) + S_G(q_c, b)$$

&

$$\int_{r(\frac{\tau}{2})=r(-\frac{\tau}{2})} [d\,r(t)]\, \exp\left[-\frac{S_0(r)}{\hbar}\right] = \operatorname{tr} U_0\left(\frac{\tau}{2}, -\frac{\tau}{2}\right)$$

eq(2.43) becomes

$$\operatorname{tr} U_G\left(\frac{\tau}{2}, -\frac{\tau}{2}\right) = \operatorname{tr} U_0\left(\frac{\tau}{2}, -\frac{\tau}{2}\right) \exp\left[-\frac{S_G(q_c, b)}{\hbar}\right]$$

$$\mathcal{Z}_G(b, \beta) = \operatorname{tr} U_G\left(\hbar\frac{\beta}{2}, -\hbar\frac{\beta}{2}\right)$$

$$= \mathcal{Z}_0(\beta) \exp\left[\frac{1}{2m}\int_{-\hbar\beta/2}^{\hbar\beta/2} d\,t \int_{-\hbar\beta/2}^{\hbar\beta/2} d\,u\; b(t)\,\Delta(t-u)\,b(u)\right] \quad (2.47)$$

where

$$\mathcal{Z}_0(\beta) = \operatorname{tr} U_0\left(\hbar\frac{\beta}{2}, -\hbar\frac{\beta}{2}\right)$$

is the partition function of the harmonic oscillator.

2.5.2. Correlation Functions, Wick's Theorem

Taking the functional derivative of eq(2.43), we get

$$\hbar\frac{\delta}{\delta\, b(t_1)} \mathcal{Z}_G(b, \beta) = \int_{q(\frac{\tau}{2})=q(-\frac{\tau}{2})} [d\,q(t)]\; q(t_1) \exp\left[-\frac{S_G(q, b)}{\hbar}\right]$$

$$\rightarrow \quad \hbar\frac{\delta}{\delta\, b(t_1)} \mathcal{Z}_G(b, \beta)\bigg|_{b=0} = \int_{q(\frac{\tau}{2})=q(-\frac{\tau}{2})} [d\,q(t)]\; q(t_1) \exp\left[-\frac{S_0(q)}{\hbar}\right]$$

$$= \mathcal{Z}_0(\beta)\,\langle\, q(t_1)\,\rangle_0$$

Similarly,

$$\hbar^p \prod_{j=1}^{p} \frac{\delta}{\delta\, b(t_j)} \mathcal{Z}_G(b, \beta)\bigg|_{b=0} = \int_{q(\frac{\tau}{2})=q(-\frac{\tau}{2})} [d\,q(t)] \prod_{j=1}^{p} q(t_j) \exp\left[-\frac{S_0(q)}{\hbar}\right]$$

$$= \mathcal{Z}_0(\beta)\left\langle\, q(t_1)\, q(t_2) \ldots q(t_p)\right\rangle_0 \quad (2.48a)$$

Note that the order of the 2 products are opposite to each other. This is immaterial if q is a commuting variable.

Using $\mathcal{Z}_G(b, \beta)$ given by eq(2.47) & the symmetry

$$\Delta(t-u) = \Delta(u-t)$$

we have

$$\hbar\frac{\delta}{\delta\, b(t_1)} \mathcal{Z}_G(b, \beta) = \frac{1}{m}\int_{-\hbar\beta/2}^{\hbar\beta/2} d\,u\,\Delta(t_1-u)\,b(u)\,\mathcal{Z}_G(b, \beta)$$

$$\hbar^2 \frac{\delta}{\delta\, b(t_2)} \frac{\delta}{\delta\, b(t_1)} \mathcal{Z}_G(b, \beta) = \left\{\frac{1}{m}\Delta(t_1 - t_2) + \frac{1}{m^2}\int_{-\hbar\beta/2}^{\hbar\beta/2} d\,u\,\Delta(t_1-u)\,b(u) \int_{-\hbar\beta/2}^{\hbar\beta/2} d\,v\,\Delta(t_2-v)\,b(v)\right\} \mathcal{Z}_G(b, \beta)$$

$$\rightarrow \quad \langle\, q(t_1)\, q(t_2)\,\rangle_0 = \frac{1}{\mathcal{Z}_0(\beta)}\,\hbar^2 \frac{\delta^2}{\delta\, b(t_2)\,\delta\, b(t_1)} \mathcal{Z}_G(b, \beta)\bigg|_{b=0}$$

$$= \frac{\hbar}{m}\Delta(t_1 - t_2) \quad (2.48b)$$

In general

$$\langle \mathcal{F}(q) \rangle_0 = \frac{1}{\mathcal{Z}_0(\beta)} \mathcal{F}\left(\hbar \frac{\delta}{\delta b(t)}\right) \mathcal{Z}_G(b, \beta)\bigg|_{b=0}$$

For the $\mathcal{Z}_G(b, \beta)$ given by eq(2.47), it is easy to see from the derivation of eq(2.48b) that only products of $\Delta(t_i - t_j)$ can survive in the $b \to 0$ limit. We have thus proved the Wick's theorem

$$\langle q(t_1)\, q(t_2) \ldots q(t_k) \rangle_0 = \sum_P \langle q(t_{P1})\, q(t_{P2}) \rangle_0 \ldots \langle q(t_{P(k-1)})\, q(t_{Pk}) \rangle_0 \qquad (2.49)$$

where P is any permutation of $1 \ldots k$. Note that the correlation function vanishes if k is odd.

$\mathcal{Z}_0(\beta)$

From

$$\mathcal{Z}_0(\beta) = \mathrm{tr}\, U_0\left(\hbar \frac{\beta}{2}, -\hbar \frac{\beta}{2}\right) = \int_{q\left(\hbar \frac{\beta}{2}\right) = q\left(-\hbar \frac{\beta}{2}\right)} [d\, q(t)] \exp\left[-\frac{S_0(q)}{\hbar}\right]$$

&

$$S_0(q) = \int_{-\hbar\beta/2}^{\hbar\beta/2} d\, t \left(\frac{1}{2} m \dot{q}^2 + \frac{1}{2} m\, \omega^2 q^2\right)$$

we have

$$\begin{aligned}
\frac{\partial}{\partial \omega} \mathcal{Z}_0(\beta) &= -\frac{1}{\hbar} \int_{q\left(\hbar \frac{\beta}{2}\right) = q\left(-\hbar \frac{\beta}{2}\right)} [d\, q(t')] \left(\int_{-\hbar\beta/2}^{\hbar\beta/2} d\, t\, m\, \omega\, q(t)^2\right) \exp\left[-\frac{S_0(q)}{\hbar}\right] \\
&= -\frac{m\, \omega}{\hbar} \int_{-\hbar\beta/2}^{\hbar\beta/2} d\, t \int_{q\left(\hbar \frac{\beta}{2}\right) = q\left(-\hbar \frac{\beta}{2}\right)} [d\, q(t')]\, q(t)^2 \exp\left[-\frac{S_0(q)}{\hbar}\right] \\
&= -\mathcal{Z}_0(\beta) \frac{m\, \omega}{\hbar} \int_{-\hbar\beta/2}^{\hbar\beta/2} d\, t \left\langle q(t)^2 \right\rangle_0
\end{aligned}$$

$$\begin{aligned}
\therefore \quad \frac{\partial}{\partial \omega} \ln \mathcal{Z}_0(\beta) &= \frac{1}{\mathcal{Z}_0(\beta)} \frac{\partial}{\partial \omega} \mathcal{Z}_0(\beta) \\
&= -\frac{m\, \omega}{\hbar} \int_{-\hbar\beta/2}^{\hbar\beta/2} d\, t \left\langle q(t)^2 \right\rangle_0 \\
&= -\omega \int_{-\hbar\beta/2}^{\hbar\beta/2} d\, t\, \Delta(0) && \text{[see eq(2.48b)]} \\
&= -\omega \int_{-\hbar\beta/2}^{\hbar\beta/2} d\, t \frac{\cosh \frac{\omega \hbar \beta}{2}}{2\, \omega \sinh \frac{\omega \hbar \beta}{2}} && \text{[see eq(2.45) with } \tau = \hbar\beta\text{]} \\
&= -\frac{\hbar\, \beta}{2} \frac{\cosh \frac{\omega \hbar \beta}{2}}{\sinh \frac{\omega \hbar \beta}{2}} && (2.50)
\end{aligned}$$

$$\begin{aligned}
\to \quad \ln \mathcal{Z}_0(\beta) &= -\frac{\hbar\, \beta}{2} \int d\, \omega \coth \frac{\omega \hbar \beta}{2} + C \\
&= -\ln \sinh \frac{\hbar\, \beta}{2} + C
\end{aligned}$$

$$= \ln \frac{e^C}{\sinh \frac{\omega \hbar \beta}{2}}$$

$$\therefore \qquad \mathcal{Z}_0(\beta) = \mathcal{N}' \frac{1}{\sinh \frac{\omega \hbar \beta}{2}} \qquad \text{where} \quad \mathcal{N}' = e^C \qquad (2.51)$$

Since a partition function is dimensionless, so is $\mathcal{N}'$.

As discussed in §2.4,

$$\mathcal{Z}(\beta \to \infty) = e^{-\beta e_0}$$

For a harmonic oscillator, $e_0 = \frac{1}{2} \hbar \omega$, so that

$$\mathcal{Z}_0(\beta \to \infty) = e^{-\beta \hbar \omega / 2}$$

From eq(2.51), we have

$$\mathcal{Z}_0(\beta \to \infty) = \mathcal{N}' \lim_{\beta \to \infty} \frac{2}{e^{\beta \hbar \omega / 2} - e^{-\beta \hbar \omega / 2}}$$

$$= 2 \mathcal{N}' e^{-\beta \hbar \omega / 2}$$

Hence,

$$\mathcal{N}' = \frac{1}{2}$$

$$\& \qquad \mathcal{Z}_0(\beta) = \frac{1}{2 \sinh \frac{\omega \hbar \beta}{2}}$$

$$= \frac{1}{e^{\beta \hbar \omega / 2} - e^{-\beta \hbar \omega / 2}}$$

$$= \frac{e^{-\beta \hbar \omega / 2}}{1 - e^{-\beta \hbar \omega}} \qquad (2.52)$$

2.5.3. Harmonic Oscillator: Paths & Square Integrable Functions

In this section, G-R stands for the handbook “Table of Integrals, Series, & Products” by I.S.Gradshteyn, I.M.Ryzshik.

k-Space

The calculations can also be performed in k-space.

The periodic B.C.

$$q_n = q_0$$

allows us to define the Fourier series

$$q_k = \frac{1}{\sqrt{n}} \sum_{l=0}^{n-1} \exp\left(\frac{2 i \pi k l}{n} \right) c_l \qquad (2.53)$$

so that

$$q_n = \frac{1}{\sqrt{n}} \sum_{l=0}^{n-1} \exp(2 i \pi l)\, c_l = \frac{1}{\sqrt{n}} \sum_{l=0}^{n-1} c_l = q_0$$

Taking the complex conjugate of eq(2.53), we have

$$q_k^* = \frac{1}{\sqrt{n}} \sum_{l=0}^{n-1} \exp\left(-\frac{2 i \pi k l}{n}\right) c_l^*$$

$$= \frac{1}{\sqrt{n}} \sum_{l=0}^{n-1} \exp(2 i \pi k) \exp\left(-\frac{2 i \pi k l}{n}\right) c_l^*$$

$$= \frac{1}{\sqrt{n}} \sum_{l=0}^{n-1} \exp\left(\frac{2 i \pi k (n-l)}{n}\right) c_l^*$$

$$= \frac{1}{\sqrt{n}} \sum_{l=1}^{n} \exp\left(\frac{2 i \pi k l}{n}\right) c_{n-l}^*$$

$$= \frac{1}{\sqrt{n}} \left[c_0^* + \sum_{l=1}^{n-1} \exp\left(\frac{2 i \pi k l}{n}\right) c_{n-l}^* \right]$$

Reality of q_k thus requires

$$c_{n-l}^* = c_l \qquad \text{for} \qquad l = 1, \ldots, n-1$$

& $$c_0^* = c_0 \qquad (2.54)$$

From eqs(2.44b & 2.34a), we set

$$S_0(q) = \frac{\varepsilon}{\hbar} \sum_{k=1}^{n} \left[\frac{1}{2} m \left(\frac{q_k - q_{k-1}}{\varepsilon}\right)^2 + \frac{1}{2} m \omega^2 q_k^2 \right]$$

Using the geometric series formula

$$\sum_{k=1}^{n} a^k = \frac{a - a^{n+1}}{1-a}$$

we have, for l integers,

$$\sum_{k=1}^{n} \exp\left(\frac{2 i \pi k l}{n}\right) =$$

$$\begin{cases} n & \text{if } l = 0, n, 2n, \ldots \\ \left(\exp\left(\frac{2 i \pi l}{n}\right) - \exp\left(\frac{1}{n} 2 i \pi (n+1) l\right)\right) \Big/ \left(1 - \exp\left(\frac{2 i \pi l}{n}\right)\right) = 0 & \text{otherwise} \end{cases}$$

Hence,

$$\frac{1}{n} \sum_{k=1}^{n} \exp\left(\frac{2 i \pi k l}{n}\right) = \begin{cases} 1 & \text{if } l = 0 \bmod n \\ 0 & \text{otherwise} \end{cases} \qquad (2.54a)$$

$$= \delta_{l,\, 0 \bmod n}$$

$$= \sum_{p=0}^{\infty} \delta_{l,\, p n}$$

$$\therefore \qquad \sum_{k=1}^{n} q_k^2 = \frac{1}{n} \sum_{k=1}^{n} \sum_{l=0}^{n-1} \sum_{l'=0}^{n-1} \exp\left(\frac{2 i \pi k (l + l')}{n}\right) c_l c_{l'}$$

$$= \sum_{l=0}^{n-1} \sum_{l'=0}^{n-1} \delta_{l+l',\, 0 \bmod n} c_l c_{l'}$$

$$= \sum_{l=0}^{n-1} c_l c_{n-l} \qquad (\; l + l' = n \text{ so that } 0 \le l, l' \le n-1 \;)$$

$$= \sum_{l=0}^{n-1} c_l\, c_l^* \qquad \text{[see eq(2.54)]}$$

$$\sum_{k=1}^{n} q_k\, q_{k-1} = \frac{1}{n} \sum_{k=1}^{n} \sum_{l=0}^{n-1} \sum_{l'=0}^{n-1} \exp\left(\frac{2\, i\, \pi\, k\, (l+l')}{n}\right) \exp\left(-\frac{2\, i\, \pi\, l'}{n}\right) c_l\, c_{l'}$$

$$= \sum_{l=0}^{n-1} \sum_{l'=0}^{n-1} \delta_{l+l',\, 0 \bmod n} \exp\left(-\frac{2\, i\, \pi\, l'}{n}\right) c_l\, c_{l'}$$

$$= \sum_{l=0}^{n-1} \exp\left(\frac{2\, i\, \pi\, l}{n}\right) c_l\, c_{n-l}$$

$$= \sum_{l=0}^{n-1} \exp\left(\frac{2\, i\, \pi\, l}{n}\right) c_l\, c_l^*$$

Since $\sum_{k=1}^{n} q_k\, q_{k-1}$ is real, the imaginary part in the sum must vanishes. Alternatively,

$$\sum_{k=1}^{n} q_k\, q_{k-1} = \frac{1}{2}\left[\sum_{k=1}^{n} q_k\, q_{k-1} + \left(\sum_{k=1}^{n} q_k\, q_{k-1}\right)^* \right]$$

$$= \sum_{l=0}^{n-1} \cos\left(\frac{2\, \pi\, l}{n}\right) c_l\, c_l^*$$

$$\therefore \qquad \frac{1}{2} \sum_{k=1}^{n} (q_k - q_{k-1})^2 = \frac{1}{2} \sum_{k=1}^{n} \left(q_k^2 + q_{k-1}^2 - 2\, q_k\, q_{k-1}\right)$$

$$= \sum_{k=1}^{n} \left(q_k^2 - q_k\, q_{k-1}\right) \qquad [\, q_0 = q_n \,]$$

$$= \sum_{l=0}^{n-1} \left[1 - \cos\left(\frac{2\, \pi\, l}{n}\right)\right] c_l\, c_l^*$$

The discrete action

$$S_0(q) = \frac{\varepsilon}{\hbar} \sum_{k=1}^{n} \left[\frac{1}{2}\, m \left(\frac{q_k - q_{k-1}}{\varepsilon}\right)^2 + \frac{1}{2}\, m\, \omega^2\, q_k^2 \right]$$

thus becomes

$$S_0(q) = \frac{\varepsilon}{\hbar}\, m \sum_{l=0}^{n-1} \left\{ \frac{1}{\varepsilon^2} \left[1 - \cos\left(\frac{2\, \pi\, l}{n}\right)\right] + \frac{1}{2}\, \omega^2 \right\} c_l\, c_l^* \qquad (2.55)$$

Jacobian

From (2.53), we have

$$\frac{\partial q_k}{\partial c_l} = \frac{1}{\sqrt{n}} \exp\left(\frac{2\, i\, \pi\, k\, l}{n}\right)$$

$$\rightarrow \qquad \frac{\partial(\, q_1,\ \ldots,\ q_n\,)}{\partial(\, c_0,\ \ldots,\ c_{n-1}\,)} = \det \left| \frac{\partial q_k}{\partial c_l} \right|$$

$$= n^{-n/2} \det \begin{vmatrix} 1 & e^{2i\pi/n} & e^{4i\pi/n} & \ldots & e^{2i\pi(n-1)/n} \\ 1 & e^{4i\pi/n} & e^{8i\pi/n} & \cdots & e^{4i\pi(n-1)/n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & e^{2i\pi(n-1)/n} & e^{4i\pi(n-1)/n} & \cdots & e^{2i\pi(n-1)^2/n} \\ 1 & 1 & 1 & 1 & 1 \end{vmatrix}$$

$$= (-)^{n-1} n^{-n/2} \prod_{0\le k<j\le n-1} \left(e^{2i\pi j/n} - e^{2i\pi k/n} \right)$$

where we've used the formula for Vandermonde's determinant

$$\det \begin{vmatrix} 1 & 1 & \ldots & 1 \\ x_1 & x_2 & \ldots & x_n \\ x_1^2 & x_2^2 & \cdots & x_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{n-1} & x_2^{n-1} & \cdots & x_n^{n-1} \end{vmatrix} = \prod_{1\le i<j\le n} (x_j - x_i)$$

(See, for example, §14.311 of G-R.)

Using

$$e^{2i\pi j/n} - e^{2i\pi k/n} = e^{i\pi(j+k)/n}\left(e^{i\pi(j-k)/n} - e^{-i\pi(j-k)/n} \right)$$

$$= 2\,i\,e^{i\pi(j+k)/n} \sin \frac{(j-k)\pi}{n}$$

we have

$$\frac{\partial(q_1, \ldots, q_n)}{\partial(c_0, \ldots, c_{n-1})} = (-)^{n-1} n^{-n/2} (2\,i)^{n(n-1)/2} \prod_{0\le k<j\le n-1} e^{i\pi(j+k)/n} \sin \frac{(j-k)\pi}{n}$$

Using (see §1.392 of R-G)

$$\sin n\,x = 2^{n-1} \prod_{k=0}^{n-1} \sin\left(x + \frac{k\pi}{n} \right)$$

we have

$$\frac{\sin n\,x}{\sin x} = 2^{n-1} \prod_{k=1}^{n-1} \sin\left(x + \frac{k\pi}{n} \right)$$

$$\prod_{k=1}^{n-1} \sin\left(\frac{k\pi}{n}\right) = \frac{1}{2^{n-1}} \lim_{x\to 0} \frac{\sin n\,x}{\sin x} = \frac{n}{2^{n-1}}$$

$$\therefore \qquad P = \prod_{0\le k<j\le n-1} \sin \frac{(j-k)\pi}{n} = \prod_{j=1}^{n-1} \prod_{k=1}^{j} \sin \frac{k\pi}{n}$$

Since

$$\sin \frac{(n-k)\pi}{n} = \sin \frac{k\pi}{n}$$

we have

$$P = \prod_{j=1}^{n-1} \prod_{k=n-j}^{n-1} \sin \frac{k\pi}{n}$$

$$\to \qquad P^2 = \left(\prod_{j=1}^{n-1} \prod_{k=1}^{j} \sin \frac{k\pi}{n} \right) \left(\prod_{j'=1}^{n-1} \prod_{k'=n-j'}^{n-1} \sin \frac{k'\pi}{n} \right)$$

By combining each k product for j with the k' product for $j' = n - j - 1$, we get the full range product

$$\prod_{k=1}^{n-1} \sin \frac{k\pi}{n}$$

This takes care of j, $j' = 1, \ldots, n-2$. However, $j = n-1$ & $j' = n-1$ require no pairings. P^2 thus contains $(n-2)+2 = n$ full range products.

$$P^2 = \left(\prod_{k=1}^{n-1} \sin\frac{k\pi}{n}\right)^n = \left(\frac{n}{2^{n-1}}\right)^n$$

$$\rightarrow \qquad P = \frac{n^{n/2}}{2^{n(n-1)/2}}$$

$$\therefore \qquad \frac{\partial(q_1, \ldots, q_n)}{\partial(c_0, \ldots, c_{n-1})} = (-)^{n-1}\, i^{n(n-1)/2} \prod_{0\le k<j\le n-1} e^{i\pi(j+k)/n} = A$$

is a phase factor of magnitude 1.

A can be evaluated as follows.

$$\prod_{0\le k<j\le n-1} e^{i\pi(j+k)/n} = \exp\left[\frac{i\pi}{n}\sum_{j=1}^{n-1}\sum_{k=0}^{j-1}(j+k)\right]$$

$$\sum_{j=1}^{n-1}\sum_{k=0}^{j-1}(j+k) = \sum_{j=1}^{n-1}\left[j^2 + \frac{1}{2}j(j-1)\right]$$

$$= \frac{3}{2}\cdot\frac{1}{6}n(n-1)(2n-1) - \frac{1}{2}\cdot\frac{1}{2}(n-1)n$$

$$= \frac{1}{2}n(n-1)^2$$

$$\rightarrow \qquad A = e^{i\pi(n-1)}\, e^{i\pi n(n-1)/4}\, e^{i\pi(n-1)^2/2}$$

$$= \exp\left[i\frac{\pi}{4}(n-1)(3n+2)\right]$$

$\mathcal{Z}_0$

For convenience, assume n to be even.

Eq(2.54) implies half of the variables c_l can be replaced by the complex conjugated ones. Thus

$$\left\{c_0, c_1, \ldots, c_{n/2-1}, c_{n/2}, c_{n/2+1} \ldots, c_{n-1}\right\} = \left\{c_0, c_1, \ldots, c_{n/2-1}, c_{n/2}^*, c_{n/2-1}^* \ldots, c_1^*\right\}$$

where

$$c_0^* = c_0 \quad \& \qquad c_{n/2} = c_{n/2}^*$$

$$\rightarrow \qquad \mathcal{Z}_0 = \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{n/2} \int \prod_{k=1}^{n} d\,q_k\, e^{-S(q)}$$

$$= \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{n/2} A \int_{-\infty}^{\infty} d\,c_0 \int_{-\infty}^{\infty} d\,c_{n/2} \int \prod_{l=1}^{n/2-1} d\,c_l\, d\,c_l^*\, e^{-S(q)}$$

For $l = 0$ & $l = \frac{n}{2}$, the integrals

$$\int_{-\infty}^{\infty} d\,c_0 \exp\left(-\frac{\varepsilon}{2\hbar} m\omega^2 c_0^2\right) = \sqrt{\frac{2\pi\hbar}{m\varepsilon\omega^2}}$$

$$\int_{-\infty}^{\infty} d\,c_{n/2} \exp\left[-\frac{2}{\hbar\,\varepsilon} m\left(1+\frac{1}{4}\varepsilon^2\,\omega^2\right) c_{n/2}^2\right] = \sqrt{\frac{2\,\pi\,\hbar\,\varepsilon}{m\left(4+\varepsilon^2\,\omega^2\right)}}$$

For $l \neq 0$, we have

$$\int d\,c_l\, d\,c_l^* \exp\left[-\frac{\varepsilon}{\hbar} m\left\{\frac{1}{\varepsilon^2}\left[1-\cos\left(\frac{2\,\pi\,l}{n}\right)\right]+\frac{1}{2}\omega^2\right\} c_l\, c_l^*\right]$$
$$= 2\,\pi \int_0^{\infty} d\,r\, r \exp\left[-\frac{\varepsilon}{\hbar} m\left\{\frac{1}{\varepsilon^2}\left[1-\cos\left(\frac{2\,\pi\,l}{n}\right)\right]+\frac{1}{2}\omega^2\right\} r^2\right]$$
$$= \left(\frac{\pi\,\hbar\,\varepsilon}{m}\right) \frac{1}{1-\cos\left(\frac{2\,\pi\,l}{n}\right)+\frac{1}{2}\varepsilon^2\,\omega^2}$$

Hence,

$$\int_{-\infty}^{\infty} d\,c_0 \int_{-\infty}^{\infty} d\,c_{n/2} \int \prod_{l=1}^{n/2-1} d\,c_l\, d\,c_l^*\, e^{-S(q)} = \frac{2}{\varepsilon\,\omega\sqrt{4+\varepsilon^2\,\omega^2}} \left(\frac{\pi\,\hbar\,\varepsilon}{m}\right)^{n/2} \prod_{l=1}^{n/2-1} \frac{1}{1-\cos\left(\frac{2\,\pi\,l}{n}\right)+\frac{1}{2}\varepsilon^2\,\omega^2}$$

$$\therefore \qquad \mathcal{Z}_0 = \frac{2^{-n/2+1}}{\varepsilon\,\omega\sqrt{4+\varepsilon^2\,\omega^2}} \prod_{l=1}^{n/2-1} \frac{1}{1-\cos\left(\frac{2\,\pi\,l}{n}\right)+\frac{1}{2}\varepsilon^2\,\omega^2} \qquad (2.56a)$$

where we've set $A = 1$ since $\mathcal{Z}_0$ is real.

Since

$$\cos\left(\frac{2\,\pi\,l}{n}\right) = \cos\left(\frac{2\,\pi\,(n-l)}{n}\right)$$

we can write eq(2.56a) as

$$\mathcal{Z}_0 = \frac{2^{-n/2+1}}{\varepsilon\,\omega\sqrt{4+\varepsilon^2\,\omega^2}} \prod_{l=n/2+1}^{n-1} \frac{1}{1-\cos\left(\frac{2\,\pi\,l}{n}\right)+\frac{1}{2}\varepsilon^2\,\omega^2}$$
$$= \frac{2^{-n/2}}{\varepsilon\,\omega}\sqrt{4+\varepsilon^2\,\omega^2} \prod_{l=n/2}^{n-1} \frac{1}{1-\cos\left(\frac{2\,\pi\,l}{n}\right)+\frac{1}{2}\varepsilon^2\,\omega^2}$$

$$\rightarrow \qquad \mathcal{Z}_0 = \frac{2^{-(n-1)/2}}{\varepsilon\,\omega} \prod_{l=1}^{n-1} \left[1-\cos\left(\frac{2\,\pi\,l}{n}\right)+\frac{1}{2}\varepsilon^2\,\omega^2\right]^{-1/2}$$
$$= 2^{-n/2} \prod_{l=0}^{n-1} \left[1-\cos\left(\frac{2\,\pi\,l}{n}\right)+\frac{1}{2}\varepsilon^2\,\omega^2\right]^{-1/2} \qquad (2.56)$$

In order to use (see eq.1 in §1.396 of G-R)

$$\prod_{k=1}^{m-1} \left(1-2\,x\cos\frac{k\,\pi}{m}+x^2\right) = \frac{x^{2\,m}-1}{x^2-1}$$

to evaluate eq(2.56a), we set

$$\alpha + \beta = 1$$

$$\to \quad 1-\cos\left(\frac{2\pi l}{n}\right)+\frac{1}{2}\varepsilon^2\omega^2 = (\alpha+\beta)\left(1+\frac{1}{2}\varepsilon^2\omega^2\right)-\cos\left(\frac{2\pi l}{n}\right)$$
$$= \alpha\left(1+\frac{1}{2}\varepsilon^2\omega^2\right)\left[1+\frac{\beta}{\alpha}-\frac{1}{\alpha\left(1+\frac{1}{2}\varepsilon^2\omega^2\right)}\cos\left(\frac{2\pi l}{n}\right)\right]$$

The quantity inside the square bracket is of the desired form if

$$\frac{n}{2}=m \qquad \frac{\beta}{\alpha}=x^2 \qquad \frac{1}{\alpha\left(1+\frac{1}{2}\varepsilon^2\omega^2\right)}=2x$$

$$\to \quad \alpha=\frac{1}{\left(2+\varepsilon^2\omega^2\right)x} \qquad \beta=\frac{1}{2+\varepsilon^2\omega^2}x$$

$$\& \quad 1+\frac{1}{2}\varepsilon^2\omega^2=\frac{1}{2}\left(x+\frac{1}{x}\right)$$

which can be “solved” by setting

$$\cosh\theta = 1+\frac{1}{2}\varepsilon^2\omega^2 \qquad (2.56b)$$

$$\to \quad x=e^{\pm\theta}$$

$$\alpha=\frac{1}{\left(x+\frac{1}{x}\right)x}=\frac{1}{1+x^2}=\frac{1}{1+e^{\pm 2\theta}}$$

$$\alpha\left(1+\frac{1}{2}\varepsilon^2\omega^2\right)=\frac{1}{2x}=\frac{1}{2}e^{\mp\theta}$$

Hence,

$$\prod_{l=1}^{n/2-1}\left[1-\cos\left(\frac{2\pi l}{n}\right)+\frac{1}{2}\varepsilon^2\omega^2\right]=\left(\frac{1}{2x}\right)^{n/2-1}\frac{x^n-1}{x^2-1}$$
$$=\left(\frac{1}{2^{n/2-1}}e^{\mp(n/2-1)\theta}\right)\left(\frac{e^{\pm n\theta}-1}{e^{\pm 2\theta}-1}\right)$$
$$=\frac{1}{2^{n/2-1}}\left(\frac{e^{\pm n\theta/2}-e^{\mp n\theta/2}}{e^{\pm\theta}-e^{\mp\theta}}\right)$$
$$=\frac{1}{2^{n/2-1}}\left(\frac{e^{n\theta/2}-e^{-n\theta/2}}{e^{\theta}-e^{-\theta}}\right)$$

$$\to \quad \mathcal{Z}_0=\frac{1}{\varepsilon\omega\sqrt{\left(4+\varepsilon^2\omega^2\right)}}\left(\frac{e^{\theta}-e^{-\theta}}{e^{n\theta/2}-e^{-n\theta/2}}\right)$$

In the limit

$$n\to\infty,\ \varepsilon\to 0,\ n\varepsilon\to\beta\hbar$$

eq(2.56b) gives

$$\theta\to\varepsilon\omega$$
$$n\theta\to\beta\hbar\omega$$

so that

$$\frac{e^{\theta}-e^{-\theta}}{\varepsilon\,\omega\sqrt{(4+\varepsilon^2\,\omega^2)}} \approx \frac{2\,\varepsilon\,\omega}{\varepsilon\,\omega\sqrt{4}} = 1$$

$$\rightarrow \qquad \mathcal{Z}_0 = \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}}$$

$$= \frac{e^{-\beta\,\omega/2}}{1 - e^{-\beta\,\omega}}$$

Continuum Calculation

For q a continuous variable, we set

$$q_k = q(k\,\varepsilon) \rightarrow q(t)$$

Eq(2.53) can be written as

$$q_k = \frac{1}{\sqrt{n}} \sum_{l=-n/2}^{n/2} \exp\left(\frac{2\,i\,\pi\,k\,\varepsilon\,l}{n\,\varepsilon}\right) c_l'$$

$$= \frac{1}{\sqrt{n\,\varepsilon}} \sum_{l=-n/2}^{n/2} \exp\left(\frac{2\,i\,\pi\,k\,\varepsilon\,l}{n\,\varepsilon}\right) \sqrt{\varepsilon}\; c_l'$$

$$\rightarrow \qquad q(t) = \frac{1}{\sqrt{\beta\hbar}} \sum_{l=-\beta\hbar/2}^{\beta\hbar/2} \exp\left(\frac{2\,i\,\pi\,l\,t}{\beta\hbar}\right) c_l \qquad\qquad (\,c_l = \sqrt{\varepsilon}\; c_l'\,)$$

Reality of q then demands

$$c_{-l} = c_l^* \qquad\qquad c_0 = c_0^*$$

As before, the jacobian is 1 so that

$$[d\,q(t)\,] = d\,c_0 \prod_{l>0} d\,c_l\,d\,c_l^* \tag{2.57}$$

The continuum version of eq(2.55) is

$$S_0(q) = \frac{m}{2\,\hbar} \int_0^{\beta\hbar} d\,t\,\left(\dot{q}^2 + \omega^2\,q^2\right)$$

Using

$$\frac{1}{\beta\hbar} \int_0^{\beta\hbar} d\,t\,\exp\left(\frac{2\,i\,\pi\,l\,t}{\beta\hbar}\right) = \frac{1}{2\,i\,\pi\,l}\left(e^{2\,i\,\pi\,l} - 1\right) = \begin{cases} 1 & \text{for } l = 0 \\ 0 & \text{otherwise} \end{cases}$$

we have

$$\int_0^{\beta\hbar} d\,t\,q^2 = \frac{1}{\beta\hbar} \sum_{l=-\beta\hbar/2}^{\beta\hbar/2}\; \sum_{l'=-\beta\hbar/2}^{\beta\hbar/2} \int_0^{\beta\hbar} d\,t\,\exp\left(\frac{2\,i\,\pi\,(l+l')\,t}{\beta\hbar}\right) c_l\,c_{l'}$$

$$= \sum_{l=-\beta\hbar/2}^{\beta\hbar/2} c_l\,c_{-l}$$

$$= c_0^2 + 2\sum_{l=1}^{\beta\hbar/2} c_l\,c_{-l}$$

$$= c_0^2 + 2\sum_{l=1}^{\beta\hbar/2} c_l\,c_l^*$$

$$\dot{q}(t) = \frac{1}{\sqrt{\beta\hbar}} \sum_{l=-\beta\hbar/2}^{\beta\hbar/2} \exp\left(\frac{2 i \pi l t}{\beta\hbar}\right) \frac{2 i \pi l}{\beta\hbar} c_l$$

$$\rightarrow \quad \int_0^{\beta\hbar} dt\, \dot{q}^2 = \frac{1}{\beta\hbar} \sum_{l=-\beta\hbar/2}^{\beta\hbar/2} \sum_{l'=-\beta\hbar/2}^{\beta\hbar/2} \int_0^{\beta\hbar} dt \exp\left(\frac{2 i \pi (l+l') t}{\beta\hbar}\right) \left(\frac{2 i \pi}{\beta\hbar}\right)^2 l\, l'\, c_l\, c_{l'}$$

$$= \left(\frac{2\pi}{\beta\hbar}\right)^2 \sum_{l=-\beta\hbar/2}^{\beta\hbar/2} l^2 c_l c_{-l}$$

$$= 2\left(\frac{2\pi}{\beta\hbar}\right)^2 \sum_{l=1}^{\beta\hbar/2} l^2 c_l c_l^*$$

$$\therefore \quad S_0(q) = \frac{m}{\hbar}\left\{ \frac{1}{2}\omega^2 c_0^2 + \sum_{l=1}^{\beta\hbar/2} \left[\left(\frac{2\pi}{\beta\hbar}\right)^2 l^2 + \omega^2 \right] c_l c_l^* \right\}$$

Without the knowledge of the prefactor in the continuum limit, we write

$$\mathcal{Z}_0 \propto \int \prod_{l=0}^{\beta\hbar/2} d c_l\, d c_l^*\, e^{-S_0(q)}$$

For $l = 0$, the integral is

$$\int_{-\infty}^{\infty} d c_0 \exp\left(-\frac{m}{2\hbar}\omega^2 c_0^2\right) = \sqrt{\frac{2\pi\hbar}{m\omega^2}}$$

For $l \geq 1$, the integral is

$$\int d c_l\, d c_l^* \exp\left\{ -\frac{m}{\hbar}\left[\left(\frac{2\pi}{\beta\hbar}\right)^2 l^2 + \omega^2 \right] c_l c_l^* \right\}$$

$$= 2\pi \int_0^{\infty} d r\, r \exp\left\{ -\frac{m}{\hbar}\left[\left(\frac{2\pi}{\beta\hbar}\right)^2 l^2 + \omega^2 \right] r^2 \right\}$$

$$= \frac{\pi\hbar}{m\left[\left(\frac{2\pi}{\beta\hbar}\right)^2 l^2 + \omega^2 \right]}$$

$$\rightarrow \quad \mathcal{Z}_0 \propto \sqrt{\frac{2\pi\hbar}{m\omega^2}} \prod_{l=1}^{\beta\hbar/2} \frac{\pi\hbar}{m\left[\left(\frac{2\pi}{\beta\hbar}\right)^2 l^2 + \omega^2 \right]}$$

$$\propto \frac{1}{\omega} \prod_{l=1}^{\beta\hbar/2} \frac{1}{\left(\frac{2\pi}{\beta\hbar}\right)^2 l^2 + \omega^2} \qquad (2.58)$$

For $\beta\hbar \to \infty$, the infinite product

$$\prod_{l=1}^{\infty} \left[1 + \left(\frac{2\pi}{\beta\hbar\omega}\right)^2 l^2 \right]$$

diverges & $\mathcal{Z}_0$ is ill-defined.

$$\ln \mathcal{Z}_0 = \text{const} - \ln \omega - \sum_{l=1}^{\beta\hbar/2} \ln\left[\left(\frac{2\pi}{\beta\hbar}\right)^2 l^2 + \omega^2\right]$$

$$\to \qquad \frac{\partial}{\partial \omega} \ln \mathcal{Z}_0 = -\frac{1}{\omega} - \sum_{l=1}^{\beta\hbar/2} \frac{2\omega}{\left(\frac{2\pi}{\beta\hbar}\right)^2 l^2 + \omega^2}$$

In order to use (see eq.4 in §1.421 of G-R)

$$\coth \pi x = \frac{1}{\pi x} + \frac{2x}{\pi} \sum_{k=1}^{\infty} \frac{1}{x^2 + k^2}$$

we set

$$\frac{\partial}{\partial \omega} \ln \mathcal{Z}_0 = -\frac{\beta\hbar}{2\pi} \left\{ \frac{2\pi}{\beta\hbar\omega} + 2\left(\frac{\beta\hbar\omega}{2\pi}\right) \sum_{l=1}^{\beta\hbar/2} \frac{1}{l^2 + \left(\frac{\beta\hbar\omega}{2\pi}\right)^2} \right.$$

$$= -\frac{\beta\hbar}{2} \coth\left(\frac{\beta\hbar\omega}{2}\right)$$

which agrees with eq(2.51).

2.5.4. Perturbed Harmonic Oscillator

Consider

$$H = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 q^2 + V_1(q) \qquad (2.59)$$

where

$$V_1(q) = \sum_n v_n q^n \qquad (2.59a)$$

$$\to \qquad S(q) = \frac{1}{\hbar} \int_{-\beta\hbar/2}^{\beta\hbar/2} dt \left(\frac{1}{2} m \dot{q}^2 + \frac{1}{2} m \omega^2 q^2 + V_1\right)$$

$$\mathcal{Z}(\beta) = \int_{q\left(-\frac{\beta}{2}\right) = q\left(\frac{\beta}{2}\right)} [dq] \exp\left[-\frac{1}{\hbar} \int_{-\beta\hbar/2}^{\beta\hbar/2} dt \left(\frac{1}{2} m \dot{q}^2 + \frac{1}{2} m \omega^2 q^2 + V_1\right)\right] \qquad (2.60)$$

Using eqs(2.48a, 2.43), we have

$$\mathcal{Z}(\beta) = \exp\left[-\frac{1}{\hbar} \int_{-\beta\hbar/2}^{\beta\hbar/2} dt\, V_1\left(\hbar \frac{\delta}{\delta b(t)}\right)\right] \mathcal{Z}_G(b, \beta) \Bigg|_{b=0} \qquad (2.61)$$

With $\mathcal{Z}_G$ given by eq(2.47), we have

$$\mathcal{Z}(\beta) = \mathcal{Z}_0(\beta) \exp\left[-\frac{1}{\hbar} \int_{-\beta\hbar/2}^{\beta\hbar/2} dt\, V_1\left(\hbar \frac{\delta}{\delta b(t)}\right)\right] \exp\left[\frac{1}{2} \int du\, dv\, b(u)\, \Delta(u-v)\, b(v)\right] \Bigg|_{b=0}$$

(2.62)

Assuming V_1 to be well-behaved,

$$\exp\left[-\frac{1}{\hbar} \int_{-\beta\hbar/2}^{\beta\hbar/2} dt\, V_1\left(\hbar \frac{\delta}{\delta b(t)}\right)\right] = \sum_{k=0}^{\infty} \frac{1}{k!} \left[-\frac{1}{\hbar} \int_{-\beta\hbar/2}^{\beta\hbar/2} dt\, V_1\left(\hbar \frac{\delta}{\delta b(t)}\right)\right]^k$$

$$= \sum_{k=0}^{\infty} \frac{(-)^k}{k!\, \hbar^k} \int_{-\beta\hbar/2}^{\beta\hbar/2} dt_1 \ldots dt_k\, V_1\left(\hbar \frac{\delta}{\delta b(t_1)}\right) \ldots V_1\left(\hbar \frac{\delta}{\delta b(t_k)}\right)$$

Using eq(2.48), we have

$$\frac{\mathcal{Z}(\beta)}{\mathcal{Z}_0(\beta)} = \sum_{k=0}^{\infty} \frac{(-)^k}{k!\,\hbar^k} \int_{-\beta\hbar/2}^{\beta\hbar/2} d\,t_1 \ldots d\,t_k \langle V_1[q(t_1)] \ldots V_1[q(t_k)] \rangle_0$$

If V_1 is given by eq(2.59a), Wick's theorem can be applied for further calculations.

Example

Let

$$V_1(q) = \lambda\, q^4$$

then to 2nd order in λ,

$$\frac{\mathcal{Z}(\beta)}{\mathcal{Z}_0(\beta)} = 1 - \frac{\lambda}{\hbar} \int_{-\beta\hbar/2}^{\beta\hbar/2} d\,t \left\langle q(t)^4 \right\rangle_0 + \frac{1}{2}\left(\frac{\lambda}{\hbar}\right)^2 \int_{-\beta\hbar/2}^{\beta\hbar/2} d\,t_1\, d\,t_2 \left\langle q(t_1)^4\, q(t_2)^4 \right\rangle_0$$

Using the Wick's theorem [eq(2.49)], we have

$$\begin{aligned}
\left\langle q(t)^4 \right\rangle_0 &= \lim_{t_1\to t_2\to t_3\to t_4\to t} \langle q(t_1)\, q(t_2)\, q(t_3)\, q(t_4) \rangle_0 \\
&= \lim_{t_1\to t_2\to t_3\to t_4\to t} \{ \langle q(t_1)\, q(t_2) \rangle_0 \langle q(t_3)\, q(t_4) \rangle_0 + \langle q(t_1)\, q(t_3) \rangle_0 \langle q(t_2)\, q(t_4) \rangle_0 \\
&\qquad + \langle q(t_1)\, q(t_4) \rangle_0 \langle q(t_2)\, q(t_3) \rangle_0 \} \\
&= 3 \left\langle q(t)^2 \right\rangle_0 \left\langle q(t)^2 \right\rangle_0 \\
&= 3 \left[\left\langle q(t)^2 \right\rangle_0 \right]^2 \\
&= 3 \left[\frac{\hbar}{m} \Delta(0) \right]^2 \qquad\qquad [\text{ se eq(2.48b)}
\end{aligned}$$

To simplify the notations, let $q_k = q(t_k)$.

To calculate $\left\langle q_a^4\, q_b^4 \right\rangle_0$, we need to consider all the pairing permutations in

$$\lim_{\substack{1\to2\to3\to4\to a \\ 5\to6\to7\to8\to b}} \langle q_1\, q_2\, q_3\, q_4\, q_5\, q_6\, q_7\, q_8 \rangle_0$$

Permutations within each group $\{1, 2, 3, 4\}$ & $\{5, 6, 7, 8\}$ gives

$$3\left[\left\langle q_a^2 \right\rangle_0\right]^2 \cdot 3\left[\left\langle q_b^2 \right\rangle_0\right]^2 = 9\left[\left\langle q_a^2 \right\rangle_0\right]^2 \left[\left\langle q_b^2 \right\rangle_0\right]^2$$

Permutations that make an odd number of mixings between groups is not possible since one is then left with the problem of pairing an odd number of q's within each group.

Permutations that allows 2 pairs of mixing between groups are of the form

$$\left\langle q_a^2 \right\rangle_0 [\langle q_a\, q_b \rangle_0]^2 \left\langle q_b^2 \right\rangle_0$$

The number of such permutations is calculated as follows.
The number of ways to pick the 1st mixing pair is 4×4.
The number of ways to pick the 2nd mixing pair is then 3×3.
What remains must pair within each group so there is only 1 way.
Since the order of the 2 mixing pairs does not matter, the number of distinct pairings is

$$\frac{(4\times4)\times(3\times3)}{2} = 72$$

Finally, permutations that allows 4 pairs of mixing between groups are of the form

$$[\langle q_a\, q_b \rangle_0]^4$$

The number of such permutations is calculated as follows.
The number of ways to pick the 1st mixing pair is 4×4.
The number of ways to pick the 2nd mixing pair is then 3×3.
The number of ways to pick the 2nd mixing pair is then 2×2.

What remains must pair within each other so there is only 1 way.
Since the order of the 4 mixing pairs does not matter, the number of distinct pairings is

$$\frac{(4\times 4)\times(3\times 3)\times(2\times 2)}{4!} = 4! = 24$$

Putting everything together, we have

$$\langle q_a^4 q_b^4\rangle_0 = 9\left[\langle q_a^2\rangle_0\right]^2\left[\langle q_b^2\rangle_0\right]^2 + 72\langle q_a^2\rangle_0\left[\langle q_a q_b\rangle_0\right]^2\langle q_b^2\rangle_0 + 24\left[\langle q_a q_b\rangle_0\right]^4$$
$$= \left(\frac{\hbar}{m}\right)^4\left\{9\,\Delta(0)^4 + 72\,\Delta(0)^2\,\Delta(t_a-t_b)^2 + 24\,\Delta(t_a-t_b)^4\right\}$$

Thus,

$$\frac{\lambda}{\hbar}\int_{-\beta\hbar/2}^{\beta\hbar/2} dt\,\langle q(t)^4\rangle_0 = \frac{\lambda}{\hbar}\int_{-\beta\hbar/2}^{\beta\hbar/2} dt\,3\left[\frac{\hbar}{m}\Delta(0)\right]^2$$
$$= 3\lambda\beta\left(\frac{\hbar}{m}\right)^2\Delta(0)^2$$

$$\frac{1}{2}\left(\frac{\lambda}{\hbar}\right)^2\int_{-\beta\hbar/2}^{\beta\hbar/2} dt_1\,dt_2\,\langle q_1^4 q_2^4\rangle_0 = \frac{1}{2}\left(\frac{\lambda}{\hbar}\right)^2\left(\frac{\hbar}{m}\right)^4\left\{9(\beta\hbar)^2\,\Delta(0)^4\right.$$
$$\left. + 72\,\Delta(0)^2\int_{-\beta\hbar/2}^{\beta\hbar/2} dt_1\,dt_2\,\Delta(t_1-t_2)^2 + 24\int_{-\beta\hbar/2}^{\beta\hbar/2} dt_1\,dt_2\,\Delta(t_1-t_2)^4\right\}$$
$$= \frac{1}{2}\left(\frac{\lambda}{\hbar}\right)^2\left(\frac{\hbar}{m}\right)^4\beta\hbar\left[9\,\hbar\beta\,\Delta(0)^4 + 72\,\Delta(0)^2\int_{-\beta\hbar/2}^{\beta\hbar/2} dt\,\Delta(t)^2 + 24\int_{-\beta\hbar/2}^{\beta\hbar/2} dt\,\Delta(t)^4\right]$$

$$\frac{\mathcal{Z}(\beta)}{\mathcal{Z}_0(\beta)} = 1 - 3\lambda\beta\left(\frac{\hbar}{m}\right)^2\Delta(0)^2 + \frac{9}{2}(\lambda\beta)^2\left(\frac{\hbar}{m}\right)^4\Delta(0)^4 \tag{2.63}$$
$$+36\,\beta\hbar\left(\frac{\lambda}{\hbar}\right)^2\left(\frac{\hbar}{m}\right)^4\Delta(0)^2\int_{-\beta\hbar/2}^{\beta\hbar/2} dt\,\Delta(t)^2$$
$$+12\,\beta\hbar\left(\frac{\lambda}{\hbar}\right)^2\left(\frac{\hbar}{m}\right)^4\int_{-\beta\hbar/2}^{\beta\hbar/2} dt\,\Delta(t)^4 + \ldots$$

The 1st three terms exponentiate, i.e., they are the terms in the Taylor expansion

$$\exp\left[-3\lambda\beta\left(\frac{\hbar}{m}\right)^2\Delta(0)^2\right] \approx 1 - 3\lambda\beta\left(\frac{\hbar}{m}\right)^2\Delta(0)^2 + \frac{9}{2}(\lambda\beta)^2\left(\frac{\hbar}{m}\right)^4\Delta(0)^4 + \ldots$$

This is in agreement of eq(1.18).