CHAPTER III

PATH INTEGRALS IN QUANTUM STATISTICS

The interplay quantum-mechanical and thermodynamical fluctuations in physical system has attracted much interest. In principle, the thermodynamic properties of a quantum-mechanical system are completely determined if the partition function is known. As we shall see in the sequel, it much more economical to work with the path integrals.

Path Integral Approach

The path integral approach is useful to understand also the thermal equilibrium properties of a system [Feynman and Hibbs 1965, Feynman 1972]. We first assume the system to have a *time independent Hamiltonian* and to be in contact with a reservoir of temperature T. As explained in Chapter I, the bulk thermodynamic quantities can be determined from the quantum statistical partition function [Kleinert 1990]

$$Z = tr\left(e^{-\hat{H}/k_BT}\right) = \sum_n e^{-E_n/k_BT} . \qquad (3.1)$$

This, in turn, may be viewed as an analytic continuation of the quantum mechanical partition function

$$Z_{QM} = tr\left(e^{-i(t_b-t_a)\hat{H}/\hbar}\right) \qquad (3.2)$$

with the imaginary time

$$t_b - t_a = -\frac{i\hbar}{k_BT} \equiv -i\hbar\beta . \qquad (3.3)$$

In the local basis $|x\rangle$, the quantum mechanical trace corresponds to an integral over positions so that the quantum statistical partition function can be obtained from the time displacement amplitude or propagator by integrating over $x_b = x_a$ at the analytically continued time,

$$Z = \int_{-\infty}^{\infty} dx \langle x \left| e^{-\beta\hat{H}} \right| x \rangle = \int_{-\infty}^{\infty} dx (x\, t_b \, | x\, t_a)|_{t_b - t_a = -i\hbar\beta} \cdot \qquad (3.4)$$

By splitting the Boltzmann factor $e^{-\beta\hat{H}}$ into a product of $N+1$ factors $e^{-\varepsilon\hat{H}/\hbar}$ with $e = \hbar / k_B T \ (N+1)$, we can derive for Z a similar path integral representation.

$$Z = \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} dx_n \right]$$

$$\times \langle x_{N+1} \left| e^{-\varepsilon\hat{H}/\hbar} \right| x_n \rangle \langle x_n \left| e^{-\varepsilon\hat{H}/\hbar} \right| x_{n-1} \rangle \times \ldots \times \langle x_1 \left| e^{-\varepsilon\hat{H}/\hbar} \right| x_{N+1} \rangle.$$

(3.5)

The matrix elements $\langle x_n \left| e^{-\varepsilon\hat{H}/\hbar} \right| x_{n-1} \rangle$ are expressed, just as in the quantum mechanical case, as

$$\langle x_n \left| e^{-\varepsilon\hat{H}} \right| x_{n-1} \rangle \approx \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} e^{i p_n (x_n - x_{n-1})/\hbar - \varepsilon H(p_n, x_n)/\hbar}, \qquad (3.6)$$

with the only difference, that there is now no imaginary factor i in front of the Hamiltonian. The product (3.5) can thus be written as

$$Z \approx \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} dx_n \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right] exp \left\{ -\frac{1}{\hbar} S_e^N \right\}, \qquad (3.7)$$

where S_e^N denotes the sum

$$S_e^N = \sum_{n=1}^{N+1} [-i\,p_n(x_n - x_{n-1}) + \varepsilon H(p_n, x_n)]\,. \tag{3.8}$$

In the continuum limit $\varepsilon \to 0$, the sum goes over into the integral

$$S_e[p, x] = \int_0^{\hbar\beta} d\tau [-ip(\tau)\dot{x}(\tau) + H(p(\tau), x(\tau))]\,. \tag{3.9}$$

In this limit we shall write the partition function as the path integral

$$Z = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{-S_e[p,x]/\hbar}\,. \tag{3.10}$$

In this expression, $p(\tau)$, $x(\tau)$ may be considered as paths running along the "imaginary time axis" $\tau = it$. The expression $S_e[p, x]$ is very similar to the mechanical canonical action (2.16). Since it governs the quantum statistical path integrals it will be called quantum statistical action. Another name for S_e is euclidean action, recorded by the subscript e.

The Density Matrix

The partition function does not determine local thermodynamic quantities which may also be accessible to experiment. Important observable information resides, for example, in the thermal analog of the time displacement amplitude $\langle x_b | e^{-\hat{H}/k_B T} | x_a \rangle$. Consider, for instance, the diagonal elements of this, renormalized by a factor Z^{-1}, to be denoted by $\rho(x_a)$ [Kleinert 1990] :

$$\rho(x_a) \equiv Z^{-1} \langle x_a | e^{-\hat{H}/k_B T} | x_a \rangle\,. \tag{3.11}$$

It determines the thermal average of the particle density of a quantum statistical system. Due to (3.11), the factor Z^{-1} makes the spatial integral over ρ equal to unity,

$$\int_{-\infty}^{\infty} dx\, \rho(x) \;=\; 1 . \tag{3.12}$$

By inserting a complete set of eigenfunctions $\psi_n(x)$ of the Hamiltonian operator $\widehat{H}$ into (3.11) we find that $\rho(x_a)$ has spectral decomposition

$$\rho(x_a) \;=\; \sum_n |\psi_n(x_a)|^2 e^{-\beta E_n} / \sum_n e^{-\beta E_n} . \tag{3.13}$$

Since $|\psi_n(x_a)|^2$ is the probability distribution of the system in the eigenstate $|n\rangle$ in configuration space, and $e^{-\beta E_n} / \sum_n e^{-\beta E_n}$ is the normalized probability to encounter the system in the state $|n\rangle$, the quantity $\rho(x_a)$ represents the normalized average particle density in space as a function of temperature.

Note the limiting properties of $\rho(x_a)$. In the limit $T \to 0$, only the lowest energy state survives and $\rho(x_a)$ tends towards the particle distribution in the ground state

$$\rho(x_a) \;\xrightarrow{T \to 0}\; |\psi_0(x_a)|^2 . \tag{3.14}$$

In the opposite limit of high temperatures, quantum effects are expected to become irrelevant and the partition function should converge to the classical expression given in Section 1.4, which is the integral over the phase space of the Boltzmann distribution,

$$Z \;\xrightarrow{T \to \infty}\; Z_{cl} \;=\; \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dx}{2\pi\hbar}\, e^{-H(p,x)/k_B T} . \tag{3.15}$$

We therefore expect the large-T limit of $\rho(x_a)$ to be equal to the *classical particle distribution*

$$\rho(x) \xrightarrow{T\to\infty} \rho_{cl}(x) = Z_{cl}^{-1}\int_{-\infty}^{\infty}\frac{dx}{2\pi\hbar}e^{-H(p,x)/k_BT}. \tag{3.16}$$

At this place we may be satisfied to argue as follows: Take the original time-sliced path integral (3.5). For large T, i.e., small $\tau_b - \tau_a = \hbar / k_B T$, we may keep only a single time slice and write

$$Z \approx \left[\int_{-\infty}^{\infty} dx\right]\left\langle x\middle| e^{-\varepsilon\hat{H}/\hbar}\middle| x\right\rangle \tag{3.17}$$

with

$$\left\langle x\middle| e^{-\varepsilon\hat{H}}\middle| x\right\rangle \approx \int_{-\infty}^{\infty}\frac{dp_n}{2\pi\hbar}e^{-\varepsilon H(p_n,x)/\hbar}. \tag{3.18}$$

Substituting $\varepsilon \approx \tau_b - \tau_a$ this gives directly (3.16). Physically speaking, for high temperature, the path has "no (imaginary) time" to fluctuate and only one term in the product of integrals needs to be considered.

If $H(p, x)$ has the standard form

$$H(p,x) = p^2/2M + V(x), \tag{3.19}$$

the momentum integral is Gaussian in p and can be done using the Gaussian formula

$$\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}e^{-ap^2/2\hbar} = \frac{1}{\sqrt{2\pi\hbar a}}. \tag{3.20}$$

Then we obtain the pure x-integral for the classical partition function

$$Z_{cl} = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi \hbar^2 / M k_B T}} e^{-V(x)/k_B T} . \tag{3.21}$$

In this case the large-T limit of $p(x)$ becomes simply

$$\rho(x) \xrightarrow{T \to \infty} \rho_{cl}(x) = Z_{cl}^{-1} \frac{1}{\sqrt{2\pi \hbar^2 / M k_B T}} e^{-V(x)/k_B T} . \tag{3.22}$$

The expression in the denominator of the measure has the dimension of a length. In fact,

$$l_e(T) \equiv \sqrt{2\pi \hbar^2 / M k_B T} \tag{3.23}$$

in the thermal (or euclidean) analog of the length $l(t_b - t_a)$ introduced earlier, in (2.81).

Let us now turn to the general temperature case and write down the path integral representation for $p(x)$. We simply omit in (3.10) the final trace integration over $x_b \equiv x_a$ and normalize the expression by a factor Z^{-1}, obtaining

$$\rho(x_a) = Z^{-1} \int_{x(\hbar\beta) = x(0)} \mathcal{D}'x \frac{\mathcal{D}p}{2\pi\hbar} e^{-S_e(p,x)/\hbar} . \tag{3.24}$$

But not only the diagonal elements of the amplitude $\langle x_b | e^{-\beta H} | x_a \rangle$ are important. The thermal equilibrium expectation of an arbitrary hermitian operator $\widehat{O}$ is given by

$$\langle \widehat{O} \rangle_T \equiv Z^{-1} \sum_n e^{-\beta E_n} \langle n | \widehat{O} | n \rangle . \tag{3.25}$$

In the local basis $|x\rangle$, this becomes

$$\langle\widehat{O}\rangle_T \equiv Z^{-1}\int\int_{-\infty}^{\infty} dx_b\, dx_a \langle x_b | e^{-\beta\widehat{H}} | x_a \rangle \langle x_a | \widehat{O} | x_b \rangle . \qquad (3.26)$$

Thus, unless one wants to calculate only expectations of functions of the position operator $\widehat{x}$ in (3.25),

$$\langle f(\widehat{x})\rangle_T = \int\int_{-\infty}^{\infty} dx_b\, dx_a \langle x_b | e^{-\beta\widehat{H}} | x_a \rangle\, \delta(x_b - x_a) f(x_a) = \int dx\, \rho(x) f(x), \qquad (3.27)$$

the off-diagonal elements of the amplitude $\langle x_b | e^{-\beta\widehat{H}} | x_a \rangle$ are also relevant. One therefore defines a *density matrix*

$$\rho(x_b, x_a) \equiv Z^{-1} \langle x_b | e^{-\beta\widehat{H}} | x_a \rangle . \qquad (3.28)$$

Its diagonal values give the above particle density $\rho(x_a)$.

It is then useful to keep the analogy between quantum mechanics and quantum statistics as close as possible and treat both cases at the same time, by considering the time translation operator along the imaginary time axis

$$\widehat{U}_e(\tau_b, \tau_a) \equiv e^{-(\tau_b - \tau_a)\widehat{H}/\hbar}, \quad \tau_b > \tau_a, \qquad (3.29)$$

and defining its local matrix elements as *imaginary* or *euclidean* time displacement amplitudes

$$(x_b \tau_b | x_a \tau_a) \equiv \langle x_b | \widehat{U}_e(\tau_b, \tau_a) | x_a \rangle, \qquad \tau_b > \tau_a . \qquad (3.30)$$

As in the real-time case, we shall only consider the causal time ordering $\tau_b > \tau_a$. Here it is essential to do so since the partition function and density matrix does not exist for $\tau_b < \tau_a$ if the system has energies up to infinity. Given these imaginary-time amplitudes, the partition function is found by integrating over the diagonal elements

$$Z = \int_{-\infty}^{\infty} dx \left(x\,\hbar\beta \mid x\,0\right), \tag{3.31}$$

and the density matrix by dividing out Z,

$$\rho(x_b, x_a) = Z^{-1}\left(x_b\,\hbar\beta \mid x_a 0\right). \tag{3.32}$$

For the sake of generality we may sometimes consider also the imaginary-time displacement operators for time dependent Hamiltonians and the associated amplitudes. They are obtained by time slicing the local matrix elements of the operator

$$\widehat{U}(\tau_b, \tau_a) = T_\tau\, exp\left\{-\frac{1}{\hbar}\int_{\tau_a}^{\tau_a} d\tau\,\widehat{H}(-i\tau)\right\}. \tag{3.33}$$

Here T_τ is an ordering operator along the imaginary times axis τ. It must be kept in mind, however, that for this to be physically usual in solving thermodynamic problems, the time dependence of the Hamiltonian operator $\widehat{H}(t)$ must be extremely slow, must slower than the time required for equilibriation. Only then can the system remain close enough to equilibrium that equilibrium methods can be used to evaluate the physical response of the system as a function of time. This is the range of validity of the so-called *linear response theory.*

In any case, the imaginary-time displacement amplitude (3.31) has certainly a path integral representation analogous to (3.7), obtained by dropping the final integration in that expression and relaxing the condition $x_b = x_a$:

$$(x_b\,\tau_b \mid x_a\,\tau_a) \approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} dx_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dp_n}{2\pi\hbar}\right] exp\left\{-S_e^N/\hbar\right\}, \tag{3.34}$$

with the time-sliced euclidean action

$$S_e^N = \prod_{n=1}^{N+1} [-i p_n (x_n - x_{n-1}) + \varepsilon H(p_n, x_n, \tau_n)], \tag{3.35}$$

where we have omitted the factor $-i$ in the τ-argument of H. In the continuum limit this is written just as (3.10) as a path integral

$$(x_b \tau_b | x_a \tau_a) = \int \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} \exp\left\{ -\frac{1}{\hbar} S_e [p, x] \right\}. \tag{3.36}$$

For a Hamiltonian in the standard form $H = p^2/2M + V(x, \tau)$ with a smooth potential $V(x, \tau)$, the momenta can be integrated out, just as in (2.25), and we find the euclidean version of the pure x-space path integral (2.26), (2.27)

$$\begin{aligned}(x_b \tau_b | x_a \tau_a) &= \int \mathcal{D}x \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[\frac{M}{2} (\partial_\tau x)^2 + V(x, \tau)\right]\right\} \\ &\approx \frac{1}{\sqrt{2\pi\hbar\varepsilon/M}} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \frac{dx_n}{2\pi\hbar\varepsilon/M} \right] \\ &\quad \times \exp\left\{ -\frac{1}{\hbar} \varepsilon \sum_{n=1}^{N+1} \left[\frac{M}{2} \left(\frac{x_n - x_{n-1}}{\varepsilon} \right)^2 + V(x_n, \tau_n) \right] \right\}. \end{aligned} \tag{3.37}$$

In the case that $V(x, \tau)$ is independent of τ we calculate the quantum statistical partition function with the path integral

$$Z = \int_{-\infty}^{\infty} dx \left(x\, \hbar\beta \; | x_a 0 \right) \approx \int_{x(\hbar\beta) = x(0)} \mathcal{D}x \, e^{-S_e[x, \dot{x}]/\hbar}, \tag{3.38}$$

where $S_e[x, \dot{x}]$ is the euclidean version of the Langrangian action

$$S_e[x, \dot{x}] = \int_{\tau_a}^{\tau_b} d\tau \left[\frac{M}{2}\dot{x}^2 + V(x)\right]. \tag{3.39}$$

Here the dot denotes differentiation with respect to the imaginary time. As in the quantum mechanical partition function in (2.30), the path integral $\int \mathcal{D}x$ now stands for

$$\int \mathcal{D}x = \prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{2\pi\hbar\varepsilon / M}}. \tag{3.40}$$

It contains no extra $1/\sqrt{2\pi\hbar\varepsilon / M}$ factor, as in (3.37), due to the trace integration over the exterior x.

The condition $x(\hbar\beta) = x(0)$ is most easily enforced by expanding $x(\tau)$ into a Fourier series

$$x(\tau) = \sum_{m=-\infty}^{\infty} \frac{1}{\sqrt{N+1}} e^{-i\omega_m \tau} x_m , \tag{3.41}$$

where the frequencies ω_m are integer multiples of $2\pi k_B T / \hbar$, i.e.,

$$\omega_m \equiv 2\pi k_B T / \hbar = \frac{2\pi m}{\hbar\beta}. \tag{3.42}$$

They are called *Matsubara frequencies.* They ensure the boundary condition $x(0) = x(\hbar\beta)$. Moreover, when considered as functions on the entire τ axis, the paths are seen to be periodic in $\hbar\beta$, i.e.,

$$x(\tau) = x(\tau + \hbar\beta). \tag{3.43}$$

Thus the path integral for the quantum statistical partition function comprises all periodic paths with period $\hbar\beta$. In the time-sliced path integral (3.37), the coordinates $x(\tau)$ are needed only at the discrete times $\tau_n = n\varepsilon$. Correspondingly, the sum over m in (3.41) can be restricted to run from $m = -N/2$ to $N/2$ for $N =$ even and from $-(N-1)/2$ to $(N+1)/2$ for N = odd (see Fig. 3.1). In order to have a real $x(\tau_n)$ we have to require that

$$x_m = x^*_{-m} \qquad \text{(modulo } N+1\text{)}. \tag{3.44}$$

Note that the Matsubara frequencies in the expansion of the paths $x(\tau)$ are now twice as big as the frequencies υ_m in the quantum fluctuations (2.65) (after the analytic continuation of $t_b - t_a$ to $-i\hbar/k_B T$). Still, they have about the same total number since they run over positive and negative integers. The only exception is the zero frequency $\omega_m = 0$ which, contrary to the frequencies υ_m which ran over positive $m = 1, 2, 3, \ldots$, is now included. This is necessary to describe paths with arbitrary nonzero end points $x_b = x_a = x$ to be integrated over when forming the trace.

Quantum Statistics of Harmonic Oscillator

As a particular example for the treatment of a quantum statistical path integral [Kleinert 1990], consider the harmonic oscillator. If the τ-axis is sliced at $\tau_n = n\varepsilon$, with $\varepsilon \equiv \hbar\beta/(N+1)(n=0,\ldots,N+1)$, the partition function is given by the limit $N \to \infty$ of the sliced expression

$$Z_\omega^N = \prod_{n=0}^{N}\left[\int_{-\infty}^{\infty}\frac{dx_n}{\sqrt{2\pi\hbar\varepsilon/M}}\right] exp\left\{-S_e^N/\hbar\right\}, \tag{3.45}$$

where S_e^N is the sliced euclidean oscillator action

$$S_e^N = \frac{M}{2\varepsilon}\sum_{n=1}^{N+1} x_n\left(-\varepsilon^2\nabla\overline{\nabla} + \varepsilon^2\omega^2\right)x_n . \tag{3.46}$$

Integrating out the x_n's we find immediately

$$Z_{\omega}^{N} = \frac{1}{\sqrt{det_{N+1}\left(-\varepsilon^2\nabla\overline{\nabla} + \varepsilon^2\omega^2\right)}}. \tag{3.47}$$

Let us evaluate the fluctuation determinant via the product of eigenvalues which diagonalize the matrix $-\varepsilon^2\nabla\overline{\nabla} + \varepsilon^2\omega^2$ in the sliced action (3.46). They are

$$\varepsilon^2\Omega_m\overline{\Omega_m} + \varepsilon^2\omega^2 = 2 - 2\cos\omega_m\varepsilon + \varepsilon^2\omega^2, \tag{3.48}$$

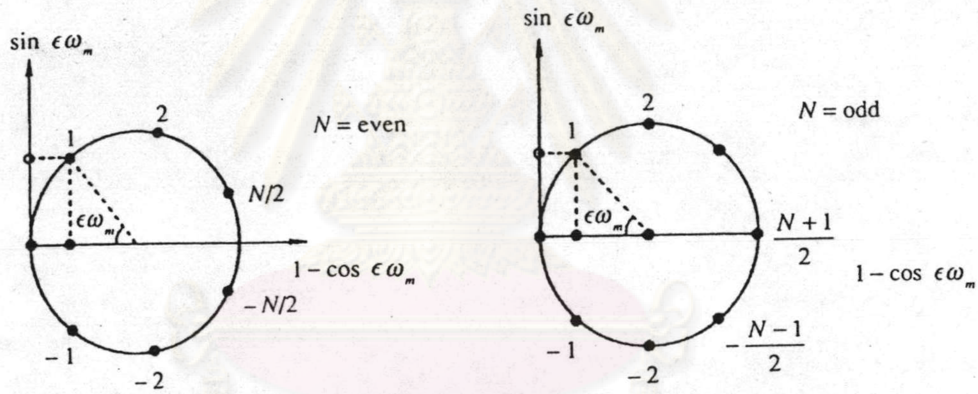

Figure 3.1 Geometric illustration of the eigenvalues of the fluctuation matrix in the action (3.46) for even and odd N

with the Matsubara frequencies ω_m. The eigenvalues $2 - \cos\omega_m\varepsilon$, are pictured in Fig. 3.1. The action (3.46) is diagonal on the Fourier components x_m. Their real and imaginary parts of the diagonal Fourier components $Re\, x_m$, $Im\, x_m$, when arranged to a row vector

$$(Re\ x_1, Im\ x_1\ ; Re\ x_2, Im\ x_2\ ; \ldots ; Re\ x_n\ , Im\ x_n\ ; \ldots)\ ,$$

are related to the time-sliced positions $x_n = x(\tau_n)$ by a transformation matrix with the rows

$$T_{mn} x_n = (T_m)_n x_n = \sqrt{\frac{2}{N+1}} \Big(\frac{1}{\sqrt{2}}, cos \frac{m}{N+1} 2\pi \cdot 1, sin \frac{m}{N+1} 2\pi \cdot 1,$$
$$cos \frac{m}{N+1} 2\pi \cdot 2, sin \frac{m}{N+1} 2\pi \cdot 2, \ldots$$
$$\ldots, cos \frac{m}{N+1} 2\pi \cdot n, sin \frac{m}{N+1} 2\pi \cdot n, \ldots \Big)_n x_n\ . \tag{3.49}$$

For each row index $m = 0, \ldots, N$, the column index n runs from zero to $N\ /\ 2$ for even N, and to $(N + 1)\ /\ 2$ for odd N. In the odd case, the last column $sin \frac{m}{N+1} 2\pi \cdot n$ with $n = (N + 1) / 2$, vanishes identically and must be dropped so that the number of columns in T_{mn} is $N + 1$, as it should. In this case, the second-last column of T_{mn} becomes the alternating sequence ± 1. Hence, for a proper normalization, the sequence has to be multiplied by an extra normalization factor $1\ /\ \sqrt{2}$, similar to the elements in the first column. It is easy to verify, by an argument similar to (2.70), (2.71), that the resulting matrix is orthogonal. Hence, we can diagonalize the sliced action in (3.46) as follows

$$S_e^N = \frac{M}{2} \varepsilon \begin{cases} \left[\omega^2 x_0^2 + 2 \sum_{m=0}^{N/2} \left(\Omega_m \overline{\Omega}_m + \omega^2\right) | x_m |^2\right] & \text{for } N = \text{even} \\ \left[\omega^2 x_0^2 + \left(\Omega_{(N+1)/2} \overline{\Omega}_{(N+1)/2} + \omega^2\right) x_{N+1}^2\right. & \\ \left. + 2 \sum_{m=0}^{(N-1)/2} \left(\Omega_m \overline{\Omega}_m + \omega^2\right) | x_m |^2\right] & \text{for } N = \text{odd}\ . \end{cases} \tag{3.50}$$

The orthogonality of T_{mn} implies that the measure $\prod_n \int_{-\infty}^{\infty} dx(\tau_n)$ is transformed into

$$\int_{-\infty}^{\infty} dx_0 \prod_{m=1}^{N/2} \int_{-\infty}^{\infty} d\,Re\, x_m \int_{-\infty}^{\infty} d\,Im\, x_m \qquad \text{for} \quad N = \text{even},$$

$$\int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dx_{N+1/2} \prod_{m=1}^{(N-1)/2} \int_{-\infty}^{\infty} d\,Re\, x_m \int_{-\infty}^{\infty} d\,Im\, x_m \qquad \text{for} \quad N = \text{odd}\,. \tag{3.51}$$

Performing the Gauss integrals gives the partition function

$$\begin{aligned} Z_{\omega}^{N} &= \left[det_{N+1}\left(-\varepsilon^2 \nabla\overline{\nabla} + \varepsilon^2 \omega^2 \right) \right]^{-1/2} \\ &= \left[\prod_{m=0}^{N} \left(\varepsilon^2 \Omega_m \overline{\Omega}_m + \varepsilon^2 \omega^2 \right) \right]^{-1/2} \\ &= \left\{ \prod_{m=0}^{N} \left[2\left(1 - cos\, \omega_m \varepsilon\right) + \varepsilon^2 \omega^2 \right] \right\}^{-1/2} \\ &= \left\{ \prod_{m=0}^{N} \left(4\, sin^2 \frac{\varepsilon\, \omega_m}{2} + \varepsilon^2 \omega^2 \right) \right\}^{-1/2} . \end{aligned} \tag{3.52}$$

Notice that the result has become a unique product expression in both case $N =$ even or odd thanks to the periodicity of the eigenvalues under the replacement $n \rightarrow n + N + 1$.

It is important to realize that in contrast to the fluctuation factor (2.100) in the real-time amplitude, the partition function contains only positive square roots of positive quantities, the unique result of Gaussian integrations, and there is no phase distinction as in the Fresnel integral (2.23). In order to calculate the product we observe that if we decompose

$$\sin^2\frac{\varepsilon\,\omega_m}{2} \;=\; \left(1+\cos\frac{\varepsilon\,\omega_m}{2}\right)\left(1-\cos\frac{\varepsilon\,\omega_m}{2}\right), \tag{3.53}$$

the sequence of first factors

$$1+\cos\frac{\varepsilon\,\omega_m}{2} \;\equiv\; 1+\cos\frac{\pi m}{N+1} \tag{3.54}$$

runs, for $m = 1, \ldots N$, through the same values as the sequence of second factors

$$1-\cos\frac{\varepsilon\,\omega_m}{2} \;=\; 1-\cos\frac{\pi m}{N+1} \;\equiv\; 1+\cos\pi\,\frac{N+1-m}{N+1}\;, \tag{3.55}$$

except in opposite order. Thus, separating out the $m = 0$ term, we can rewrite (3.52) in the form:

$$Z_\omega^N \;=\; \frac{1}{\varepsilon\omega}\left\{\prod_{m=1}^{N} 2\left(1-\cos\frac{\varepsilon\,\omega_m}{2}\right)\right\}^{-1}\left[\prod_{m=1}^{N}\left(1+\frac{\varepsilon^2\omega^2}{4\sin^2\frac{\varepsilon\,\omega_m}{2}}\right)\right]^{-1/2}. \tag{3.56}$$

The factor in curly brackets on the right-hand side is the quantum mechanical determinant of the free-particle problem $det_N\left(-\varepsilon^2\nabla\overline{\nabla}\right) = N+1$, see (2.78), so that we obtain for both even and odd N.

$$Z_\omega^N \;=\; \frac{k_B T}{\hbar\omega}\left[\prod_{m=1}^{N}\left(1+\frac{\varepsilon^2\omega^2}{4\sin^2\frac{\omega_m\varepsilon}{2}}\right)\right]^{-1/2}. \tag{3.57}$$

To evaluate the remaining product we must distinguish again the cases N = even or odd. For N = even where every eigenvalue occurs twice (see Fig. 3.1) we obtain

$$Z_\omega^N \;=\; \frac{k_B T}{\hbar\omega}\left[\prod_{m=1}^{N/2}\left(1+\frac{\varepsilon^2\omega^2}{4\sin^2\frac{m\pi}{N+1}}\right)\right]^{-1}. \tag{3.58}$$

For N = odd the term with $m = (N+1)/2$ occurs only once and must be treated separately so that

$$Z_\omega^N = \frac{k_B T}{\hbar\omega}\left[\left(1+\frac{\varepsilon^2\omega^2}{4}\right)^{1/2}\prod_{m=1}^{(N-1)/2}\left(1+\frac{\varepsilon^2\omega^2}{4\sin^2\frac{\pi m}{N+1}}\right)\right]^{-1}. \tag{3.59}$$

In the odd case we can use once more a parameter $\tilde{\omega}_e$, the euclidean analog of (2.101), defined by

$$\sinh\frac{\tilde{\omega}_e\varepsilon}{2} \equiv \frac{\omega\varepsilon}{2}, \tag{3.60}$$

together with the product formula related to the one used already in (2.103)

$$\prod_{m=1}^{(N-1)/2}\left(1-\frac{\sin^2 x}{\sin^2\frac{m\pi}{(N+1)}}\right) = \frac{2}{\sin 2x}\frac{\sin[(N+1)x]}{(N+1)}. \tag{3.61}$$

and we find

$$Z_\omega^N = \frac{k_B T}{\hbar\omega}\left[\frac{1}{\sinh(\tilde{\omega}_e\varepsilon/2)}\frac{\sinh[(N+1)\tilde{\omega}_e\varepsilon/2]}{N+1}\right]^{-1}. \tag{3.62}$$

In the case of even N we use the formula

$$\prod_{m=1}^{N/2}\left(1-\frac{\sin^2 x}{\sin^2\frac{m\pi}{(N+1)}}\right) = \frac{1}{\sin x}\frac{\sin[(N+1)x]}{(N+1)}, \tag{3.63}$$

and find again (3.62). Using the relation (3.60) for the parameter $\tilde{\omega}_e$ we see that in both cases, the partition function on the sliced imaginary time axis is given by

$$Z_\omega^N = \frac{1}{2\sinh(\hbar\tilde{\omega}_e\beta/2)}. \tag{3.64}$$

The partition function can be expanded in the following series

$$Z_\omega^N = e^{-\hbar\tilde{\omega}_e/2k_BT} + e^{-3\hbar\tilde{\omega}_e/2k_BT} + e^{-5\hbar\tilde{\omega}_e/2k_BT} + \dots. \tag{3.65}$$

This is the usual spectral expansion of a partition function, displaying the energy eigenvalues

$$E_n = \left(n + \frac{1}{2}\right)\hbar\tilde{\omega}_e \tag{3.66}$$

of the system. They show the typical linearly rising oscillator sequence with

$$\tilde{\omega}_e = \frac{2}{\varepsilon}\, arsinh\frac{\omega\varepsilon}{2} \tag{3.67}$$

playing the role of the frequency.

In the continuum limit $\varepsilon \to 0$, this goes over into the well-known oscillator partition function

$$Z_\omega = \frac{1}{2\, sinh\left(\hbar\omega\beta / 2\right)}. \tag{3.68}$$

Now that the continuum limit $\varepsilon \to 0$ of the product in (3.57) can also be taken factor by factor. Then Z_ω becomes

$$Z_\omega = \frac{k_B T}{\hbar\omega}\left[\prod_{n=1}^{\infty}\left(1 + \frac{\omega^2}{(2\pi\, n\, k_B T / \hbar)^2}\right)\right]^{-1}. \tag{3.69}$$

The product converges rapidly as in formula (2.129) and we find

$$Z_\omega = \frac{k_B T}{\hbar\omega}\,\frac{\hbar\omega / 2k_B T}{sinh(\hbar\omega / 2k_B T)} = \frac{1}{2 sinh\left(\hbar\omega\beta\ / 2\right)}. \tag{3.70}$$

The reason why we are allowed to take the continuum limit in each factor of (3.57) is, of course, that the product involves only ratios of frequencies. Just as in the quantum mechanical case, this procedure of obtaining the continuum limit can be summarized in the sequence of equations arriving at a ratio of differential operators

$$Z_\omega^N = \left[det_{N+1}\left(-\varepsilon^2\nabla\overline{\nabla} + \varepsilon^2\omega^2\right)\right]^{-1/2}$$

$$= \left[det_{N+1}\left(-\varepsilon^2\nabla\overline{\nabla}\right)\right]^{-1/2}\left[\frac{det_{N+1}\left(-\varepsilon^2\nabla\overline{\nabla}+\varepsilon^2\omega^2\right)}{det_{N+1}\left(-\varepsilon^2\nabla\overline{\nabla}\right)}\right]^{-1/2}$$

$$\xrightarrow{\varepsilon\to 0} \frac{k_B T}{\hbar\omega}\left[\prod_{m=1}^{\infty}\frac{\omega_m^2+\omega^2}{\omega_m^2}\right]^{-1/2} = \frac{k_B T}{\hbar}\left[\frac{det\left(-\partial_\tau^2+\omega^2\right)}{det'\left(-\partial_\tau^2\right)}\right]^{-1/2}. \quad (3.71)$$

Here ∂_τ is the differential operator acting on real functions which are periodic under the replacement $\tau \rightarrow \tau + \hbar\beta$. Remember that each eigenvalues ω_m^2 of $-\partial_\tau^2$ occurs twice, except for the zero frequency $\omega_0 = 0$ which appears only once. In the lower determinant, this eigenvalue must be excluded from the product to reproduce the left-hand side. This fact is recorded by the prime.

Let us finally mention that the results of this section could also have been obtained directly from the quantum mechanical amplitude (2.112) by an analytic continuation of the time difference $t_b - t_a$ to imaginary values $-i(\tau_b - \tau_a)$,

$$(x\tau_b|x\tau_a) = \frac{1}{\sqrt{2\pi\hbar/M}}\sqrt{\frac{\omega}{sinh\,\omega(\tau_b-\tau_a)}}$$

$$\times exp\left\{-\frac{1}{2\hbar}\frac{M\omega}{sinh\,\omega(\tau_b-\tau_a)}\left[\left(x_b^2+x_a^2\right)cosh\,\omega(\tau_b-\tau_a)-2x_b x_a\right]\right\}. \quad (3.72)$$

By setting $x = x_b = x_a$ and integrating over x we obtain

$$Z_\omega = \int_{-\infty}^{\infty} dx(x\tau_b|x\tau_a) = \frac{1}{\sqrt{2\pi\hbar(\tau_b-\tau_a)/M}}\sqrt{\frac{\omega(\tau_b-\tau_a)}{sinh\,[\omega(\tau_b-\tau_a)]}}$$

$$\times\sqrt{\frac{2\pi\hbar sinh\,[\omega(\tau_b-\tau_a)]/\omega M}{2sinh\,[\omega(\tau_b-\tau_a)/2]}} = \frac{1}{2sinh\,[\omega(\tau_b-\tau_a)/2]}. \quad (3.73)$$

Upon inserting $\tau_b - \tau_a = \hbar\beta$ we retrieve the partition function (3.68). The main reason for presenting an independent direct evaluation in the space of real periodic functions was to display the different frequency structure of ω_m 's of periodic paths, as compared with the frequencies υ_m 's of the quantum mechanical fluctuations with fixed ends, and to show how to handle the ensuing product expressions.