2.6. Semi-Classical Expansion

2.6.1. Quantum Partition Function

In the classical limit ($\hbar \to 0$), the dominant term in the imaginary time action [see eq(2.32)]

$$\frac{S(q)}{\hbar} = \int_0^\beta d\tau \left\{ \frac{1}{2\hbar^2} m \dot{q}^2(\tau) + V[q(\tau)] \right\} \qquad \left(\tau = \frac{t}{\hbar} \right)$$

is the kinetic term.

Consider

$$\langle q_0 | e^{-\beta H} | q_0 \rangle = \int_{q(0)=q(\beta)=q_0} [d\,q(\tau)]\, e^{-S(q)/\hbar} \tag{2.64}$$

Let

$$q = q_0 + r$$

$\rightarrow$ $\quad d\,q = d\,r \qquad \& \qquad r(0) = r(\beta) = 0$

$$\therefore \quad \langle q_0 | e^{-\beta H} | q_0 \rangle = \int_{r(0)=r(\beta)=0} [d\,r(\tau)]\, e^{-\Sigma(r)} \tag{2.65}$$

where

$$\Sigma(r) = \int_0^\beta d\tau \left[\frac{1}{2\hbar^2} m \dot{r}^2 + V(q_0 + r) \right] \tag{2.66}$$

As $\hbar \to 0$, the kinetic term restricts r to be of order $\hbar$. Hence,

$$V(q_0 + r) = V(q_0) + V'(q_0)\, r + \frac{1}{2} V''(q_0)\, r^2 + O(\hbar^3) \tag{2.66a}$$

$$\rightarrow \quad e^{-\Sigma} = e^{-\beta V(q_0)} \exp\left(-\int_0^\beta d\tau \frac{1}{2\hbar^2} m \dot{r}^2 \right) \exp\left\{ -\int_0^\beta d\tau \left[V'(q_0)\, r + \frac{1}{2} V''(q_0)\, r^2 + O(\hbar^3) \right] \right\}$$

$$= e^{-\beta V(q_0)} \exp\left(-\int_0^\beta d\tau \frac{1}{2\hbar^2} m \dot{r}^2 \right) \left\{ 1 - \int_0^\beta d\tau \left[V'(q_0)\, r(\tau) + \frac{1}{2} V''(q_0)\, r(\tau)^2 \right] + \frac{1}{2} V'(q_0)^2 \int_0^\beta d\tau \int_0^\beta d\tau'\; r(\tau)\, r(\tau') + O(\hbar^3) \right\}$$

Let

$$\langle f(r) \rangle = \frac{1}{\mathcal{N}(\beta)} \int_{r(0)=r(\beta)=0} [d\,r(\tau)]\; e^{-\Sigma_0(r)}\, f(r) \tag{2.66b}$$

with

$$\Sigma_0(r) = \int_0^\beta d\tau \frac{1}{2\hbar^2} m \dot{r}^2$$

i.e., $\langle \ldots \rangle$ is the expectation value with respect to the free action Σ_0. We have

$$\langle q_0 | e^{-\beta H} | q_0 \rangle = \mathcal{N}(\beta)\, e^{-\beta V(q_0)} \left\{ 1 - V'(q_0) \int_0^\beta d\tau \, \langle r(\tau) \rangle - \frac{1}{2} V''(q_0) \int_0^\beta d\tau \langle r(\tau)^2 \rangle + \frac{1}{2} V'(q_0)^2 \int_0^\beta d\tau \int_0^\beta d\tau' \, \langle r(\tau)\, r(\tau') \rangle + O(\hbar^3) \right\} \tag{2.66 c}$$

Following the procedure of §2.5.1, we set

$$\Sigma_{0\,G}(r, b) = \int_0^\beta d\tau \left(\frac{1}{2\hbar^2} m \dot{r}^2 - b\, r \right) \qquad \text{[see eq(2.42)]}$$

$$= -\int_0^\beta d\tau\, L$$

The Euler-Lagrange eq. for L is

$$\frac{1}{\hbar^2} m \ddot{r} = -b$$

with solution

$$r(\tau) = \frac{\hbar^2}{m} \int_0^\beta d\,u\,\Delta(\tau, u)\, b(u)\, d\,u$$

where

$$\ddot{\Delta}(\tau, u) = -\delta(\tau - u) \qquad \text{[see eq(2.45c)]}$$

with B.C.

$$\Delta(0, u) = \Delta(\beta, u) = 0$$

$\Delta(\tau, u)$

We follow the procedure of §2.5.1 to find Δ.

The independent solutions to the homogeneous eq.

$$\ddot{\psi} = 0$$

are

$$\psi_1 = \text{const} \qquad \& \qquad \psi_2 = c\,\tau$$

Integrating the E-L eq. gives the discontinuity of $\dot{\Delta}$ at $\tau = u$:

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

In order to satisfy the symmetry relation

$$\Delta(\tau, \mu) = \Delta(u, \tau)$$

& the B.C.

$$\Delta(0, u) = \Delta(\beta, u) = 0$$

we use ψ_2 & set

$$\Delta(\tau, u) = \begin{cases} A\,(\beta - \tau)\,u & \text{for } \tau > u \\ A\,\tau\,(\beta - u) & \text{for } \tau < u \end{cases} \qquad (\,A = \text{const}\,)$$

$$\rightarrow \qquad \dot{\Delta}(\tau, u) = \begin{cases} -A\,u & \text{for } \tau > u \\ A\,(\beta - u) & \text{for } \tau < u \end{cases}$$

so that the discontinuity condition becomes

$$-A\,u - A(\beta - u) = -1$$

$$\rightarrow \qquad A = \frac{1}{\beta}$$

$$\therefore \qquad \Delta(\tau, u) = \begin{cases} (\beta - \tau)\,\dfrac{u}{\beta} & \text{for } \tau > u \\ \tau\left(1 - \dfrac{u}{\beta}\right) & \text{for } \tau < u \end{cases}$$

$$= \begin{cases} u - \dfrac{1}{\beta}\,u\,\tau & \text{for } \tau > u \\ \tau - \dfrac{1}{\beta}\,u\,\tau & \text{for } \tau < u \end{cases}$$

$$= \frac{1}{2}\,(\,\tau + u - |\,\tau - u\,|\,) - \frac{1}{\beta}\,u\,\tau$$

$$= -\frac{1}{2}\left|\tau-u\right| + \frac{1}{2}\left(\tau+u-2\frac{u\,\tau}{\beta}\right) \tag{2.67}$$

$\mathcal{Z}(\beta)$

As in §2.5.2, we set

$$\mathcal{Z}_{0\,G}(b,\beta) = \int [d\,r(\tau)]\, e^{-\Sigma_{0\,G}(r,b)}$$

$$\to \quad \frac{\delta}{\delta\, b(\tau_1)}\mathcal{Z}_{0\,G}(b,\beta) = \int [d\,r(\tau)]\, r(\tau_1)\, e^{-\Sigma_{0\,G}(r,b)}$$

$$= \frac{\hbar^2}{m}\int_0^\beta d\,u\,\Delta(\tau_1,u)\, b(u)\, d\,u\,\mathcal{Z}_{0\,G}(b,\beta) \tag{2.67a}$$

so that

$$\langle r(\tau)\, r(u)\rangle = \frac{1}{\mathcal{Z}_0(\beta)}\frac{\delta^2}{\delta\, b(u)\,\delta\, b(\tau)}\mathcal{Z}_{0\,G}(b,\beta)\bigg|_{b=0} \qquad \text{[see eq(2.48b)]}$$

$$= \frac{\hbar^2}{m}\Delta(\tau,u)$$

$$= \frac{\hbar^2}{m}\left[\frac{1}{2}\left(\tau+u-\left|\tau-u\right|\right) - \frac{1}{\beta}u\,\tau\right] \tag{2.67b}$$

From eq(2.66b), we have

$$\langle 1\rangle = 1$$

$$\to \quad \mathcal{N}(\beta) = \int_{r(0)=r(\beta)=0} [d\,r(\tau)]\, e^{-\Sigma_0(r)}$$

$$= \left\langle r\left|\, e^{-\beta H_0}\right| r\right\rangle_{r=0}$$

$$= \left\langle 0\left|\, e^{-\beta H_0}\right| 0\right\rangle$$

where

$$\Sigma_0(r) = \int_0^\beta d\,\tau\,\frac{1}{2\,\hbar^2}m\,\dot{r}^2 = \beta\, H_0$$

From §2.2, the 1-D version of eq(2.10) gives

$$\langle q\,|\,U(t,t')\,|\,q'\rangle = \left(\frac{m}{2\,\pi\,\hbar\,(t-t')}\right)^{1/2}\exp\left[-\frac{m}{2\,\hbar\,(t-t')}(q-q')^2\right]$$

where

$$U(t,t') = \exp\left(-\frac{1}{\hbar}\int_t^{t'} d\,t''\,\frac{1}{2}m\,\dot{q}^2\right)$$

Setting

$$\tau = \frac{t}{\hbar} \qquad \& \qquad r = q$$

we get

$$U(\beta\,\hbar,0) = e^{-\beta H_0}$$

$$\to \quad \mathcal{N}(\beta) = \left(\frac{m}{2\,\pi\,\hbar^2\,\beta}\right)^{1/2} \tag{2.68}$$

Furthermore, from eq(2.67a,b), we have

$$\left\langle r(\tau_1)\ldots r(\tau_p)\right\rangle = 0 \qquad \forall\; p = \text{odd}$$

$$\int_0^\beta d\tau \left\langle r(\tau)^2 \right\rangle = \frac{\hbar^2}{m} \int_0^\beta d\tau \left(\tau - \frac{1}{\beta} \tau^2 \right)$$
$$= \frac{1}{6} \frac{\hbar^2}{m} \beta^2$$

$$\int_0^\beta d\tau \int_0^\beta du \, \langle r(\tau)\, \tau(u) \rangle = \frac{\hbar^2}{m} \int_0^\beta d\tau \left[\int_0^\tau du \left(u - \frac{1}{\beta} u \tau \right) + \int_\tau^\beta du \left(\tau - \frac{1}{\beta} u \tau \right) \right]$$
$$= \frac{\hbar^2}{m} \int_0^\beta d\tau \left\{ \frac{1}{2} \tau^2 \left(1 - \frac{\tau}{\beta} \right) + \tau \left[\beta - \tau - \frac{1}{2\beta} (\beta^2 - \tau^2) \right] \right\}$$
$$= \frac{1}{2} \frac{\hbar^2}{m} \int_0^\beta d\tau \, (\beta - \tau)\, \tau$$
$$= \frac{1}{12} \frac{\hbar^2}{m} \beta^3$$

Eq(2.66c) thus becomes

$$\mathcal{Z}(\beta) = \operatorname{tr} e^{-\beta H}$$
$$= \int dr \left\langle r \,\middle|\, e^{-\beta H} \,\middle|\, r \right\rangle$$
$$= \left(\frac{m}{2\pi\hbar^2\beta} \right)^{1/2} \int_{-\infty}^{\infty} dr \, e^{-\beta V(r)} \left\{ 1 - \frac{1}{12} V''(r) \frac{\hbar^2}{m} \beta^2 + \frac{1}{24} V'(r)^2 \frac{\hbar^2}{m} \beta^3 + O(\hbar^4) \right\}$$

$$d\, e^{-\beta V} = -\beta V' e^{-\beta V} dr$$

$$\rightarrow \quad \int_{-\infty}^{\infty} dr \, e^{-\beta V} V'^2 = -\frac{1}{\beta} \int V' \, d\, e^{-\beta V}$$
$$= -\frac{1}{\beta} \left[V' e^{-\beta V} \Big|_{r=-\infty}^{r=\infty} - \int_{-\infty}^{\infty} dr \, V'' e^{-\beta V} \right]$$
$$= \frac{1}{\beta} \int_{-\infty}^{\infty} dr \, V'' e^{-\beta V} \qquad \text{since } V \text{ is bounded}$$

$$\therefore \quad \mathcal{Z}(\beta) = \left(\frac{m}{2\pi\hbar^2\beta} \right)^{1/2} \int_{-\infty}^{\infty} dr \, e^{-\beta V(r)} \left\{ 1 - \frac{1}{24} V''(r) \frac{\hbar^2}{m} \beta^2 + O(\hbar^4) \right\}$$
$$= \left(\frac{m}{2\pi\hbar^2\beta} \right)^{1/2} \int_{-\infty}^{\infty} dr \left\{ \exp\left[-\beta V(r) - \frac{1}{24} V''(r) \frac{\hbar^2}{m} \beta^2 \right] + O(\hbar^4) \right\} \qquad (2.69)$$

where we've used

$$\exp\left[-\frac{1}{24} V''(r) \frac{\hbar^2}{m} \beta^2 \right] = 1 - \frac{1}{24} V''(r) \frac{\hbar^2}{m} \beta^2 + O(\hbar^4)$$

Discussion

(i) The classical partition function for

$$H = \frac{p^2}{2m} + V(q)$$

is given by

$$\mathcal{Z}_{\text{cl}}(\beta) = \int \frac{dp\, dq}{2\pi\hbar} e^{-\beta H} = \left(\frac{m}{2\pi\hbar^2\beta} \right)^{1/2} \int dq \, e^{-\beta V}$$

which is just eq(2.69) for $\hbar \rightarrow 0$.

(ii) The thermal length is defined as

$$\lambda_{\text{th}} = \hbar \sqrt{\frac{\beta}{m}}$$

A length scale for the potential that increases as $\beta \to 0$ (high temperature limit) is

$$l_{pot} \propto \sqrt{\left| \frac{\langle V(q) \rangle}{\langle V''(q) \rangle} \right|}$$

The relative strength of the quantum correction is

$$\left| \frac{\frac{1}{24} \langle V''(r) \rangle \frac{\hbar^2}{m} \beta^2}{\beta \langle V(r) \rangle} \right| \propto \left(\frac{\lambda_{th}}{l_{pot}} \right)^2$$

(iii) Dimensional reduction:

dim. of $\mathcal{Z}_{cl}(\beta)$ is 1 less than that of the quantum $\mathcal{Z}(\beta)$.

(See Zinn-Justin's text.)

2.6.2. WKB Spectrum

WKB limit means $\hbar \to 0$ at fixed energy.
It can be obtained from the semi-classical expansion discussed in §2.6.1.

For a hamiltonian with a discrete spectrum

$$\mathcal{Z}(\beta) = \text{tr}\, e^{-\beta H} = \sum_n e^{-\beta E_n}$$

The Laplace transform $G(E)$ of $\mathcal{Z}(\beta)$ is

$$\begin{aligned} G(E) &= \int_0^\infty d\beta\, e^{\beta E}\, \mathcal{Z}(\beta) \\ &= \sum_n \int_0^\infty d\beta\, e^{-\beta (E_n - E)} \\ &= \sum_n \frac{1}{E_n - E} \end{aligned} \qquad (2.70a)$$

where we've used

$$\int_0^\infty dx\, e^{-a x} = \frac{1}{a} \qquad \text{for } a \text{ real \& positive}$$

Eq(2.70a) is thus obtained assuming E to be real & less than E_n for all n.
We then assume it to be valid for all complex E, i.e., analytic continue it into the complex plane.
Its behavior near the poles at E_n is represented by the limit

$$\lim_{\delta \to 0} [\, G(E + i\delta) - G(E - i\delta)\,] = \sum_n \left(\frac{1}{E_n - E - i\delta} - \frac{1}{E_n - E + i\delta} \right)$$

Using

$$\lim_{x \to 0} \frac{1}{x + i\delta} = P \frac{1}{x} - i\pi\, \delta(x)$$

where $P f$ = principal value of f, we have

$$\lim_{\delta \to 0} [\, G(E + i\delta) - G(E - i\delta)\,] = 2\pi i \sum_n \delta(E - E_n)$$

The integrated spectral distribution is given by

$$\begin{aligned} \int_{-\infty}^{E} dE' \frac{G(E' + i\delta) - G(E' - i\delta)}{2\pi i} &= \sum_n \int_{-\infty}^{E} dE'\, \delta(E - E_n) \\ &= \sum_n \theta(E - E_n) \end{aligned} \qquad (2.70b)$$

where θ is the step function

$$\theta(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x < 0 \\ \frac{1}{2} & \text{for } x = 0 \end{cases}$$

For E on the spectrum, i.e., $E = E_k$, we have

$$\int_{-\infty}^{E_k} d\,E' \,\frac{G(E' + i\,\delta) - G(E' - i\,\delta)}{2\,\pi\,i} = \frac{1}{2} + \sum_{n=0}^{k-1} 1$$

$$= k + \frac{1}{2} \qquad (2.70)$$

Keeping only the leading term in the semi-classical result [eq(2.69)], we have

$$\mathcal{Z}(\beta) \approx \left(\frac{m}{2\,\pi\,\hbar^2\,\beta}\right)^{1/2} \int_{-\infty}^{\infty} d\,r\, e^{-\beta\,V(r)}$$

Eq(2.70a) then becomes

$$G_{\rm cl}(E) = \left(\frac{m}{2\,\pi\,\hbar^2}\right)^{1/2} \int_0^{\infty} d\,\beta\, e^{\beta\,E} \int_{-\infty}^{\infty} d\,r\, \frac{e^{-\beta\,V(r)}}{\sqrt{\beta}}$$

Using

$$\int_0^{\infty} d\,\beta\, \frac{e^{-\beta\,(V-E)}}{\sqrt{\beta}} = \sqrt{\frac{\pi}{V-E}}$$

we have

$$G_{\rm cl}(E) = \left(\frac{m}{2\,\hbar^2}\right)^{1/2} \int_{-\infty}^{\infty} \frac{d\,r}{\sqrt{V(r) - E}}$$

$$\to \qquad G_{\rm cl}(E' + i\,\delta) - G_{\rm cl}(E' - i\,\delta) = \left(\frac{m}{2\,\hbar^2}\right)^{1/2} \int_{-\infty}^{\infty} d\,r \left(\frac{1}{\sqrt{V(r) - E' - i\,\delta}} - \frac{1}{\sqrt{V(r) - E' + i\,\delta}}\right)$$

For $\delta \to 0$,

$$\frac{1}{\sqrt{x + i\,\delta}} = \frac{1}{\sqrt{x}\left(1 + \frac{i}{x}\,\delta\right)^{1/2}} = \frac{1}{\sqrt{x}\left(1 + \frac{i}{2\,x}\,\delta\right)}$$

$$= \frac{2\sqrt{x}}{2\,x + i\,\delta} = 2\sqrt{x}\left[P\,\frac{1}{2\,x} - i\,\pi\,\delta(2\,x)\right] = 2\sqrt{x}\left[P\,\frac{1}{2\,x} - i\,\frac{\pi}{2}\,\delta(x)\right]$$

where

$$\delta(a\,x) = \frac{1}{|\,a\,|}\,\delta(x)$$

Alternatively, with $a\,\delta \sim \delta$, we get the same result

$$\frac{2\sqrt{x}}{2\,x + i\,\delta} = \frac{\sqrt{x}}{x + i\,\delta} = \sqrt{x}\left[P\,\frac{1}{x} - i\,\pi\,\delta(x)\right]$$

Hence

$$G_{\rm cl}(E' + i\,\delta) - G_{\rm cl}(E' - i\,\delta) = \left(\frac{m}{2\,\hbar^2}\right)^{1/2} 2\,i\,\pi \int_{-\infty}^{\infty} d\,r\, \sqrt{V(r) - E'}\;\delta[V(r) - E']$$

The integrated spectral distribution [eq(2.70b)] becomes

$$\int_{-\infty}^{E} dE' \, \frac{G_{cl}(E'+i\delta) - G_{cl}(E'-i\delta)}{2\pi i} = \left(\frac{m}{2\hbar^2}\right)^{1/2} \int_{-\infty}^{\infty} dr \int_{-\infty}^{E} dE' \, \sqrt{V(r) - E'} \, \delta[V(r) - E']$$

$$= \left(\frac{m}{2\hbar^2}\right)^{1/2} \int_{-\infty}^{\infty} dr \, \sqrt{E - V(r)} \, \theta[E - V(r)]$$

Setting $E = E_k$ & using eq(2.70), we have

$$\left(\frac{m}{2\hbar^2}\right)^{1/2} \int_{-\infty}^{\infty} dr \, \sqrt{E_k - V(r)} \, \theta[E_k - V(r)] = k + \frac{1}{2}$$

$$\int_{-\infty}^{\infty} dr \, \sqrt{2m[E_k - V(r)]} \, \theta[E_k - V(r)] = 2\hbar\left(k + \frac{1}{2}\right)$$

If the motion is periodic, it may be compared with the Bohr–Sommerfeld quantization condition

$$\oint_{H=E} \boldsymbol{p} \cdot d\boldsymbol{q} = 2\pi n \hbar \qquad\qquad H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$$