2.13. Classical Limit

As discussed in the last section, using the Fourier expansion

$$x(\tau) = x_0 + {\sum_{m=-\infty}^{\infty}}' x_m e^{-i\omega_m \tau} \qquad \omega_m = \frac{2\pi m}{\beta\hbar} \tag{2.457a}$$

where the prime on the summation symbol denotes the omission of the $m = 0$ term, we have

$$\frac{1}{2} M \int_0^{\beta\hbar} d\tau\, \dot{x}^2 = M\beta\hbar \sum_{m=1}^{\infty} \omega_m^2 \,|x_m|^2 \tag{2.457}$$

The partition function for a system with a imaginary-time Lagrangian

$$L = \frac{1}{2} M \dot{x}^2 + V$$

becomes

$$Z = \oint \mathcal{D} x \exp\left[-M\beta \sum_{m=1}^{\infty} \omega_m^2 \,|x_m|^2 - \frac{1}{\hbar} \int_0^{\beta\hbar} d\tau\, V\left(x_0 + {\sum_{m=-\infty}^{\infty}}' x_m e^{-i\omega_m \tau} \right) \right] \tag{2.458}$$

For high temperatures, $\beta \to 0$ and $\omega_m \to \infty$ for $m \neq 0$. The Boltzmann factor

$$\exp\left(-\beta M \omega_m^2 \,|x_m|^2 \right)$$

is therefore a Gaussian sharply peaked around $|x_m| = 0$ with a standard deviation

$$\frac{1}{\sqrt{2\beta M}\ \omega_m} = \frac{\hbar}{2\pi m} \sqrt{\frac{\beta}{2M}} \tag{2.458a}$$

If V is a smooth function, then $V[x(\tau)] \approx V(x_0)$. Hence, (2.458) becomes

$$Z \xrightarrow[\beta\to 0]{} \oint \mathcal{D} x \exp\left[-M\beta \sum_{m=1}^{\infty} \omega_m^2 \,|x_m|^2 - \beta V(x_0) \right] \tag{2.459}$$

$$= \int_{-\infty}^{\infty} \frac{dx_0}{l_e} \prod_{m=1}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\,\mathrm{Re}\, x_m \; d\,\mathrm{Im}\, x_m}{\pi / M\beta\omega_m^2} \qquad \text{[(2.445) used.]}$$

$$\times \exp\left[-M\beta \sum_{m=1}^{\infty} \omega_m^2 \,|x_m|^2 - \beta V(x_0) \right]$$

$$= \int_{-\infty}^{\infty} \frac{dx_0}{l_e} \exp[-\beta V(x_0)] \tag{2.460}$$

$$= Z_{\text{cl}}$$

Thus, for high T, Z goes to the classical value, as already stated in (2.344).

This derivation also reveals an important criterion for the validity of the classical limit (2.460), namely, that V must be a smooth function. Notable examples of breakdown of this include the Coulomb potential $-\frac{1}{r}$, the centrifugal barrier $\frac{1}{r^2}$, and the angular barrier $\frac{1}{\sin^2\theta}$. See Chapter 8 for details.

On the other hand, the particle distribution $\rho(x)$ does not have this problem. It always tends to the classical limit (2.352):

$$\rho(x) \xrightarrow[\beta\to 0]{} \frac{1}{Z_{\text{cl}}} \exp[-\beta V(x)] \tag{2.461}$$

although the convergence is non-uniform in x, thus accounting for the occasional failures of (2.460). See Chapter 12 for more details.