2.14. Calculation Techniques on Sliced Time Axis via the Poisson Formula

Consider the time-sliced partition function for a harmonic oscillator

$$Z = \prod_{m=0}^{N} \left[2\,(1 - \cos\omega_m\,\epsilon) + \epsilon^2\,\omega^2 \right]^{-1/2} \qquad \omega_m = \frac{2\,\pi\,m}{\beta\,\hbar} \tag{2.462}$$

Instead of evaluating the products directly, one may deal instead of the free energy

$$\begin{aligned} F &= -\frac{1}{\beta}\ln Z \\ &= \frac{1}{2\,\beta}\sum_{m=0}^{N} \ln\left[2\,(1 - \cos\omega_m\,\epsilon) + \epsilon^2\,\omega^2 \right] \end{aligned} \tag{2.463}$$

Using Poisson's summation formula (1.197)

$$\sum_{n=-\infty}^{\infty} e^{i\,2\,\pi\,n\,\mu} = \sum_{m=-\infty}^{\infty} \delta(\mu - m)$$

which implies (1.205)

$$\int d\,\mu \sum_{n=-\infty}^{\infty} e^{i\,2\,\pi\,n\,\mu}\, f(\mu) = \sum_{m} f(m)$$

we can write (2.463) as

$$F = \frac{1}{2\,\beta}\int_0^N d\,\mu \sum_{n=-\infty}^{\infty} e^{i\,2\,\pi\,n\,\mu} \ln\left[2\left(1 - \cos\frac{2\,\pi\,\mu}{\beta\,\hbar}\,\epsilon\right) + \epsilon^2\,\omega^2 \right] \tag{2.463a}$$

Note: The L.H.S. of (1.197) is just the Fourier series expansion of the periodic function, of period 1, on the R.H.S.

Setting

$$\lambda = \frac{2\,\pi\,\mu}{\beta\,\hbar}\,\epsilon = \frac{2\,\pi\,\mu}{N+1}$$

turns (2.463a) into

$$F = \frac{N+1}{2\,\beta}\int_0^{2\,\pi} \frac{d\,\lambda}{2\,\pi} \sum_{n=-\infty}^{\infty} e^{i\,n\,(N+1)\,\lambda} \ln\left[2\,(1 - \cos\lambda) + \epsilon^2\,\omega^2 \right] \tag{2.464}$$

where we've replaced the upper integration limit $\frac{2\,\pi\,N}{N+1}$ with $2\,\pi$.

The next task is to calculate the integral

$$\mathcal{I} = \int_0^{2\,\pi} \frac{d\,\lambda}{2\,\pi}\, e^{i\,n\,(N+1)\,\lambda} \ln\left[2\,(1 - \cos\lambda) + \epsilon^2\,\omega^2 \right] \tag{2.465}$$

Consider the small-x expansion of the exponential integral [Gradshteyn & L Ryzhik, Formula 8.214.2]

$$E_1(x) = -E_i(-x) \equiv \int_x^{\infty} d\,t\,\frac{e^{-t}}{t} \qquad x > 0 \tag{2.468}$$

$$= -\gamma - \ln x - \sum_{k=1}^{\infty} \frac{(-x)^k}{k\,k!} \tag{2.469}$$

where

$$\gamma \equiv -\frac{\Gamma'(1)}{\Gamma(1)} = \lim_{N\to\infty}\left(\sum_{n=1}^{N} \frac{1}{n} - \ln N \right) \approx 0.5773156649\ldots \tag{2.467}$$

is the Euler-Mascheroni constant.

With $t = a\,\tau$, (2.468) becomes

$$E_1(x) = \int_{x/a}^{\infty} d\,\tau\,\frac{e^{-a\,\tau}}{\tau}$$

$$\rightarrow \qquad E_1(a\,\delta) = \int_{\delta}^{\infty} d\,\tau\,\frac{e^{-a\,\tau}}{\tau}$$

$$= -\gamma - \ln(a\,\delta) - \sum_{k=1}^{\infty} \frac{(-a\delta)^k}{k\,k!}$$

$$\therefore \qquad \ln a = -\int_{\delta}^{\infty} d\,\tau\,\frac{e^{-a\,\tau}}{\tau} - \gamma - \ln\delta - \sum_{k=1}^{\infty} \frac{(-a\delta)^k}{k\,k!}$$

$$\xrightarrow[\delta\to 0]{} -\int_{\delta}^{\infty} d\,\tau\,\frac{e^{-a\,\tau}}{\tau} - \gamma - \ln\delta \qquad (2.466)$$

(2.465) then becomes

$$\mathcal{I} = \lim_{\delta\to 0} \int_0^{2\pi} \frac{d\,\lambda}{2\,\pi}\, e^{i\,n\,(N+1)\,\lambda} \left\{ -\int_{\delta}^{\infty} d\,\tau\,\frac{e^{-\left[2\,(1-\cos\lambda) + \epsilon^2\,\omega^2\right]\,\tau}}{\tau} - \gamma - \ln\delta \right\} \qquad (2.470a)$$

Using [Arfken, 3rd ed., Ex.11.1.16(b)]

$$J_n(x) = \frac{i^{-n}}{2\,\pi} \int_0^{2\pi} d\,\theta\, e^{i\,(n\,\theta + x\cos\theta)}$$

we have

$$\int_0^{2\pi} \frac{d\,\lambda}{2\,\pi}\, e^{i\,n\,(N+1)\,\lambda + 2\,\tau\cos\lambda} = i^{n\,(N+1)}\, J_{n\,(N+1)}(-2\,i\,\tau)$$

$$= i^{n\,(N+1)}\, e^{-i\,n\,(N+1)\,\pi/2}\, I_{n\,(N+1)}(2\,\tau)$$

$$= I_{n\,(N+1)}(2\,\tau) \qquad (2.470b)$$

where [Gradshteyn & L Ryzhik, Formula 8.406.1]

$$I_\nu(z) = e^{-i\,\nu\,\pi/2}\, J_\nu(i\,z)$$

is the modified Bessel function. Since I_n & J_n are real for real arguments, we have

$$I_n(x) = e^{i\,n\,\pi/2}\, J_n^*(i\,x) \;= e^{i\,n\,\pi/2}\, J_n(-i\,x)$$

Together with

$$\int_0^{2\pi} \frac{d\,\lambda}{2\,\pi}\, e^{i\,n\,(N+1)\,\lambda} = \delta_{n\,0} \qquad (2.470c)$$

(2.470a) becomes

$$\mathcal{I} = -\lim_{\delta\to 0} \left\{ \int_{\delta}^{\infty} d\,\tau\; I_{n\,(N+1)}(2\,\tau)\, \frac{e^{-\left(2+\epsilon^2\,\omega^2\right)\,\tau}}{\tau} + \delta_{n\,0}(\gamma + \ln\delta) \right\}$$

$$= -\lim_{\delta\to 0} \left\{ \int_{2\,\delta}^{\infty} d\,\tau\; I_{n\,(N+1)}(\tau)\, \frac{e^{-\left(2+\epsilon^2\,\omega^2\right)\,\tau/2}}{\tau} + \delta_{n\,0}(\gamma + \ln\delta) \right\}$$

(2.464) becomes

$$F = -\frac{\hbar}{2\,\epsilon} \sum_{n=-\infty}^{\infty} \lim_{\delta\to 0} \left\{ \int_{2\,\delta}^{\infty} d\,\tau\; I_{n\,(N+1)}(\tau)\, \frac{e^{-\left(2+\epsilon^2\,\omega^2\right)\,\tau/2}}{\tau} + \delta_{n\,0}(\gamma + \ln\delta) \right\}$$

$$= -\frac{\hbar}{2\,\epsilon} \sum_{n=-\infty}^{\infty} \lim_{\delta\to 0} \left\{ \int_{\delta}^{\infty} d\,\tau\; I_{n\,(N+1)}(\tau)\, \frac{e^{-\left(2+\epsilon^2\,\omega^2\right)\,\tau/2}}{\tau} + \delta_{n\,0}\left(\gamma + \ln\frac{\delta}{2}\right) \right\} \qquad (2.471)$$

Setting $m^2 = \epsilon^2\,\omega^2$, we have

$$\frac{\partial F}{\partial m^2} = \frac{\hbar}{4\,\epsilon} \sum_{n=-\infty}^{\infty} \lim_{\delta\to 0} \int_{\delta}^{\infty} d\,\tau\; I_{n\,(N+1)}(\tau)\, e^{-\left(2+m^2\right)\,\tau/2} \qquad (2.472)$$

Using [Gradshteyn & L Ryzhik, Formula 6.611.4]

$$\int_0^\infty d\,x\, e^{-\alpha x} I_\nu(\beta x) = \frac{\beta^\nu}{\sqrt{\alpha^2-\beta^2}\left(\alpha+\sqrt{\alpha^2-\beta^2}\right)^\nu} \tag{2.473}$$

where $\mathrm{Re}\,\nu > -1$ & $\mathrm{Re}\,\alpha > |\,\mathrm{Re}\beta\,|$, and

$I_{-n}(x) = I_n(x)$ for n integers

we have

$$\frac{\partial F}{\partial m^2} = \frac{\hbar}{4\epsilon}\sum_{n=-\infty}^{\infty} 1\Big/\sqrt{\frac{1}{4}(2+m^2)^2-1}\left[\frac{1}{2}(2+m^2)+\sqrt{\frac{1}{4}(2+m^2)^2-1}\right]^{|n|(N+1)}$$

$$= \frac{\hbar}{2\epsilon}\sum_{n=-\infty}^{\infty}\frac{1}{\sqrt{(2+m^2)^2-4}\left[\frac{(2+m^2)+\sqrt{(2+m^2)^2-4}}{2}\right]^{|n|(N+1)}}$$

$$= \frac{\hbar}{2\epsilon}\sum_{n=-\infty}^{\infty}\frac{1}{\sqrt{(2+m^2)^2-4}}\left[\frac{(2+m^2)-\sqrt{(2+m^2)^2-4}}{2}\right]^{|n|(N+1)} \tag{2.474}$$

Integrating (2.474) gives

$$F = \int d(2+m^2)\,\frac{\partial F}{\partial m^2} + \text{const}$$

$$= \sum_{n=-\infty}^{\infty}\mathcal{F}_n \tag{2.474a}$$

Using

$$\int d\,x\,\frac{1}{\sqrt{x^2-4}}\left(x-\sqrt{x^2-4}\right)^\alpha = -\frac{1}{\alpha}\left(x-\sqrt{x^2-4}\right)^\alpha \qquad \alpha \neq 0$$

$$\int d\,x\,\frac{1}{\sqrt{x^2-4}} = \ln\left(x+\sqrt{x^2-4}\right)$$

we have

$$\mathcal{F}_0 = \frac{\hbar}{2\epsilon}\ln\left[\frac{(2+m^2)+\sqrt{(2+m^2)^2-4}}{2}\right] + C_0 \tag{2.475}$$

and for $n \neq 0$,

$$\mathcal{F}_n = -\frac{\hbar}{2\epsilon}\,\frac{1}{|\,n\,|\,(N+1)}\left[\frac{(2+m^2)-\sqrt{(2+m^2)^2-4}}{2}\right]^{|n|(N+1)}\Bigg\} + C_n \tag{2.476}$$

where C_n are constants.

These constants can be obtained from the $m^2 \to \infty$ limit of (2.471). Owing to the factor $e^{-m^2\tau/2}$, the integral in (2.741) is dominated by the contribution from the small τ region where

$$I_\alpha(\tau) \approx \frac{1}{|\,\alpha\,|\,!}\left(\frac{\tau}{2}\right)^\alpha\left[1+O(\tau^2)\right] \tag{2.477}$$

Comparing (2.471) with (2.474a) gives, for $m^2 \to \infty$,

$$\mathcal{F}_0 \approx -\frac{\hbar}{2\epsilon}\left[\int_\delta^\infty d\,\tau\,\frac{e^{-m^2\tau/2}}{\tau} + \gamma + \ln\frac{\delta}{2}\right]$$

$$= -\frac{\hbar}{2\,\epsilon}\left[E_1\left(\frac{m^2}{2}\,\delta\right) + \gamma + \ln\frac{\delta}{2}\right]$$
$$\approx -\frac{\hbar}{2\,\epsilon}\left[-\gamma - \ln\left(\frac{m^2}{2}\,\delta\right) + \gamma + \ln\frac{\delta}{2}\right]$$
$$= \frac{\hbar}{\epsilon}\ln m \qquad (2.477a)$$

Setting $m^2 \to \infty$ to (2.475) gives

$$\mathcal{F}_0 \approx \frac{\hbar}{\epsilon}\ln m + C_0 \qquad (2.477b)$$

so that

$$C_0 = 0$$

Similarly, the $m^2 \to \infty$ limit of (2.474a) for $n \neq 0$ gives

$$\mathcal{F}_n = -\frac{\hbar}{2\,\epsilon}\int_0^\infty d\,\tau\; I_{n(N+1)}(\tau)\,\frac{e^{-m^2\,\tau/2}}{\tau}$$
$$\approx -\frac{\hbar}{2\,\epsilon}\,\frac{1}{[\;|\,n\,|\;(N+1)]\,!\,2^{|n|\,(N+1)}}\int_\delta^\infty d\,\tau\,\tau^{|n|\,(N+1)-1}\,e^{-m^2\,\tau/2}$$
$$= -\frac{\hbar}{2\,\epsilon}\,\frac{1}{[\;|\,n\,|\;(N+1)]\,!\,2^{|n|\,(N+1)}}\left(\frac{m^2}{2}\right)^{-|n|\,(N+1)}[\;|\,n\,|\;(N+1)-1]!$$
$$= -\frac{\hbar}{2\,\epsilon}\,\frac{1}{|\,n\,|\;(N+1)}\,m^{-2|n|\,(N+1)} \qquad (2.477c)$$

Setting $m^2 \to \infty$ to (2.476) gives

$$\mathcal{F}_n = -\frac{\hbar}{2\,\epsilon}\,\frac{1}{|\,n\,|\;(N+1)}\left(\frac{1}{m^2}\right)^{|n|\,(N+1)} + C_n \qquad (2.477d)$$

so that

$$C_n = 0 \qquad \forall\; n$$

Combining (2.474a) with (2.475-6) then re-write (2.463) as

$$F = \frac{1}{2\,\beta}\sum_{m=0}^{N}\ln\left[2\,(1-\cos\omega_m\,\epsilon) + \epsilon^2\,\omega^2\right]$$
$$= \frac{\hbar}{2\,\epsilon}\left\{\ln\left[\frac{(2+\epsilon^2\,\omega^2) + \sqrt{(2+\epsilon^2\,\omega^2)^2-4}}{2}\right]\right.$$
$$\left. - \sum_{n=-\infty}^{\infty}{}' \frac{1}{|\,n\,|\;(N+1)}\left[\frac{(2+\epsilon^2\,\omega^2) - \sqrt{(2+\epsilon^2\,\omega^2)^2-4}}{2}\right]^{|n|\,(N+1)}\right\}$$
$$= \frac{\hbar}{2\,\epsilon}\left\{\ln\left[\frac{(2+\epsilon^2\,\omega^2) + \sqrt{(2+\epsilon^2\,\omega^2)^2-4}}{2}\right]\right. \qquad (2.479)$$
$$\left. - \frac{2}{N+1}\sum_{n=1}^{\infty}\frac{1}{n}\left[\frac{(2+\epsilon^2\,\omega^2) + \sqrt{(2+\epsilon^2\,\omega^2)^2-4}}{2}\right]^{-n\,(N+1)}\right\}$$

We now introduce the parameter

$$\epsilon\,\tilde{\omega}_e \equiv \ln\left[\frac{(2+\epsilon^2\,\omega^2) + \sqrt{(2+\epsilon^2\,\omega^2)^2-4}}{2}\right] \qquad (2.480)$$

which satisfies

$$\cosh(\epsilon\,\tilde{\omega}_e) = \frac{1}{2}\left(e^{\epsilon\,\tilde{\omega}_e} + e^{-\epsilon\,\tilde{\omega}_e}\right)$$

$$= \frac{1}{2}\left[\frac{(2+\epsilon^2\,\omega^2) + \sqrt{(2+\epsilon^2\,\omega^2)^2 - 4}}{2} + \frac{2}{(2+\epsilon^2\,\omega^2) + \sqrt{(2+\epsilon^2\,\omega^2)^2 - 4}}\right]$$

$$= \frac{1}{2}\left[\frac{(2+\epsilon^2\,\omega^2) + \sqrt{(2+\epsilon^2\,\omega^2)^2 - 4}}{2} + \frac{(2+\epsilon^2\,\omega^2) - \sqrt{(2+\epsilon^2\,\omega^2)^2 - 4}}{2}\right]$$

$$= \frac{1}{2}(2+\epsilon^2\,\omega^2) \qquad (2.481)$$

and

$$\sinh(\epsilon\,\tilde{\omega}_e) = \frac{1}{2}\left(e^{\epsilon\,\tilde{\omega}_e} - e^{-\epsilon\,\tilde{\omega}_e}\right)$$

$$= \frac{1}{2}\sqrt{(2+\epsilon^2\,\omega^2)^2 - 4} \qquad (2.481a)$$

Hence,

$$\sinh^2\frac{\epsilon\,\tilde{\omega}_e}{2} = \frac{1}{2}[\cosh(\epsilon\,\tilde{\omega}_e) - 1] = \frac{1}{4}\epsilon^2\,\omega^2$$

$$\rightarrow \qquad \sinh\frac{\epsilon\,\tilde{\omega}_e}{2} = \frac{\epsilon\,\omega}{2}$$

which is simply (2.397).

(2.479) thus becomes

$$F = \frac{\hbar}{2\,\epsilon}\left(\epsilon\,\tilde{\omega}_e - \frac{2}{N+1}\sum_{n=1}^{\infty}\frac{1}{n}e^{-n\,(N+1)\,\epsilon\,\tilde{\omega}_e}\right)$$

$$= \frac{1}{2}\left(\hbar\,\tilde{\omega}_e - \frac{2}{\beta}\sum_{n=1}^{\infty}\frac{1}{n}e^{-n\,\beta\,\hbar\,\tilde{\omega}_e}\right)$$

$$= \frac{1}{2}\left[\hbar\,\tilde{\omega}_e + \frac{2}{\beta}\ln\left(1 - e^{-\beta\,\hbar\,\tilde{\omega}_e}\right)\right] \qquad (2.482a)$$

Using

$$\ln(1 - e^{-x}) = \ln\left[e^{-x/2}\left(e^{x/2} - e^{-x/2}\right)\right]$$

$$= -\frac{x}{2} + \ln\left(2\sinh\frac{x}{2}\right)$$

(2.482a) becomes

$$F = \frac{1}{\beta}\ln\left(2\sinh\frac{\beta\,\hbar\,\tilde{\omega}_e}{2}\right) \qquad (2.482)$$

In the continuum limit

$$F \xrightarrow[\epsilon\to 0]{} \frac{1}{\beta}\ln\left(2\sinh\frac{\beta\,\hbar\,\omega}{2}\right) = \frac{1}{2}\hbar\omega + \frac{1}{\beta}\ln\left(1 - e^{-\beta\,\hbar\,\omega}\right) \qquad (2.483)$$