2.8. Path Integrals and Quantum Statistics

The quantum statistical partition function was defined in §1.7 for a time-independent Hamiltonian H as

$$Z = \operatorname{Tr} e^{-\hat{H}/k_B T} = \sum_n e^{-E_n/k_B T} \tag{2.326}$$

which may be taken as the analytic continuation of the quantum mechanical partition function

$$Z_{\rm QM} = \operatorname{Tr} e^{-i(t_b - t_a)\hat{H}/\hbar} \tag{2.327}$$

to the imagianary time

$$t_b - t_a = -i\,\beta\,\hbar \qquad\qquad \beta = \frac{1}{k_B T} > 0 \tag{2.328}$$

In the local basis $|\,\boldsymbol{x}\,\rangle$, (2.326) becomes

$$\begin{aligned} Z &\equiv \int d\boldsymbol{x}\; z(\boldsymbol{x}) && (2.239\text{a})\\ &= \int d\boldsymbol{x}\,\left\langle \boldsymbol{x}\,\middle|\, e^{-\beta\hat{H}} \,\middle|\, \boldsymbol{x}\right\rangle \\ &= \int d\boldsymbol{x}\,\left\langle \boldsymbol{x}\,\middle|\, e^{-i(t_b-t_a)\hat{H}/\hbar} \,\middle|\, \boldsymbol{x}\right\rangle_{t_b-t_a=-i\beta\hbar} \\ &= \int d\boldsymbol{x}\,(\boldsymbol{x}\,t_b\,|\,\boldsymbol{x}\,t_a)_{t_b-t_a=-i\beta\hbar} && (2.329) \end{aligned}$$

From (2.239a), the diagonal element

$$z(\boldsymbol{x}) \equiv \left\langle \boldsymbol{x}\,\middle|\, e^{-\beta\hat{H}} \,\middle|\, \boldsymbol{x}\right\rangle = (\boldsymbol{x}\,t_b\,|\,\boldsymbol{x}\,t_a)_{t_b-t_a=-i\beta\hbar} \tag{2.330}$$

can be taken as the partition function density at $\boldsymbol{x}$.

For a 1-D harmonic oscillator, (2.173) gives

$$z_\omega(x) = \sqrt{\frac{M}{2\pi\hbar}}\sqrt{\frac{\omega}{\sinh\beta\omega}}\,\exp\left[-\frac{M\omega}{\hbar}\tanh\left(\frac{\hbar\beta\omega}{2}x^2\right)\right] \tag{2.331}$$

As in (2.4), the time-sliced version of Z is

$$\begin{aligned} Z &= \left(\prod_{n=1}^{N+1}\int_{-\infty}^{\infty} d\boldsymbol{x}_n\right)\left\langle \boldsymbol{x}_{N+1}\,\middle|\, e^{-\epsilon\hat{H}/\hbar}\,\middle|\,\boldsymbol{x}_N\right\rangle\left\langle \boldsymbol{x}_N\,\middle|\, e^{-\epsilon\hat{H}/\hbar}\,\middle|\,\boldsymbol{x}_{N-1}\right\rangle && (2.332)\\ &\quad\times\ldots\times\left\langle \boldsymbol{x}_2\,\middle|\, e^{-\epsilon\hat{H}/\hbar}\,\middle|\,\boldsymbol{x}_1\right\rangle\left\langle \boldsymbol{x}_1\,\middle|\, e^{-\epsilon\hat{H}/\hbar}\,\middle|\,\boldsymbol{x}_{N+1}\right\rangle \\ &= \prod_{n=1}^{N+1}\int d\boldsymbol{x}_n\left\langle \boldsymbol{x}_n\,\middle|\, e^{-\epsilon\hat{H}/\hbar}\,\middle|\,\boldsymbol{x}_{n-1}\right\rangle && (2.332\text{a}) \end{aligned}$$

where $\boldsymbol{x}_0 = \boldsymbol{x}_{N+1}$ and

$$\epsilon = \frac{\hbar\beta}{N+1} = \frac{\hbar}{(N+1)\,k_B T} \tag{2.332b}$$

Note that the $\boldsymbol{x}_{N+1}$ integration comes from taking the trace.

From (2.13), we get

$$\left\langle \boldsymbol{x}_n\,\middle|\, e^{-\epsilon\hat{H}/\hbar}\,\middle|\,\boldsymbol{x}_{n-1}\right\rangle = \int\frac{d\boldsymbol{p}_n}{(2\pi\hbar)^D}\exp\left[\frac{i}{\hbar}\boldsymbol{p}_n\cdot(\boldsymbol{x}_n - \boldsymbol{x}_{n-1}) - \frac{\epsilon}{\hbar}H(\boldsymbol{x}_n,\boldsymbol{p}_n)\right] \tag{2.333}$$

so that (2.332) becomes

$$Z = \left(\prod_{n=1}^{N+1} \int_{\mathbf{x}_{N+1}=\mathbf{x}_0} d\,\mathbf{x}_n \int \frac{d\,\mathbf{p}_n}{(2\,\pi\,\hbar)^D} \right) e^{-\mathcal{A}_e^N/\hbar} \tag{2.334}$$

where

$$\mathcal{A}_e^N = \sum_{n=1}^{N+1} \left[-i\,\mathbf{p}_n \cdot (\mathbf{x}_n - \mathbf{x}_{n-1}) + \epsilon\, H(\mathbf{x}_n, \mathbf{p}_n) \right] \tag{2.335}$$

and the subscript e stands for Euclidean.

In the continuum limit, $\epsilon \to 0$ and [c.f. (2.16c)]

$$\mathcal{A}^N \to \mathcal{A}_e[\mathbf{x}, \mathbf{p}] = \int_0^{\beta\hbar} d\,\tau \left[-i\,\mathbf{p} \cdot \dot{\mathbf{x}} + H(\mathbf{x}, \mathbf{p}) \right] \qquad \dot{\mathbf{x}} = \frac{d\,\mathbf{x}}{d\,\tau} \tag{2.336}$$

where $\mathcal{A}_e$ is called the quantum-statistical action or Euclidean action since, in relativity theory, the imaginary time $\tau = i\,t$ is just another dimension in the (spatial) Euclidean space. Thus, the event interval

$$d\,x^2 = g_{\mu\nu}\, d\,x^\mu\, d\,x^\nu = -(c\,d\,t)^2 + (d\,\mathbf{x})^2$$

can be attributed to the Minskowski metric tensor $g_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$ or taken simply as the length squared

$$d\,x^2 = (c\,d\,\tau)^2 + (d\,\mathbf{x})^2$$

in a $(D+1)$-dimensional Euclidean space of vectors $x = (c\,\tau, \mathbf{x})$.

(2.334) thus becomes

$$Z = \oint \mathcal{D}\,\mathbf{x} \int \frac{\mathcal{D}\,\mathbf{p}}{(2\,\pi\,\hbar)^D}\, e^{-\mathcal{A}_e[\mathbf{x},\mathbf{p}]/\hbar} \tag{2.337}$$

where the circle in $\oint$ indicates the periodic B.C., $\mathbf{x}_{N+1} = \mathbf{x}_0$.

The integrand of (2.336) defines a Euclidean Lagrangian L_e (for imaginary times) so that

$$H = i\,\mathbf{p} \cdot \dot{\mathbf{x}} + L_e = i\,\frac{\partial L_e}{\partial \dot{\mathbf{x}}} \cdot \dot{\mathbf{x}} + L_e \tag{2.338}$$

where the Euclidean Hamiltonian H was without a subscript e due to the notations used in (2.336). The real-time Legendre transformation is recovered by setting $L(t) = i\,L_e(\tau = i\,t)$ and similarly for the Hamiltonians.

As shown in (2.46), the periodic B.C. can be imposed either on $\mathcal{D}\,\mathbf{x}$ or $\mathcal{D}\,\mathbf{p}$, i.e.,

$$\oint \mathcal{D}\,\mathbf{x} \int \frac{\mathcal{D}\,\mathbf{p}}{(2\,\pi\,\hbar)^D} = \int \mathcal{D}\,\mathbf{x} \oint \frac{\mathcal{D}\,\mathbf{p}}{(2\,\pi\,\hbar)^D}$$

$$= \prod_{n=1}^{N+1} \int_{\mathbf{x}_{N+1}=\mathbf{x}_0} d\,\mathbf{x}_n \int \frac{d\,\mathbf{p}_n}{(2\,\pi\,\hbar)^D} = \prod_{n=1}^{N+1} \int d\,\mathbf{x}_n \int_{\mathbf{p}_{N+1}=\mathbf{p}_0} \frac{d\,\mathbf{p}_n}{(2\,\pi\,\hbar)^D} \tag{2.339}$$

since it does not matter whether the trace is taken in x- or p-space.

See Kleinert’s remark in the final paragraph.