Chapter 4

Effective Classical Theory for Quantum Systems

We have shown in Section 3.3.1 that the quantum statistical density matrix can be expressed with the help of a bilocal potential $V_{\mathrm{eff,cl}}(\mathbf{x}_b, \mathbf{x}_a)$, which makes the density matrix classically looking (3.83). In the following we will develop a similar formalism for the quantum statistical partition function and the free energy. Since the path integral counts all paths in phase space, which satisfy periodic boundary conditions $\mathbf{x}(0) = \mathbf{x}(\hbar\beta)$, we first investigate the Fourier decomposition of such paths, and the influence of the zero modes on the Green functions (3.157)–(3.160) [4,20]. Then, we consider the fluctuations of paths with fixed end points.

After having separated the zero-frequency Fourier modes, which lead to diverging correlations in the classical limit of high temperatures $\beta \equiv 1/k_B T \to 0$, we finally turn to the derivation of the smearing formula for restricted partition functions.

4.1 The Zero-Mode Problem

In order to illustrate the relation between zero-mode fluctuations and classical statistical properties more obviously, we consider, once more, the example of the harmonic oscillator with the action

$$\mathcal{A}_\omega[x] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}^2(\tau) + \frac{1}{2}M\omega^2 x^2(\tau) \right], \tag{4.1}$$

where the dot means differentiation with respect to τ.

4.1.1 Harmonic Fluctuation Width for Periodic Paths

According to Eq. (3.175), the partition function of the harmonic oscillator with the action (4.1) is given by

$$Z_\omega = \oint \mathcal{D}x \, e^{-\mathcal{A}_\omega[x]/\hbar} = \frac{1}{2\sinh \hbar\beta\omega/2}. \tag{4.2}$$

Correlation functions of local quantities $O_1(x(\tau_1))O_2(x(\tau_2))\cdots$ are then defined as

$$\langle O_1(x(\tau_1))O_2(x(\tau_2))\cdots\rangle_\omega = Z_\omega^{-1} \oint \mathcal{D}x \, O_1(x(\tau_1))O_2(x(\tau_2))\cdots e^{-\mathcal{A}_\omega[x]/\hbar}. \tag{4.3}$$

The path $x(\tau)$ shall be periodic: $x(0) = x(\hbar\beta)$. Thus, it can be expanded into the Fourier series

$$x(\tau) = x_0 + \sum_{m=1}^{\infty} \left(x_m \, e^{-i\omega_m \tau} + x_m^\star \, e^{i\omega_m \tau} \right) . \tag{4.4}$$

Here, we have separated the zero frequency component x_0 from the sum. Since the quantities $x(\tau)$, x_0, and the fluctuations must be real, there is the constraint $x_m^\star = x_{-m}$. The Matsubara frequencies are as usual $\omega_m = 2\pi m/\hbar\beta$.

Now, we integrate (4.4) over τ and divide the result by $\hbar\beta$. This entails

$$\overline{x(\tau)} \equiv \frac{1}{\hbar\beta} \int_0^{\hbar\beta} d\tau \, x(\tau) = x_0, \tag{4.5}$$

where the contribution of the fluctuations around x_0 vanishes as a consequence of the orthogonality relation

$$\delta_{nm} = \frac{1}{\hbar\beta} \int_0^{\hbar\beta} d\tau \, e^{i(\omega_n - \omega_m)\tau}. \tag{4.6}$$

From Eq. (4.5), we conclude that the temporal mean value of the path is identical with the zero-frequency component x_0. In the following, we investigate the violence of these zero-mode fluctuations. First we calculate the particle distribution of the harmonic oscillator at a certain position $x = x(\tau)$. This yields

$$P(x) = \langle \delta(x - x(\tau)) \rangle_\omega = \frac{1}{\sqrt{2\pi a^2}} \exp\left(-\frac{x^2}{2a^2} \right), \tag{4.7}$$

where a is the Gaussian fluctuation width and is related to the Green function (3.166) for equal times:

$$a^2 = G^{\mathrm{p}}_{xx}(\tau, \tau) = \frac{\hbar}{2M\omega} \coth \frac{\hbar\beta\omega}{2}. \tag{4.8}$$

At zero temperature, this is equal to the square of the ground-state wave function of the harmonic oscillator, whose width is

$$a_0^2 = \frac{\hbar}{2M\omega}. \tag{4.9}$$

In the limit $\hbar \to 0$, from Eqs. (4.7) and (4.8) we obtain the classical distribution

$$P_{\mathrm{cl}}(x) = \frac{1}{\sqrt{2\pi a_{\mathrm{cl}}^2}} \exp\left(-\frac{x^2}{2a_{\mathrm{cl}}^2} \right), \tag{4.10}$$

with

$$a_{\mathrm{cl}}^2 = \frac{1}{\beta M \omega^2}. \tag{4.11}$$

The linear growth of this classical width is the origin of the famous Dulong-Petit law for the specific heat of a harmonic system. The classical fluctuations are governed by the integral over the Boltzmann factor

$$e^{-\beta M \omega^2 x^2/2} \tag{4.12}$$

in the classical partition function

$$Z_{\mathrm{cl}} = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar^2\beta/M}} \, e^{-\beta M\omega^2 x^2/2}. \tag{4.13}$$

From this we obtain the classical distribution (4.10) as the expectation value

$$P_{\rm cl}(x) = \langle \delta(x-\overline{x})\rangle_{\omega,{\rm cl}} = Z_{\rm cl}^{-1}\int_{-\infty}^{\infty}\frac{d\overline{x}}{\sqrt{2\pi\hbar^2\beta/M}}\,\delta(x-\overline{x})\,e^{-\beta M\omega^2 x^2/2}. \tag{4.14}$$

Which fluctuations cause the divergence of the Gaussian width (4.8) for high temperatures? In order to answer this question we exclude from the path integral (4.2) the zero-frequency contributions, which we have identified in (4.5) to be equal to the temporal mean value $\overline{x(\tau)}$ of the path. Thus, we define for each x_0 new local expectation values

$$\langle O_1(x(\tau_1))O_2(x(\tau_2))\cdots\rangle_\omega^{x_0} = \frac{\left\langle \delta(x_0-\overline{x(\tau)})O_1(x(\tau_1))O_2(x(\tau_2))\cdots\right\rangle_\omega}{\left\langle \delta(x_0-\overline{x(\tau)})\right\rangle_\omega}. \tag{4.15}$$

The original quantum statistical distribution of the harmonic oscillator (4.7) collects fluctuations of $x_0=\overline{x(\tau)}$ and those around x_0, and can therefore be written as the convolution integral

$$P(x) = \int_{-\infty}^{\infty} dx_0\, P_{x_0}(x-x_0)P_{\rm cl}(x_0) \tag{4.16}$$

over the classical distribution (4.10) and the local one

$$P_{x_0}(x) = \langle \delta(x-x(\tau))\rangle_\omega^{x_0} = \frac{1}{\sqrt{2\pi a_{x_0}^2}}\exp\left[-\frac{(x-x_0)^2}{2a_{x_0}^2}\right]. \tag{4.17}$$

Such a convolution of Gaussian distributions as in Eq. (4.16) leads to another Gaussian distribution with added widths, so that the width of the local distribution is given by the difference

$$a_{x_0}^2 = a^2 - a_{\rm cl}^2 = \frac{\hbar}{2M\omega}\left(\coth\frac{\hbar\beta\omega}{2} - \frac{2}{\hbar\beta\omega}\right), \tag{4.18}$$

which starts out at the finite value (4.9) for $T=1/k_B\beta=0$, and goes to zero for $T\to\infty$ with the asymptotic behavior $\hbar\beta\omega/12$ (see Fig. 4.1). The latter property suppresses all fluctuations around $\overline{x(\tau)}$. Thus it turns out that the zero-frequency fluctuations x_0 lead to the divergence of the fluctuation width for $T\to\infty$. Such violent fluctuations cannot be treated by perturbation theory. They must be separated from the path integral (4.2) and integrated at the end of the calculation. Thus we shall revise the perturbative treatment for the free energy in Section 3.7.

4.1.2 Fluctuation Width for Fixed Ends

Now we dwell on the question how the fluctuation width behaves for a system with fixed ends. We consider the unnormalized density matrix $\tilde\varrho(x_b,x_a)$, which is expressed by the path integral

$$\tilde\varrho(x_b,x_a) = \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}x\, e^{-\mathcal{A}[x]/\hbar} \tag{4.19}$$

over all paths with the fixed end points $x(0)=x_a$ and $x(\hbar\beta)=x_b$. For a harmonic oscillator (4.1), the path integral (4.19) can easily be done, with the result

$$\tilde\varrho_\omega(x_b,x_a) = \sqrt{\frac{M\omega}{2\pi\hbar\sinh\hbar\beta\omega}}\exp\left\{-\frac{M\omega}{2\hbar\sinh\hbar\beta\omega}\left[(x_b^2+x_a^2)\cosh\hbar\beta\omega - 2x_bx_a\right]\right\}. \tag{4.20}$$

At fixed end points x_b, x_a, the quantum mechanical correlation functions are

$$\langle O_1(x(\tau_1))\,O_2(x(\tau_2))\cdots\rangle_\omega^{x_b,x_a} = \frac{1}{\tilde\varrho_\omega(x_b,x_a)}\int_{x(0)=x_a}^{x(\hbar\beta)=x_b}\mathcal{D}x\; O_1(x(\tau_1))\,O_2(x(\tau_2))\cdots e^{-\mathcal{A}_\omega[x]/\hbar} \tag{4.21}$$

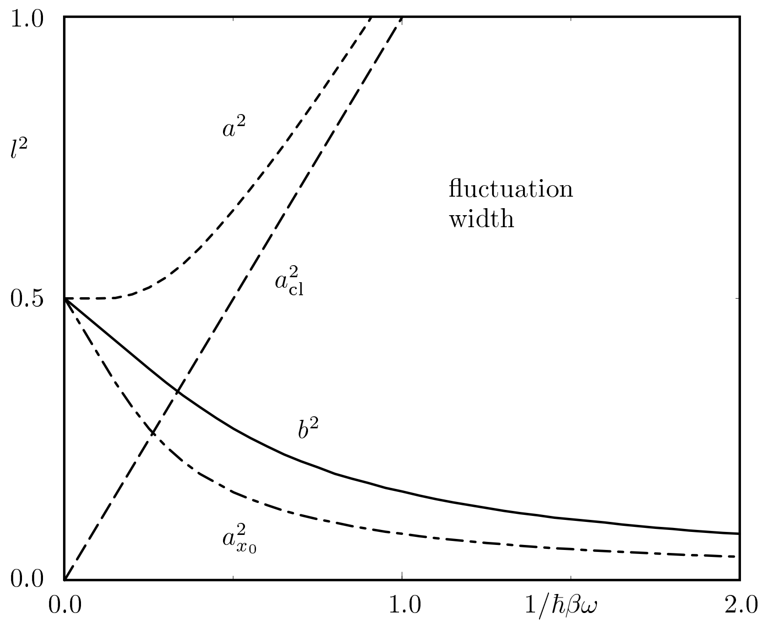

FIGURE 4.1: Temperature dependence of fluctuation widths of any point $x(\tau)$ on the path in a harmonic oscillator (l^2 is a square length in units of $\hbar/M\omega$). The quantity a^2 (dashed) is the quantum mechanical width, whereas $a_{x_0}^2$ (dash-dotted) is the width after separating out the fluctuations around the path average x_0. The quantity $a_{\rm cl}^2$ (long-dashed) is the width of the classical distribution, and b^2 (solid curve) is the fluctuation width at fixed ends.

and the distribution function is found to be

$$p(x,\tau) \equiv \langle \delta(x - x(\tau))\rangle_\omega^{x_b,x_a} = \frac{1}{\sqrt{2\pi b^2(\tau)}} \exp\left[-\frac{(x - x_{\rm cl}(\tau))^2}{2b^2(\tau)}\right]. \tag{4.22}$$

The classical path of a particle in a harmonic potential is given by Eq. (3.47), and the time-dependent width $b^2(\tau)$ is found to be

$$b^2(\tau) = G_{xx}^{\rm D}(\tau,\tau) = \frac{\hbar}{2M\omega}\left\{\coth\hbar\beta\omega - \frac{\cosh[\omega(2\tau - \hbar\beta)]}{\sinh\hbar\beta\omega}\right\}, \tag{4.23}$$

and is thus identical with the harmonic equal-time Green function (3.54) for Dirichlet boundary conditions. Since the Euclidean time τ lies in the interval $0 \le \tau \le \hbar\beta$, the width (4.23) is bounded by

$$b^2(\tau) \le \frac{\hbar}{2M\omega}\tanh\frac{\hbar\beta\omega}{2}, \tag{4.24}$$

thus remaining finite at all temperatures. The temporal average of (4.23) is

$$b^2 = \frac{1}{\hbar\beta}\int_0^{\hbar\beta} d\tau\, b^2(\tau) = \frac{\hbar}{2M\omega}\left(\coth\hbar\beta\omega - \frac{1}{\hbar\beta\omega}\right). \tag{4.25}$$

Just as $a_{x_0}^2$, this goes to zero for $T \to \infty$ with an asymptotic behavior $\hbar\beta\omega/6$, which is twice as big as that of $a_{x_0}^2$ (see Fig. 4.1). Because of the finiteness of the fluctuation width b^2 at all temperatures, which is similar to that of $a_{x_0}^2$, the special treatment of $\overline{x} = x_0$ becomes superfluous for paths with fixed end points x_b, x_a. While the separation of x_0 was necessary to deal with the diverging fluctuation

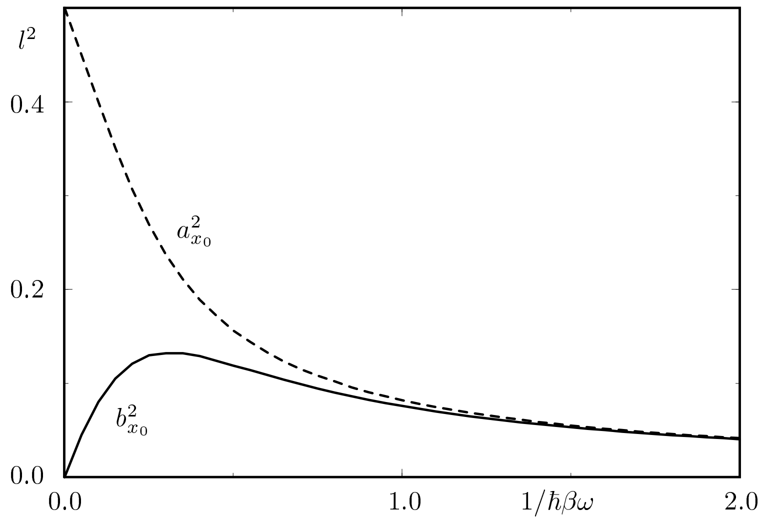

FIGURE 4.2: Temperature dependence of the width of fluctuations around the path average $x_0 = \overline{x}$ at fixed ends. For comparison we also show the width $a^2_{x_0}$ of Fig. 4.1. The vertical axis gives these square lengths l^2 in units of $\hbar/M\omega$ again.

width of the path average $\overline{x}$, paths with fixed ends have fluctuations of the path average, which are governed by the distribution

$$p_{x_0}(x_b, x_a) \equiv \langle \delta(x_0 - \overline{x}) \rangle_\omega^{x_b, x_a} = \frac{1}{\sqrt{2\pi b^2_{x_0}}} \exp\left\{ -\frac{1}{2b^2_{x_0}} \left[x_0 - \frac{1}{2}(x_b + x_a) \frac{2}{\hbar\beta\omega} \tanh \frac{\hbar\beta\omega}{2} \right]^2 \right\} \tag{4.26}$$

with the width

$$b^2_{x_0} = \frac{1}{M\beta\omega^2} \left[1 - \frac{2}{\hbar\beta\omega} \tanh \frac{\hbar\beta\omega}{2} \right], \tag{4.27}$$

which goes to zero for both limits $\beta \to \infty$ and $\beta \to 0$ (see Fig. 4.2). At each Euclidean time, $x(\tau)$ fluctuates narrowly around the classical path $x_{\rm cl}(\tau)$ connecting x_b and x_a. This is the reason why we may treat the fluctuations of $\overline{x} = x_0$ by perturbation theory, just as the other fluctuations.

Thus there is no need for particularly treating certain fluctuations for quantities with fixed bounds.

4.2 Restricted Partition Function and Effective Classical Hamiltonian

As was shown in the previous section, a separate treatment of the zero-frequency fluctuations for periodic paths is necessary. We illustrate how this separation leads to a reformulation of quantum statistics, which is then governed by an effective classical Hamiltonian.

We rewrite the partition function

$$Z = \oint \mathcal{D}^d x \mathcal{D}^d p \, e^{-\mathcal{A}[\mathbf{p},\mathbf{x}]/\hbar} \tag{4.28}$$

for an arbitrary system as

$$Z = \int \frac{d^d x_0 d^d p_0}{(2\pi\hbar)^d}\, e^{-\beta H_{\rm eff}(\mathbf{p}_0,\mathbf{x}_0)} = \int \frac{d^d x_0 d^d p_0}{(2\pi\hbar)^d}\, Z^{\mathbf{p}_0\mathbf{x}_0}, \tag{4.29}$$

where we have introduced the restricted partition function

$$Z^{\mathbf{p}_0\mathbf{x}_0} = (2\pi\hbar)^d \oint \mathcal{D}^d x \mathcal{D}^d p\, \delta(\mathbf{p}_0 - \overline{\mathbf{p}(\tau)})\delta(\mathbf{x}_0 - \overline{\mathbf{x}(\tau)})\, e^{-\mathcal{A}[\mathbf{p},\mathbf{x}]/\hbar}. \tag{4.30}$$

From (4.29) follows that the effective classical Hamiltonian $H_{\rm eff}(\mathbf{p}_0, \mathbf{x}_0)$ and the restricted partition function $Z^{\mathbf{p}_0\mathbf{x}_0}$ are related by

$$H_{\rm eff}(\mathbf{p}_0, \mathbf{x}_0) = -\frac{1}{\beta}\ln Z^{\mathbf{p}_0\mathbf{x}_0}. \tag{4.31}$$

This expression for the effective classical Hamiltonian has a similar form like a free energy, which is here local in phase space. Thus, we can also write

$$F^{\mathbf{p}_0\mathbf{x}_0} \equiv H_{\rm eff}(\mathbf{p}_0, \mathbf{x}_0). \tag{4.32}$$

Now we turn to the general Gaussian action (3.1), which we will use in the form (3.8), and calculate the restricted functional

$$\begin{aligned} Z_0^{\mathbf{w}_0}[\mathbf{C}] &= (2\pi\hbar)^d \oint \mathcal{D}^{2d} w\, \delta(\mathbf{w}_0 - \overline{\mathbf{w}(\tau)}) \\ &\times \exp\left[-\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \mathbf{w}^T(\tau) S(\tau,\tau')\mathbf{w}(\tau') - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \mathbf{C}^T(\tau)\mathbf{w}(\tau)\right], \end{aligned} \tag{4.33}$$

with $\mathbf{w}^T(\tau) = \big(\mathbf{x}^T(\tau), \mathbf{p}^T(\tau)\big)$ and $\mathbf{C}^T(\tau) = \big(\mathbf{j}^T(\tau), \mathbf{v}^T(\tau)\big)$. The temporal mean value of $\mathbf{w}(\tau)$ is defined as before, $\overline{\mathbf{w}(\tau)} = \int_0^{\hbar\beta} d\tau\, \mathbf{w}(\tau)/\hbar\beta$. The symmetric matrix S is given by (3.10). There is no difficulty to calculate $Z_0^{\mathbf{w}_0}$. Along similar lines as in Section 3.5, we express the δ function by its Fourier transform

$$\delta(\mathbf{w}_0 - \overline{\mathbf{w}(\tau)}) = \int \frac{d^{2d}k}{(2\pi)^{2d}} \exp\left[i\mathbf{w}_0^T\mathbf{k} - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \mathbf{C}_0^T \mathbf{w}(\tau)\right], \tag{4.34}$$

where $\mathbf{C}_0$ is a constant current vector,

$$\mathbf{C}_0 = \frac{i}{\beta}\mathbf{k}. \tag{4.35}$$

The functional (4.33) becomes

$$\begin{aligned} Z_0^{\mathbf{w}_0}[\tilde{\mathbf{C}}] &= (2\pi\hbar)^d \int \frac{d^{2d}k}{(2\pi)^{2d}} e^{i\mathbf{w}_0^T\mathbf{k}} \oint \mathcal{D}^{2d} w \\ &\times \exp\left[-\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \mathbf{w}^T(\tau) S(\tau,\tau')\mathbf{w}(\tau') - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \tilde{\mathbf{C}}^T(\tau)\mathbf{w}(\tau)\right], \end{aligned} \tag{4.36}$$

where we have introduced the current

$$\tilde{\mathbf{C}}(\tau) = \mathbf{C}(\tau) + \mathbf{C}_0. \tag{4.37}$$

The path integral is calculated on equal footing as for the particle density (3.144) and yields an expression similar to the partition function (3.155). We obtain

$$Z_0^{\mathbf{w}_0}[\mathbf{C}] = \frac{(2\pi\hbar)^d}{\sqrt{\det S}} \int \frac{d^{2d}k}{(2\pi)^{2d}} e^{i\mathbf{w}_0^T\mathbf{k}} \exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, \tilde{\mathbf{C}}^T(\tau) S^{-1}(\tau,\tau')\tilde{\mathbf{C}}(\tau')\right\}, \tag{4.38}$$

with the $2d$-fold k integral still to be done. Re-expressing the current $\tilde{\mathbf{C}}$ by (4.37) and inserting (4.35), the integrations over k turn out to be simple Gaussian ones. Executing the usual procedure of completing the square, rotation in phase space to find a diagonal representation to decouple the k-components, and translation of the components of k enables us to solve the k integrals, yielding

$$Z_0^{\mathbf{w}_0}[\mathbf{C}] = \frac{1}{\sqrt{\det_{\mathrm{ps}} B' \det S}} \exp\left\{-\frac{\hbar^2\beta^2}{2}\mathbf{w}_0^T {B'}^{-1}\mathbf{w}_0 - \beta\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, \mathbf{C}^T(\tau) S^{-1}(\tau,\tau'){B'}^{-1}\mathbf{w}_0\right\}$$
$$\times \exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, \mathbf{C}^T(\tau)\left[S^{-1}(\tau,\tau') - \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, S^{-1}(\tau,\tau_1){B'}^{-1}S^{-1}(\tau_2,\tau')\right]\mathbf{C}(\tau')\right\}. \tag{4.39}$$

We have introduced the $2d \times 2d$ matrix

$$B' = \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, S^{-1}(\tau,\tau'), \tag{4.40}$$

which is constant in time and therefore its determinant is calculated in phase space only. This differs from the calculation of the determinant of S, which is done in phase and time space. A similar case has been considered below Eq. (3.153).

It is revealing to continue the discussion of the expressions (4.39) and (4.40) in frequency space. We write the matrix $S(\tau,\tau')$ and its inverse in Fourier space as

$$S(\tau,\tau') = \frac{1}{\hbar\beta}S_0 + \frac{1}{\hbar\beta}\sum_{m=1}^{\infty}\left[S(\omega_m)e^{-i\omega_m(\tau-\tau')} + S(-\omega_m)e^{i\omega_m(\tau-\tau')}\right], \tag{4.41}$$

$$S^{-1}(\tau,\tau') = \frac{1}{\hbar\beta}S_0^{-1} + \frac{1}{\hbar\beta}\sum_{m=1}^{\infty}\left[S^{-1}(\omega_m)e^{-i\omega_m(\tau-\tau')} + S^{-1}(-\omega_m)e^{i\omega_m(\tau-\tau')}\right], \tag{4.42}$$

where we have abbreviated the zero-frequency components by $S_0 \equiv S(\omega_m = 0)$ and $S_0^{-1} \equiv S^{-1}(\omega_m = 0)$, respectively. In particular, we are interested in time integrations of $S^{-1}(\tau,\tau')$. Inserting the Fourier decomposition the integration over one time argument yields the result

$$\int_0^{\hbar\beta} d\tau\, S^{-1}(\tau,\tau') = S_0^{-1}, \tag{4.43}$$

which is independent of time. This is obvious, since $S^{-1}(\tau,\tau') = S^{-1}(\tau-\tau')$ is invariant under translations of time. Thus, an additional integration of (4.43) over τ' only contributes a "volume factor" $\hbar\beta$:

$$\int_0^{\hbar\beta} d\tau' \int_0^{\hbar\beta} d\tau\, S^{-1}(\tau,\tau') = \hbar\beta S_0^{-1} \equiv B'. \tag{4.44}$$

An alternative representation is to use temporal mean values:

$$\overline{\overline{S^{-1}(\tau,\tau')}} = \frac{1}{\hbar^2\beta^2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, S^{-1}(\tau,\tau') = \frac{1}{\hbar\beta}S_0^{-1}. \tag{4.45}$$

These results are very useful to simplify the expression (4.39). We obtain

$$Z_0^{\mathbf{w}_0}[\mathbf{C}] = \frac{1}{\sqrt{\det_{\mathrm{ps}} {S_0}^{-1} \det S}} \exp\left\{-\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, \mathbf{w}_0^T S(\tau,\tau')\mathbf{w}_0 - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \mathbf{C}^T(\tau)\mathbf{w}_0\right\}$$
$$\times \exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, \mathbf{C}^T(\tau) G^{\mathbf{w}_0}(\tau,\tau')\mathbf{C}(\tau')\right\}, \tag{4.46}$$

where the $2d \times 2d$ matrix $G^{\mathbf{w}_0}(\tau,\tau')$ of Green functions is defined as

$$G^{\mathbf{w}_0}(\tau,\tau') = S^{-1}(\tau,\tau') - \overline{\overline{S^{-1}(\tau,\tau')}} \equiv \begin{pmatrix} G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau,\tau') & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau,\tau') \\ G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{px}}(\tau,\tau') & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau,\tau') \end{pmatrix} . \tag{4.47}$$

The elements are $d \times d$ block matrices and identified with the Green functions (3.157)–(3.160) with *excluded* zero-frequency mode:

$$G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau,\tau') = G^{\mathrm{p}}_{\mathbf{xx}}(\tau,\tau') - \overline{\overline{G^{\mathrm{p}}_{\mathbf{xx}}(\tau,\tau')}} = G^{\mathrm{p}}_{\mathbf{xx}}(\tau,\tau') - G^{\mathrm{p}}_{\mathbf{xx},\mathrm{cl}}, \tag{4.48}$$

$$G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau,\tau') = G^{\mathrm{p}}_{\mathbf{xp}}(\tau,\tau') - \overline{\overline{G^{\mathrm{p}}_{\mathbf{xp}}(\tau,\tau')}} = G^{\mathrm{p}}_{\mathbf{xp}}(\tau,\tau') - G^{\mathrm{p}}_{\mathbf{xp},\mathrm{cl}}, \tag{4.49}$$

$$G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{px}}(\tau,\tau') = G^{\mathrm{p}}_{\mathbf{px}}(\tau,\tau') - \overline{\overline{G^{\mathrm{p}}_{\mathbf{px}}(\tau,\tau')}} = G^{\mathrm{p}}_{\mathbf{px}}(\tau,\tau') - G^{\mathrm{p}}_{\mathbf{px},\mathrm{cl}} = G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau',\tau), \tag{4.50}$$

$$G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau,\tau') = G^{\mathrm{p}}_{\mathbf{pp}}(\tau,\tau') - \overline{\overline{G^{\mathrm{p}}_{\mathbf{pp}}(\tau,\tau')}} = G^{\mathrm{p}}_{\mathbf{pp}}(\tau,\tau') - G^{\mathrm{p}}_{\mathbf{pp},\mathrm{cl}}, \tag{4.51}$$

where we have used the identity of the zero-frequency component of the quantum statistical Green functions and the classical fluctuation width. As a consequence of the relations (4.31) and (4.32), and the zero-temperature limit (3.191), the restricted partition function (4.46) is the fundamental quantity, which enables us to calculate the free energy and the effective classical Hamiltonian of any system with Gaussian action. For later use, we introduce expectation values in phase space with the zero-frequency modes excluded in a similar manner as in Eq. (4.15). Defining the restricted partition function as the functional (4.46) with vanishing currents,

$$Z_0^{\mathbf{w}_0} \equiv Z_0^{\mathbf{w}_0}[0] = \frac{1}{\sqrt{\det_{\mathrm{ps}} {S_0}^{-1} \det S}} \exp\left\{-\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, \mathbf{w}_0^T S(\tau,\tau')\mathbf{w}_0\right\}, \tag{4.52}$$

the restricted expectation value for any quantity, which depends on position and/or momentum is expressed as

$$\langle\cdots\rangle^{\mathbf{p}_0\mathbf{x}_0} = (2\pi\hbar)^d \left[Z_0^{\mathbf{w}_0}\right]^{-1} \oint \mathcal{D}^{2d}w\, \delta(\mathbf{w}_0 - \overline{\mathbf{w}(\tau)}) \cdots \exp\left[-\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, \mathbf{w}^T(\tau) S(\tau,\tau')\mathbf{w}(\tau')\right]. \tag{4.53}$$

Similar to the method of calculating expectation values and the results obtained in Section 3.2.3, we find that the one-point function is

$$\langle \mathbf{w}(\tau)\rangle^{\mathbf{p}_0\mathbf{x}_0} = \mathbf{w}_0, \tag{4.54}$$

and the two-point functions are evaluated as

$$\langle w_m(\tau) w_n(\tau')\rangle^{\mathbf{p}_0\mathbf{x}_0} = G^{\mathbf{p}_0\mathbf{x}_0}_{w_m w_n} + w_{0,m} w_{0,n}, \qquad m,n = 1,\ldots,2d\,. \tag{4.55}$$

This makes it possible to rewrite the Green functions (4.48)–(4.51) as two-point correlation functions

$$\begin{aligned} G^{\mathbf{p}_0\mathbf{x}_0}_{x_k x_l}(\tau,\tau') &= \langle \tilde{x}_k(\tau)\tilde{x}_l(\tau')\rangle^{\mathbf{p}_0\mathbf{x}_0}, & G^{\mathbf{p}_0\mathbf{x}_0}_{p_k p_l}(\tau,\tau') &= \langle \tilde{p}_k(\tau)\tilde{p}_l(\tau')\rangle^{\mathbf{p}_0\mathbf{x}_0}, \\ G^{\mathbf{p}_0\mathbf{x}_0}_{x_k p_l}(\tau,\tau') &= \langle \tilde{x}_k(\tau)\tilde{p}_l(\tau')\rangle^{\mathbf{p}_0\mathbf{x}_0}, & G^{\mathbf{p}_0\mathbf{x}_0}_{p_k x_l}(\tau,\tau') &= \langle \tilde{p}_k(\tau)\tilde{x}_l(\tau')\rangle^{\mathbf{p}_0\mathbf{x}_0}, \end{aligned} \qquad k,l = 1,\ldots,d\,, \tag{4.56}$$

with abbreviations

$$\tilde{\mathbf{x}}(\tau) = \mathbf{x}(\tau) - \mathbf{x}_0, \qquad \tilde{\mathbf{p}}(\tau) = \mathbf{p}(\tau) - \mathbf{p}_0. \tag{4.57}$$

For the calculation of an expectation value of a quantity, which is a nonpolynomial function F of $\mathbf{x}$ or $\mathbf{p}$, we need the smearing formula. The derivation of this multiple convolution integral follows along a similar procedure as presented in Section 3.3.2 for the density matrix. We do not repeat it here and give only the result for the general case of a product of $N+M$ functions, where N of which may depend on $\mathbf{x}$ and M on $\mathbf{p}$:

$$\langle F_1(\mathbf{x}(\tau_1))F_2(\mathbf{x}(\tau_2))\dots F_N(\mathbf{x}(\tau_N))F_{N+1}(\mathbf{p}(\tau_{N+1}))F_{N+2}(\mathbf{p}(\tau_{N+2}))\dots F_{N+M}(\mathbf{x}(\tau_{N+M}))\rangle^{\mathbf{p}_0\mathbf{x}_0}$$
$$= \frac{1}{\sqrt{G^{\mathbf{p}_0\mathbf{x}_0}}}\prod_{n=1}^{N}\left[\int d^dx_n\,F_n(\mathbf{x}_n)\right]\prod_{m=1}^{M}\left[\frac{d^dp_m}{(2\pi\hbar)^d}\,F_{N+m}(\mathbf{p}_m)\right]\exp\left\{-\frac{1}{2}\mathbf{y}^T[G^{\mathbf{p}_0\mathbf{x}_0}]^{-1}\mathbf{y}\right\}, \tag{4.58}$$

where $\mathbf{y}$ is the $(N+M)d$-dimensional vector

$$\mathbf{y}^T = (\mathbf{x}_1(\tau_1)-\mathbf{x}_0,\dots,\mathbf{x}_N(\tau_N)-\mathbf{x}_0,\mathbf{p}_1(\tau_{N+1})-\mathbf{p}_0,\dots\mathbf{p}_M(\tau_{N+M})-\mathbf{p}_0)\,. \tag{4.59}$$

The $(N+M)d\times(N+M)d$-matrix

$$G^{\mathbf{p}_0\mathbf{x}_0} = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \tag{4.60}$$

is composed of the $Nd\times Nd$-matrix A and the $Md\times Md$-matrix C,

$$A = \begin{pmatrix} G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_1,\tau_1) & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_1,\tau_2) & \cdots & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_1,\tau_N) \\ G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_1,\tau_2) & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_1,\tau_1) & \cdots & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_2,\tau_N) \\ \vdots & \vdots & \ddots & \vdots \\ G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_1,\tau_N) & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_2,\tau_N) & \cdots & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xx}}(\tau_1,\tau_1) \end{pmatrix}, \tag{4.61}$$

$$C = \begin{pmatrix} G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_1,\tau_1) & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_1,\tau_2) & \cdots & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_1,\tau_M) \\ G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_1,\tau_2) & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_1,\tau_1) & \cdots & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_2,\tau_M) \\ \vdots & \vdots & \ddots & \vdots \\ G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_1,\tau_M) & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_2,\tau_M) & \cdots & G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{pp}}(\tau_1,\tau_1) \end{pmatrix}, \tag{4.62}$$

as well as the $Nd\times Md$-matrix

$$B = \begin{pmatrix} -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_1,\tau_1) & -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_1,\tau_2) & \cdots & -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_1,\tau_M) \\ -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_2,\tau_1) & -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_1,\tau_1) & \cdots & -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_2,\tau_M) \\ \vdots & \vdots & \vdots & \vdots \\ -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_N,\tau_1) & -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_N,\tau_2) & \cdots & -G^{\mathbf{p}_0\mathbf{x}_0}_{\mathbf{xp}}(\tau_N,\tau_M) \end{pmatrix}. \tag{4.63}$$

The inverse and the determinant of the block matrix $G^{\mathbf{p}_0\mathbf{x}_0}$ are calculated as described in Appendix 3A.

We calculate now the appropriate Green functions and the partition function (4.46) for the harmonic oscillator. The calculation of the Green functions with the zero-frequency components excluded is simply done, since we know the complete Green functions for the harmonic oscillator from Eqs. (3.166)–(3.169). Subtracting the twice-averaged terms, we obtain

$$G^{p_0x_0}_{xx,\omega}(\tau,\tau') = G^{\mathrm{p}}_{xx,\omega}(\tau,\tau') - \frac{1}{M\beta\omega^2}, \tag{4.64}$$
$$G^{p_0x_0}_{xp,\omega}(\tau,\tau') = G^{\mathrm{p}}_{xp,\omega}(\tau,\tau'), \tag{4.65}$$
$$G^{p_0x_0}_{px,\omega}(\tau,\tau') = G^{\mathrm{p}}_{px,\omega}(\tau,\tau'), \tag{4.66}$$
$$G^{p_0x_0}_{pp,\omega}(\tau,\tau') = G^{\mathrm{p}}_{pp,\omega}(\tau,\tau') - \frac{M}{\beta}. \tag{4.67}$$

The zero-frequency modes of the mixed two-point functions vanish. Thus, the matrix of the zero components simply reads

$$S_0 = \begin{pmatrix} M\hbar^{-1}\omega^2 & 0 \\ 0 & (\hbar M)^{-1} \end{pmatrix}. \tag{4.68}$$

The determinant is easily calculated and yields $\det_{\rm ps} S_0 = \omega^2$ in units, where $\hbar = \beta = M = 1$. Together with the result (3.175) for the partition function of the harmonic oscillator, this gives the restricted partition function

$$Z_\omega^{p_0 x_0} = \frac{\hbar\beta\omega}{2\sinh\hbar\beta\omega/2} \exp\left[-\beta\left(\frac{p_0^2}{2M} + \frac{1}{2}M\omega^2 x_0^2\right)\right], \tag{4.69}$$

where the exponential contains the effective classical Hamiltonian of the harmonic oscillator, $H_{\text{eff},\omega} = p_0^2/2M + M\omega^2 x_0^2/2$. Performing the integral over the zero-frequency components x_0 and p_0 leads to the known partition function (3.175) of the harmonic oscillator.