CHAPTER 3

Smearing Formulas for Fluctuation Effects

It is well known from perturbative expansions of interacting quantum fields and quantum mechanical systems with polynomial interactions that correlation functions appearing in a certain perturbative order can be decomposed into sums of products of two-point correlation functions by applying Wick's rule [4, Chap. 3]. When the potential of a physical system is nonpolynomial, the correlation functions are more complicated, and Wick's rule fails. This case can only be treated with a so-called smearing formula, which simply turns out to be a Gaussian convolution of the original classical potential. The width of the Gaussian distribution is governed by the two-point correlation functions or Green functions of the unperturbed system. A special example was the perturbative expansion for the effective classical Hamiltonian (2.77), which will now be generalized to arbitrary Gaussian systems.

3.1 Generalized Euclidean Action in Phase Space

The most general Euclidean quadratic action in flat $2d$-dimensional phase space reads

$$\mathcal{A}_0[\mathbf{p},\mathbf{x};\mathbf{j},\mathbf{v}] = \frac{\hbar}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \left[\mathbf{x}^T(\tau) D_{\mathbf{xx}}(\tau,\tau')\mathbf{x}(\tau') + \mathbf{x}^T(\tau) D_{\mathbf{xp}}(\tau,\tau')\mathbf{p}(\tau')\right.$$
$$\left. + \mathbf{p}^T(\tau) D_{\mathbf{px}}(\tau,\tau')\mathbf{x}(\tau') + \mathbf{p}^T(\tau) D_{\mathbf{pp}}(\tau,\tau')\mathbf{p}(\tau')\right] + \int_0^{\hbar\beta} d\tau \left[\mathbf{j}^T(\tau)\mathbf{x}(\tau) + \mathbf{v}^T(\tau)\mathbf{p}(\tau)\right], \quad (3.1)$$

where $\mathbf{j}(\tau)$ and $\mathbf{v}(\tau)$ are external currents coupled linearly to the respective d-dimensional phase space coordinate $\mathbf{x}(\tau)$ or $\mathbf{p}(\tau)$. The superscript T denotes the transpose with respect to the phase space coordinates. The $d \times d$ matrices $D_{\mathbf{xx}}(\tau,\tau')$, $D_{\mathbf{xp}}(\tau,\tau')$, $D_{\mathbf{px}}(\tau,\tau')$, and $D_{\mathbf{pp}}(\tau,\tau')$ are arbitrary at the moment.

Integrating $\exp\{-\mathcal{A}_0[\mathbf{p},\mathbf{x};\mathbf{j},\mathbf{v}]/\hbar\}$ over all possible configurations satisfying periodic boundary conditions in phase space yields the partition function of the system with external sources

$$Z_0[\mathbf{j},\mathbf{v}] = \oint \mathcal{D}^d x \mathcal{D}^d p \, e^{-\mathcal{A}_0[\mathbf{p},\mathbf{x};\mathbf{j},\mathbf{v}]/\hbar}. \quad (3.2)$$

This serves as the generating functional for all correlation functions. The path integral measure is defined by slicing:

$$\oint \mathcal{D}^d x \mathcal{D}^d p = \lim_{N\to\infty} \prod_{n=1}^{N+1} \left[\int \frac{d^d x_n d^d p_n}{(2\pi\hbar)^d} \right]. \tag{3.3}$$

The partition function can also be written as an integral over the unnormalized particle density $\tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}]$,

$$Z_0[\mathbf{j},\mathbf{v}] = \int d^d x\, \tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}]. \tag{3.4}$$

The unnormalized particle density $\tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}]$ is the diagonal element of the unnormalized density matrix

$$\tilde{\varrho}_0(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}] = \int \mathcal{D}'^d x \mathcal{D}^d p\, e^{-\mathcal{A}_0[\mathbf{p},\mathbf{x};\mathbf{j},\mathbf{v}]/\hbar} \tag{3.5}$$

with the sliced measure

$$\int \mathcal{D}'^d x \mathcal{D}^d p = \lim_{N\to\infty} \prod_{n=1}^{N} \left[\int d^d x_n \right] \prod_{n=1}^{N+1} \left[\int \frac{d^d p_n}{(2\pi\hbar)^d} \right]. \tag{3.6}$$

The density matrix is normalized by the partition function (3.2):

$$\varrho_0(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}] = \frac{\tilde{\varrho}_0(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}]}{Z_0[\mathbf{j},\mathbf{v}]}. \tag{3.7}$$

For the calculation of the density matrix in the presence of external sources (3.5), it is useful to introduce natural units with $\hbar = \beta = M = 1$, where M is the particle mass. Thus, positions are measured in units of $\sqrt{\hbar^2\beta/M}$, and the Euclidean time is given as a multiple of $\hbar\beta$.

The action (3.1) can be written in the $2d \times 2d$ matrix form

$$\mathcal{A}_0[\mathbf{p},\mathbf{x};\mathbf{j},\mathbf{v}] = \frac{1}{2}\int_0^1 d\tau \int_0^1 d\tau'\, \mathbf{w}^T(\tau) S(\tau,\tau') \mathbf{w}(\tau') + \int_0^1 d\tau\, \mathbf{C}^T(\tau)\mathbf{w}(\tau), \tag{3.8}$$

with $2d$ phase space vectors $\mathbf{w}^T(\tau) = \left(\mathbf{x}^T(\tau), \mathbf{p}^T(\tau)\right)$ and currents $\mathbf{C}^T(\tau) = \left(\mathbf{j}^T(\tau), \mathbf{v}^T(\tau)\right)$. The $2d \times 2d$ matrix $S(\tau,\tau')$ is composed as follows:

$$S(\tau,\tau') = \begin{pmatrix} D_{\mathbf{xx}}(\tau,\tau') & D_{\mathbf{xp}}(\tau,\tau') \\ D_{\mathbf{px}}(\tau,\tau') & D_{\mathbf{pp}}(\tau,\tau') \end{pmatrix}. \tag{3.9}$$

Utilizing the invariance of the first term of the action (3.8) under transposing and interchanging τ and τ', we introduce a symmetrized matrix

$$S^{\mathrm{s}}(\tau,\tau') = \begin{pmatrix} D^{\mathrm{s}}_{\mathbf{xx}}(\tau,\tau') & D^{\mathrm{s}}_{\mathbf{xp}}(\tau,\tau') \\ D^{\mathrm{s}}_{\mathbf{px}}(\tau,\tau') & D^{\mathrm{s}}_{\mathbf{pp}}(\tau,\tau') \end{pmatrix}, \tag{3.10}$$

where the superscript "s" denotes the symmetry $S^{\mathrm{s}}(\tau,\tau') = S^{\mathrm{s}\,T}(\tau',\tau)$. The symmetrized kernels are

$$D^{\mathrm{s}}_{\mathbf{xx}}(\tau,\tau') = \frac{1}{2}\left[D_{\mathbf{xx}}(\tau,\tau') + D^T_{\mathbf{xx}}(\tau',\tau)\right], \quad D^{\mathrm{s}}_{\mathbf{pp}}(\tau,\tau') = \frac{1}{2}\left[D_{\mathbf{pp}}(\tau,\tau') + D^T_{\mathbf{pp}}(\tau',\tau)\right] \tag{3.11}$$

and satisfy

$$D^{\mathrm{s}}_{\mathbf{xx}}(\tau,\tau') = D^{\mathrm{s}\,T}_{\mathbf{xx}}(\tau',\tau), \quad D^{\mathrm{s}}_{\mathbf{pp}}(\tau,\tau') = D^{\mathrm{s}\,T}_{\mathbf{pp}}(\tau',\tau). \tag{3.12}$$

For the mixed kernels, we have

$$D^{\mathrm{s}}_{\mathbf{xp}}(\tau,\tau') = \frac{1}{2}\left[D_{\mathbf{xp}}(\tau,\tau') + D^T_{\mathbf{px}}(\tau',\tau)\right], \quad D^{\mathrm{s}}_{\mathbf{px}}(\tau,\tau') = \frac{1}{2}\left[D_{\mathbf{px}}(\tau,\tau') + D^T_{\mathbf{xp}}(\tau',\tau)\right], \tag{3.13}$$

which implies the symmetry

$$D^{\rm s}_{\mathbf{px}}(\tau,\tau') = D^{{\rm s}\,T}_{\mathbf{xp}}(\tau',\tau). \tag{3.14}$$

We will only use the symmetrized kernels in the following sections, where we calculate the path integrals for the unnormalized density matrix (3.5) and the partition function (3.2) in the presence of external sources. For simplicity, we omit the superscript "s" for the symmetrized matrices in the sequel.

By varying the symmetrized action without external sources,

$$\delta\mathcal{A}_0[\mathbf{p},\mathbf{x};0,0] = 0, \tag{3.15}$$

we find the general Hamiltonian equations of motion

$$\int_0^1 d\tau' \left[D_{\mathbf{xx}}(\tau,\tau')\mathbf{x}_{\rm cl}(\tau') + D_{\mathbf{xp}}(\tau,\tau')\mathbf{p}_{\rm cl}(\tau')\right] \;=\; 0, \tag{3.16}$$

$$\int_0^1 d\tau' \left[D_{\mathbf{pp}}(\tau,\tau')\mathbf{p}_{\rm cl}(\tau') + D_{\mathbf{px}}(\tau,\tau')\mathbf{x}_{\rm cl}(\tau')\right] \;=\; 0 \tag{3.17}$$

for the classical paths in phase space $\mathbf{x}_{\rm cl}(\tau)$ and $\mathbf{p}_{\rm cl}(\tau)$.

3.2 Density Matrix with External Sources

We now calculate the general path integral (3.5) by a time-slicing procedure and find in particular the generating functional and the two-point correlation functions for the one-dimensional harmonic oscillator.

3.2.1 Calculation of the Phase Space Path Integral

By dividing the time interval $[0,1]$ into $N+1$ pieces of length ε, the unnormalized density matrix in the presence of external sources (3.5) can be written as

$$\begin{aligned}\tilde{\varrho}_0(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}] = \lim_{N\to\infty}\prod_{n=1}^{N}\left[\int d^dx_n\right]\prod_{n=1}^{N+1}\left[\int\frac{d^dp_n}{(2\pi)^d}\right]\exp\left[-\sum_{n=1}^{N}(\mathbf{x}_n\mathbf{j}_n+\mathbf{p}_n\mathbf{v}_n)\right]\\ \times\exp\left[-\frac{1}{2}\sum_{n,m=1}^{N+1}\left(\mathbf{x}_n[D_{\mathbf{xx}}]_{nm}\mathbf{x}_m+2\mathbf{x}_n[D_{\mathbf{xp}}]_{nm}\mathbf{p}_m+\mathbf{p}_n[D_{\mathbf{pp}}]_{nm}\mathbf{p}_m\right)\right],\end{aligned} \tag{3.18}$$

where we have absorbed the lattice constant ε in the discrete matrices and currents, respectively. The calculation of the momentum integrals is easily done after quadratic completion and rotation into the diagonal basis of $D_{\mathbf{pp}}$. In continuum representation, we obtain

$$\begin{aligned}\tilde{\varrho}_0(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}] = \frac{1}{\sqrt{(2\pi)^d\det D_{\mathbf{pp}}}}\exp\left[-\frac{1}{2}\int_0^1 d\tau\int_0^1 d\tau'\,\mathbf{v}^T(\tau)D^{-1}_{\mathbf{pp}}(\tau,\tau')\mathbf{v}(\tau')\right]\\ \times\int_{\mathbf{x}(0)=\mathbf{x}_a}^{\mathbf{x}(1)=\mathbf{x}_b}\mathcal{D}^d_{\rm cs}x\,\exp\left[-\frac{1}{2}\int_0^1 d\tau\int_0^1 d\tau'\,\mathbf{x}^T(\tau)G^{{\rm D}\,-1}_{\mathbf{xx}}(\tau,\tau')\mathbf{x}(\tau')-\int_0^1 d\tau\,\mathbf{J}^T(\tau)\mathbf{x}(\tau)\right],\end{aligned} \tag{3.19}$$

where the path integral measure in configuration space is

$$\int\mathcal{D}^d_{\rm cs}x = \lim_{N\to\infty}\prod_{n=1}^{N}\left[\int\frac{d^dx_n}{(2\pi)^{d/2}}\right]. \tag{3.20}$$

The expression (3.19) possesses the remarkable property that the current

$$\mathbf{J}(\tau) = \mathbf{j}(\tau) - \int_0^1 d\tau_1\int_0^1 d\tau_2\,D_{\mathbf{xp}}(\tau,\tau_1)D^{-1}_{\mathbf{pp}}(\tau_1,\tau_2)\mathbf{v}(\tau_2), \tag{3.21}$$

which linearly couples to the coordinate $\mathbf{x}(\tau)$, contains a term with $\mathbf{v}(\tau)$ originally being coupled to the momentum. It is a general property of such functionals that currents coupling to momenta can always be considered as new currents, which couple to positions [17].

The other new quantity, which has been introduced in Eq. (3.19), is

$$G^{\mathrm{D}^{-1}}_{\mathbf{xx}}(\tau,\tau') = D_{\mathbf{xx}}(\tau,\tau') - \int_0^1 d\tau_1 \int_0^1 d\tau_2\, D_{\mathbf{xp}}(\tau,\tau_1) D^{-1}_{\mathbf{pp}}(\tau_1,\tau_2) D_{\mathbf{px}}(\tau_2,\tau'). \tag{3.22}$$

Enclosed by coordinates $\mathbf{x}(\tau)$ in the configuration space path integral appearing in Eq. (3.19), the quantity $G^{\mathrm{D}^{-1}}_{\mathbf{xx}}(\tau,\tau')$ is interpreted as a new kernel. It maps the Green function $G^{\mathrm{D}}_{x_i x_j}(\tau,\tau')$ to a δ function:

$$\sum_{j=1}^{d} \int_0^1 d\tau\, G^{\mathrm{D}\,-1}_{x_i x_j}(\tau_1,\tau)\, G^{\mathrm{D}}_{x_j x_k}(\tau,\tau_2) = \delta_{ik}\, \delta(\tau_1-\tau_2), \tag{3.23}$$

where the Kronecker symbol δ_{ij} is defined as

$$\delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases} \tag{3.24}$$

The δ function has the property

$$\int_0^1 d\tau\, f(\tau)\, \delta(\tau-\tau') = f(\tau'), \quad \tau' \in (0,1), \tag{3.25}$$

for any smooth test function $f(\tau)$. With Eqs. (3.22) and (3.23), we write the matrix of Green functions as

$$G^{\mathrm{D}}_{\mathbf{xx}}(\tau,\tau') = \left[D_{\mathbf{xx}}(\tau,\tau') - \int_0^1 d\tau_1 \int_0^1 d\tau_2\, D_{\mathbf{xp}}(\tau,\tau_1) D^{-1}_{\mathbf{pp}}(\tau_1,\tau_2) D_{\mathbf{px}}(\tau_2,\tau') \right]^{-1}. \tag{3.26}$$

Since the end points of the paths are fixed, $\mathbf{x}(0) = \mathbf{x}_a$ and $\mathbf{x}(1) = \mathbf{x}_b$, fluctuations are vanishing at these edges, and the Green function $G^{\mathrm{D}}_{x_i x_j}(\tau,\tau')$ must obey Dirichlet boundary conditions:

$$G^{\mathrm{D}}_{x_i x_j}(0,\tau') = G^{\mathrm{D}}_{x_i x_j}(1,\tau') = 0, \quad G^{\mathrm{D}}_{x_i x_j}(\tau,0) = G^{\mathrm{D}}_{x_i x_j}(\tau,1) = 0. \tag{3.27}$$

The calculation of the configuration space path integral in Eq. (3.19),

$$(\mathbf{x}_b\, 1|\mathbf{x}_a\, 0)[\mathbf{J}] = \int\limits_{\mathbf{x}(0)=\mathbf{x}_a}^{\mathbf{x}(1)=\mathbf{x}_b} \mathcal{D}^d_{\mathrm{cs}} x\, e^{-\mathcal{A}_{0\,\mathrm{cs}}[\mathbf{x};\mathbf{J}]/\hbar}, \tag{3.28}$$

with the action in configuration space

$$\mathcal{A}_{0\mathrm{cs}}[\mathbf{x};\mathbf{J}] = \frac{\hbar}{2} \int_0^1 d\tau \int_0^1 d\tau'\, \mathbf{x}^T(\tau) G^{\mathrm{D}^{-1}}_{\mathbf{xx}}(\tau,\tau') \mathbf{x}(\tau') + \int_0^1 d\tau\, \mathbf{J}^T(\tau)\mathbf{x}(\tau), \tag{3.29}$$

is done on usual footing. We decompose the path $\mathbf{x}(\tau)$ into a classical part $\mathbf{x}_{\mathrm{cl}}(\tau)$ and the fluctuation term $\delta\mathbf{x}(\tau)$,

$$\mathbf{x}(\tau) = \mathbf{x}_{\mathrm{cl}}(\tau) + \delta\mathbf{x}(\tau), \tag{3.30}$$

where the fluctuations may vanish at the boundaries, $\delta\mathbf{x}(0) = \delta\mathbf{x}(1) = 0$. The variation of the action (3.29) in the absence of the external current $\mathbf{J}(\tau)$ vanishes for the classical path. Performing this variation, we obtain a relation, which we need for the following considerations:

$$\delta\mathcal{A}_{0\mathrm{cs}}[\mathbf{x}_{\mathrm{cl}};\mathbf{0}] \;=\; \frac{1}{2} \int_0^1 d\tau \int_0^1 d\tau' \left[\delta\mathbf{x}^T(\tau) G^{\mathrm{D}^{-1}}_{\mathbf{xx}}(\tau,\tau') \mathbf{x}_{\mathrm{cl}}(\tau') + \mathbf{x}^T_{\mathrm{cl}}(\tau) G^{\mathrm{D}^{-1}}_{\mathbf{xx}}(\tau,\tau') \delta\mathbf{x}(\tau') \right]$$

$$= \int_0^1 d\tau \int_0^1 d\tau' \, \delta \mathbf{x}^T(\tau) G_{\mathbf{xx}}^{\mathrm{D}^{-1}}(\tau,\tau') \mathbf{x}_{\mathrm{cl}}(\tau') = 0. \tag{3.31}$$

Here we have utilized in the last line the symmetry of $G_{\mathbf{xx}}^{\mathrm{D}^{-1}}(\tau,\tau')$, which is obvious from the definition (3.22) and the properties (3.12) and (3.14). From (3.31), we read off the Euler–Lagrange equations of motion

$$\int_0^1 d\tau' \, G_{\mathbf{xx}}^{\mathrm{D}^{-1}}(\tau,\tau') \mathbf{x}_{\mathrm{cl}}(\tau') = 0. \tag{3.32}$$

Inserting now the decomposition (3.30) into the action (3.29), considering the vanishing of the coupling of fluctuations and classical path from the last line in (3.31), and acknowledging that the measure is invariant under the translation (3.30), $\mathcal{D}_{\mathrm{cs}}^d x = \mathcal{D}_{\mathrm{cs}}^d \delta x$, the functional (3.28) can be expressed as

$$\begin{aligned}
(\mathbf{x}_b\, 1|\mathbf{x}_a\, 0)[\mathbf{J}] = \exp\left\{ \frac{1}{2} \int_0^1 d\tau \int_0^1 d\tau' \left[\mathbf{J}^T(\tau) G_{\mathbf{xx}}^{\mathrm{D}}(\tau,\tau') \mathbf{J}(\tau') - \mathbf{x}_{\mathrm{cl}}^T(\tau) G_{\mathbf{xx}}^{\mathrm{D}^{-1}}(\tau,\tau') \mathbf{x}_{\mathrm{cl}}(\tau') \right] \right\} \\
\times \exp\left\{ - \int_0^1 d\tau \, \mathbf{J}^T(\tau) \mathbf{x}_{\mathrm{cl}}(\tau) \right\} \int_{\delta\mathbf{x}(0)=0}^{\delta\mathbf{x}(1)=0} \mathcal{D}_{\mathrm{cs}}^d \delta x \, \exp\left\{ -\frac{1}{2} \int_0^1 d\tau \int_0^1 d\tau' \right. \\
\left. \times \left[\delta\mathbf{x}^T(\tau) + \int_0^1 d\tau_1 \, \mathbf{J}^T(\tau_1) G_{\mathbf{xx}}^{\mathrm{D}}(\tau_1,\tau) \right] G_{\mathbf{xx}}^{\mathrm{D}^{-1}}(\tau,\tau') \left[\delta\mathbf{x}(\tau') + \int_0^1 d\tau_2 \, G_{\mathbf{xx}}^{\mathrm{D}}(\tau',\tau_2) \mathbf{J}(\tau_2) \right] \right\}.
\end{aligned} \tag{3.33}$$

The path integral over the fluctuations is a constant, since it is independent of the end points $\mathbf{x}_a$ and $\mathbf{x}_b$. For convenience, we introduce the new variable

$$\mathbf{y}(\tau) = \delta\mathbf{x}(\tau) + \int_0^1 d\tau' \, G_{\mathbf{xx}}^{\mathrm{D}}(\tau,\tau') \mathbf{J}(\tau'), \tag{3.34}$$

which also vanishes at the boundary, $\mathbf{y}(0) = \mathbf{y}(1) = 0$, since the Green functions $G_{\mathbf{xx}}^{\mathrm{D}}(\tau,\tau')$ satisfy the Dirichlet boundary conditions (3.27). The measure of the path integral over the fluctuations remains unchanged, $\mathcal{D}_{\mathrm{cs}}^d y = \mathcal{D}_{\mathrm{cs}}^d \delta x$, and the calculation of this path integral is simply done, e.g. in discrete space, yielding

$$\int_{\mathbf{y}(0)=0}^{\mathbf{y}(1)=0} \mathcal{D}_{\mathrm{cs}}^d y \, \exp\left[-\frac{1}{2} \int_0^1 d\tau \int_0^1 d\tau' \, \mathbf{y}^T(\tau) G_{\mathbf{xx}}^{\mathrm{D}^{-1}}(\tau,\tau') \mathbf{y}(\tau') \right] = \frac{1}{\sqrt{\det G_{\mathbf{xx}}^{\mathrm{D}^{-1}}}} \, . \tag{3.35}$$

Combining the results (3.19), (3.33), and (3.35), we obtain the density matrix in the presence of external sources

$$\begin{aligned}
\tilde{\varrho}_0(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}] = \left(\frac{M}{2\pi\hbar^2\beta} \right)^{d/2} \frac{1}{\sqrt{\det D_{\mathbf{pp}} \det G_{\mathbf{xx}}^{\mathrm{D}^{-1}}}} \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[\mathbf{j}^T(\tau) \mathbf{x}_{\mathrm{cl}}(\tau) + \mathbf{v}^T(\tau) \mathbf{p}_{\mathrm{cl}}(\tau) \right] \right\} \\
\times \exp\left[-\frac{1}{2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \, \mathbf{x}_{\mathrm{cl}}^T(\tau) G_{\mathbf{xx}}^{\mathrm{D}^{-1}}(\tau,\tau') \mathbf{x}_{\mathrm{cl}}(\tau') \right] \\
\times \exp\left\{ \frac{1}{2\hbar^2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \left[\mathbf{j}^T(\tau) G_{\mathbf{xx}}^{\mathrm{D}}(\tau,\tau') \mathbf{j}(\tau') + \mathbf{j}^T(\tau) G_{\mathbf{xp}}^{\mathrm{D}}(\tau,\tau') \mathbf{v}(\tau') \right. \right. \\
\left. \left. + \mathbf{v}^T(\tau) G_{\mathbf{px}}^{\mathrm{D}}(\tau,\tau') \mathbf{j}(\tau') + \mathbf{v}^T(\tau) G_{\mathbf{pp}}^{\mathrm{D}}(\tau,\tau') \mathbf{v}(\tau') \right] \right\},
\end{aligned} \tag{3.36}$$

where we have reused the standard units. In order to prevent complications, the determinants shall be treated as dimensionless quantities here. For this reason, we have already extracted the dimension-carrying prefactor $(M/\hbar^2\beta)^{d/2}$. As a rule, the determinants are calculated with $\hbar = \beta = M = 1$. At the end, powers of $\hbar$, β, and M are multiplied to the determinant to make it dimensionless.

In (3.36), we further utilized the relation

$$\mathbf{p}_{\rm cl}(\tau) = -\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, D^{-1}_{\mathbf{pp}}(\tau,\tau_1) D_{\mathbf{px}}(\tau_1,\tau_2)\mathbf{x}_{\rm cl}(\tau_2), \tag{3.37}$$

which is a direct consequence of the Hamiltonian equation of motion (3.17), when solved with respect to $\mathbf{p}_{\rm cl}(\tau)$.

Additionally to $G^{\rm D}_{\mathbf{xx}}(\tau,\tau')$, defined by (3.26), we have introduced the $d \times d$ matrices

$$G^{\rm D}_{\mathbf{xp}}(\tau,\tau') = -\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, G^{\rm D}_{\mathbf{xx}}(\tau,\tau_1) D_{\mathbf{xp}}(\tau_1,\tau_2) D^{-1}_{\mathbf{pp}}(\tau_2,\tau'), \tag{3.38}$$

$$\begin{aligned} G^{\rm D}_{\mathbf{px}}(\tau,\tau') &= \left[G^{\rm D}_{\mathbf{xp}}\right]^T(\tau',\tau) \\ &= -\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, D^{-1}_{\mathbf{pp}}(\tau,\tau_1) D_{\mathbf{px}}(\tau_1,\tau_2) G^{\rm D}_{\mathbf{xx}}(\tau_2,\tau'), \end{aligned} \tag{3.39}$$

$$\begin{aligned} G^{\rm D}_{\mathbf{pp}}(\tau,\tau') &= D^{-1}_{\mathbf{pp}}(\tau,\tau') + \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_4 \\ &\quad \times D^{-1}_{\mathbf{pp}}(\tau,\tau_1) D_{\mathbf{px}}(\tau_1,\tau_2) G^{\rm D}_{\mathbf{xp}}(\tau_2,\tau_3) D_{\mathbf{xp}}(\tau_3,\tau_4) D^{-1}_{\mathbf{pp}}(\tau_4,\tau'). \end{aligned} \tag{3.40}$$

These expressions are equivalent to position- and/or momentum-dependent two-point correlation functions, as we show in Section 3.2.3. Before embarking to this, however, we will first check the density matrix functional (3.36) for a simple example, the one-dimensional harmonic oscillator.

3.2.2 Example: Density Matrix of the One-Dimensional Harmonic Oscillator with Sources

The harmonic oscillator is usually a pretty good system for checking a general theory, since its exact quantum statistical properties are well known. Due to the Gaussian type of the Boltzmann factor, the path integrals for density matrix and partition function are simply solved. Additionally, this system is nontrivial in a sense that it possesses a nonvanishing interaction.

In what follows, we calculate the density matrix functional for the one-dimensional case, since it already contains the interesting properties that we would like to point out, e.g. the two-point correlation functions. The action of this system in the presence of external sources $j(\tau)$ and $v(\tau)$ reads

$$\mathcal{A}_\omega[p,x;j,v] = \int_0^{\hbar\beta} d\tau \left\{ -ip(\tau)\frac{d}{d\tau}x(\tau) + \frac{1}{2}\left[\frac{p^2(\tau)}{M} + M\omega^2 x^2(\tau)\right] + j(\tau)x(\tau) + v(\tau)p(\tau) \right\}. \tag{3.41}$$

By comparing this action with the general one introduced in Eq. (3.1), we identify

$$\begin{aligned} &D_{xx}(\tau,\tau') = \frac{M}{\hbar}\omega^2\delta(\tau,\tau'), \quad D_{pp}(\tau,\tau') = \frac{1}{\hbar M}\delta(\tau,\tau'), \quad D_{xp}(\tau,\tau') = \frac{i}{\hbar}\frac{\partial}{\partial\tau}\delta(\tau,\tau'), \\ &D_{px}(\tau,\tau') = -\frac{i}{\hbar}\frac{\partial}{\partial\tau}\delta(\tau,\tau') + \frac{i}{\hbar}\delta(\tau,\tau')\left[\delta(\hbar\beta,\tau) - \delta(\tau,0)\right]. \end{aligned} \tag{3.42}$$

The δ functions with two arguments act as the usual δ function with the exception of time translational invariance. It is a consequence of the Dirichlet boundary conditions the paths must satisfy due to the fixing of the end points. This will become clear after expanding the fluctuations into a complete set of orthonormal functions and is shown later on.

The symmetric splitting of the first term in the action (3.41) is necessary to ensure the symmetry of the matrix $S(\tau,\tau')$, defined in Eq. (3.9). This requires that the nondiagonal elements D_{xp} and D_{px} of S must be transposed to one another.[1] It is a nice problem to show what the transpose of the operator $i\partial/\partial\tau$ is. It is well known from quantum mechanics that the operator

$$\hat{H} \to i\frac{\partial}{\partial\tau} \tag{3.43}$$

[1] The second and third terms of $D_{px}(\tau,\tau')$ appear since operators with derivatives yield boundary terms: $\int_0^{\hbar\beta} d\tau\, f(\tau)\dot{g}(\tau) = f(\tau)g(\tau)\big|_{\tau=0}^{\tau=\hbar\beta} - \int_0^{\hbar\beta} d\tau\, \dot{g}(\tau)f(\tau)$. If $f(\tau)$ and $g(\tau)$ have periodic or Dirichlet boundary conditions, these additional terms vanish, and $D_{px}(\tau,\tau')$ is exactly the transpose of $D_{xp}(\tau,\tau')$.

is Hermitian, $\hat{H} = \hat{H}^+$. This means that any representation of this operator is identical to its transpose with complex conjugated elements. With (3.43), we obtain

$$i\frac{\partial}{\partial\tau} = \left(i\frac{\partial}{\partial\tau}\right)^+ = \left[\left(i\frac{\partial}{\partial\tau}\right)^\star\right]^T = -i\left(\frac{\partial}{\partial\tau}\right)^T \quad\Longrightarrow\quad \left(\frac{\partial}{\partial\tau}\right)^T = -\frac{\partial}{\partial\tau}. \tag{3.44}$$

This explains the different signs of D_{xp} and the first term of D_{px} in (3.42).

The first quantity we shall calculate is $G^{\mathrm{D}\,-1}_{xx,\omega}(\tau,\tau')$, defined in Eq. (3.22). Inserting the identifications from (3.42) into (3.22) yields

$$G^{\mathrm{D}\,-1}_{xx,\omega}(\tau,\tau') = \frac{M}{\hbar}\left[\delta(\hbar\beta-\tau)-\delta(\tau)\right]\frac{\partial}{\partial\tau}\delta(\tau-\tau') - \frac{M}{\hbar}\left(\frac{\partial^2}{\partial\tau^2}-\omega^2\right)\delta(\tau-\tau'). \tag{3.45}$$

Thus, calculating the classical action of the density matrix (3.36) for the one-dimensional harmonic oscillator gives the known result (without external currents):

$$\begin{aligned}\mathcal{A}_{\omega,\mathrm{cl}}[x] &= \frac{\hbar}{2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,x_{\mathrm{cl}}(\tau)G^{\mathrm{D}\,-1}_{xx,\omega}(\tau,\tau')x_{\mathrm{cl}}(\tau')\\ &= \frac{M}{2}\left[x_{\mathrm{cl}}(\hbar\beta)\dot{x}_{\mathrm{cl}}(\hbar\beta)-x_{\mathrm{cl}}(0)\dot{x}_{\mathrm{cl}}(0)-\int_0^{\hbar\beta}d\tau\,x_{\mathrm{cl}}(\tau)\left(\frac{\partial^2}{\partial\tau^2}-\omega^2\right)x_{\mathrm{cl}}(\tau)\right]\\ &= \int_0^{\hbar\beta}d\tau\,\left[\frac{1}{2}M\dot{x}^2_{\mathrm{cl}}(\tau)+\frac{1}{2}M\omega^2x^2_{\mathrm{cl}}(\tau)\right].\end{aligned} \tag{3.46}$$

Since the classical path for the harmonic oscillator is known to be [4, Chap. 2]

$$x_{\mathrm{cl}}(\tau) = \frac{1}{\sinh\hbar\beta\omega}\left[x_b\sinh\omega\tau + x_a\sinh\omega(\hbar\beta-\tau)\right], \tag{3.47}$$

the classical action (3.46) becomes the usual one

$$\mathcal{A}_{\omega,\mathrm{cl}}(x_b,x_a) = \frac{M\omega}{2\sinh\hbar\beta\omega}\left[\left(x_a^2+x_b^2\right)\cosh\hbar\beta\omega - 2x_ax_b\right]. \tag{3.48}$$

Now we consider the Green function $G^{\mathrm{D}}_{xx,\omega}(\tau,\tau')$ given by Eq. (3.26). Due to the vanishing of the fluctuations $\delta x(\tau)$ at the fixed end points of the path, this Green function is required to satisfy Dirichlet boundary conditions (3.27). The fluctuations can be expanded into a complete set of orthonormal functions [4, Chap. 3],

$$\delta x_n(\tau) = \frac{1}{\sqrt{\hbar\beta}}\sin\nu_n\tau, \tag{3.49}$$

with

$$\nu_n = \frac{\pi n}{\hbar\beta} \tag{3.50}$$

being half the Matsubara frequencies defined in Eq. (2.13).

The completeness relation is then

$$\delta(\tau,\tau') = \sum_{n=-\infty}^{\infty}\delta x_n(\tau)\delta x_n(\tau') = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}\sin\nu_n\tau\sin\nu_n\tau' = \frac{2}{\hbar\beta}\sum_{n=1}^{\infty}\sin\nu_n\tau\sin\nu_n\tau'. \tag{3.51}$$

Here we see the necessity to introduce the δ function with two arguments, since the expression on the right-hand side is not invariant under time translations. Substituting the δ functions in expression

(3.45) by the completeness relation (3.51), it turns out that the boundary terms vanish. Thus we obtain the decomposition

$$G^{\mathrm{D}\,-1}_{xx,\omega}(\tau,\tau') = \frac{2}{\hbar\beta}\sum_{n=1}^{\infty}\frac{M}{\hbar}\left(\omega^2+\nu_n^2\right)\sin\nu_n\tau\sin\nu_n\tau'. \tag{3.52}$$

Inverting the kernel yields the Green function in Fourier space

$$G^{\mathrm{D}}_{xx,\omega}(\nu_n) = \frac{\hbar}{M}\frac{1}{\omega^2+\nu_n^2}. \tag{3.53}$$

After performing the Fourier back transformation, we obtain the Green function for the harmonic oscillator with fixed end points

$$G^{\mathrm{D}}_{xx,\omega}(\tau,\tau') = \frac{\hbar}{2M\omega\sinh\hbar\beta\omega}\left[\cosh\omega(|\tau-\tau'|-\hbar\beta)-\cosh\omega(\tau+\tau'-\hbar\beta)\right]. \tag{3.54}$$

The calculation of the two-point functions (3.38)–(3.40) is straightforward, since these can be derived from $G^{\mathrm{D}}_{xx,\omega}(\tau,\tau')$. Inserting (3.42) into (3.38) leads to

$$\begin{aligned} G^{\mathrm{D}}_{xp,\omega}(\tau,\tau') &= -\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\, G^{\mathrm{D}}_{xx,\omega}(\tau,\tau_1)\frac{i}{\hbar}\frac{\partial}{\partial\tau_1}\delta(\tau_1,\tau_2)\,\hbar M\delta(\tau_2,\tau') \\ &= -iM\int_0^{\hbar\beta}d\tau_1\, G^{\mathrm{D}}_{xx,\omega}(\tau,\tau_1)\frac{\partial}{\partial\tau_1}\delta(\tau_1,\tau') = iM\frac{\partial}{\partial\tau'}G^{\mathrm{D}}_{xx,\omega}(\tau,\tau'). \end{aligned} \tag{3.55}$$

In the last line we have carried out a partial integration, where the boundary term vanishes due to the Dirichlet boundary conditions (3.27). The derivative with respect to the second argument of the Green function (3.54) is easily performed and yields

$$\begin{aligned} G^{\mathrm{D}}_{xp,\omega}(\tau,\tau') &= -\frac{i\hbar}{2}\frac{1}{\sinh\hbar\beta\omega}\big[\Theta(\tau-\tau')\sinh\omega(\tau-\tau'-\hbar\beta)-\Theta(\tau'-\tau)\sinh\omega(\tau'-\tau-\hbar\beta) \\ &\quad +\sinh\omega(\tau+\tau'-\hbar\beta)\big]. \end{aligned} \tag{3.56}$$

As the explicit calculation of (3.39) shows, it is

$$G^{\mathrm{D}}_{px,\omega}(\tau,\tau') = iM\frac{\partial}{\partial\tau}G^{\mathrm{D}}_{xx,\omega}(\tau,\tau'). \tag{3.57}$$

The difference between (3.55) and (3.57) is that the derivative now acts on the first argument of the Green function $G^{\mathrm{D}}_{xx,\omega}(\tau,\tau')$. Thus, we obtain

$$\begin{aligned} G^{\mathrm{D}}_{px,\omega}(\tau,\tau') &= \frac{i\hbar}{2}\frac{1}{\sinh\hbar\beta\omega}\big[\Theta(\tau-\tau')\sinh\omega(\tau-\tau'-\hbar\beta)-\Theta(\tau'-\tau)\sinh\omega(\tau'-\tau-\hbar\beta) \\ &\quad -\sinh\omega(\tau+\tau'-\hbar\beta)\big] = G^{\mathrm{D}}_{xp,\omega}(\tau',\tau). \end{aligned} \tag{3.58}$$

Calculating (3.40) exposes no new aspects and yields

$$\begin{aligned} G^{\mathrm{D}}_{pp,\omega}(\tau,\tau') &= \hbar M\delta(\tau,\tau') - M^2\frac{\partial^2}{\partial\tau\partial\tau'}G^{\mathrm{D}}_{xx,\omega}(\tau,\tau') \\ &= \frac{M\hbar\omega}{2\sinh\hbar\beta\omega}\left[\cosh\omega(|\tau-\tau'|-\hbar\beta)+\cosh\omega(\tau+\tau'-\hbar\beta)\right]. \end{aligned} \tag{3.59}$$

The sole task remaining to be done to specify the density matrix functional (3.36) for the one-dimensional harmonic oscillator is the calculation of the determinants. Since we know that the prefactor $\sqrt{M/\hbar^2\beta}$ carries the complete physical dimension of the density matrix, it is useful, for evaluating the determinants, to return to dimensionless natural variables by setting $M=\hbar=\beta=1$. Determining the determinant of D_{pp} is quite simple and yields $\det D_{pp} = 1$. This is a simple consequence that D_{pp} is unity in Fourier space and an infinite product of unity yields again unity. The calculation of the other determinant is much more involved and shall be presented in detail in the following. With the Fourier representation (3.52) of $G^{\mathrm{D}\,-1}_{xx,\omega}$, the appropriate fluctuation factor of (3.36) can be written as

$$\left[\det G^{\mathrm{D}\,-1}_{xx,\omega}\right]^{-1/2} = \exp\left(-\frac{1}{2}\,\mathrm{Tr}\,\ln G^{\mathrm{D}\,-1}_{xx,\omega}\right) = \exp\left[-\frac{1}{2}\int_0^1 d\tau\, 2\sum_{n=1}^{\infty}\ln(\omega^2+\nu_n^2)\,\sin^2\nu_n\tau\right]. \quad (3.60)$$

The integration of the sine-squared over τ is easily done, $\int_0^1 d\tau\,\sin^2\nu_m\tau = 1/2$, and Eq. (3.60) becomes

$$\left[\det G^{\mathrm{D}\,-1}_{xx,\omega}\right]^{-1/2} = \exp\left\{-\frac{1}{2}\ln\prod_{n=1}^{\infty}\left[\omega^2+(\pi n)^2\right]\right\}. \quad (3.61)$$

Obviously, the product diverges, but this divergence is not physical. A lattice calculation would have proved the finiteness of the determinant [4, Chap. 2]. By regularizing the expression within the product with respect to the free-particle Green function, we obtain

$$\prod_{n=1}^{\infty}\left[\omega^2+(\pi n)^2\right] \quad\Longrightarrow\quad \prod_{n=1}^{\infty}\left[\frac{\omega^2+(\pi n)^2}{(\pi n)^2}\right] = \prod_{n=1}^{\infty}\left[1+\frac{\omega^2}{(\pi n)^2}\right] = \frac{1}{\omega}\sinh\omega. \quad (3.62)$$

Inserting this result into (3.61), we eventually find

$$\left[\det G^{\mathrm{D}\,-1}_{xx,\omega}\right]^{-1/2} = \sqrt{\frac{\hbar\beta\omega}{\sinh\hbar\beta\omega}}\;, \quad (3.63)$$

with physical units.

Thus we have calculated the density matrix of the one-dimensional harmonic oscillator in the presence of external sources, with the result [17]

$$\begin{aligned}\tilde{\varrho}_\omega(x_b,x_a)[j,v] = {} & \sqrt{\frac{M\omega}{2\pi\hbar\sinh\hbar\beta\omega}}\exp\left\{-\frac{M\omega}{2\hbar\sinh\hbar\beta\omega}\left[\left(x_a^2+x_b^2\right)\cosh\hbar\beta\omega-2x_ax_b\right]\right\}\\ & \times\exp\left\{-\frac{1}{\hbar\sinh\hbar\beta\omega}\int_0^{\hbar\beta}d\tau\left[j(\tau)+iMv(\tau)\frac{\partial}{\partial\tau}\right]\left[x_b\sinh\omega\tau+x_a\sinh\omega(\hbar\beta-\tau)\right]\right\}\\ & \times\exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\Big[j(\tau)G^{\mathrm{D}}_{xx,\omega}(\tau,\tau')j(\tau')+j(\tau)G^{\mathrm{D}}_{xp,\omega}(\tau,\tau')v(\tau')\right.\\ & \left.+v(\tau)G^{\mathrm{D}}_{px,\omega}(\tau,\tau')j(\tau')+v(\tau)G^{\mathrm{D}}_{pp,\omega}(\tau,\tau')v(\tau')\Big]\right\},\end{aligned} \quad (3.64)$$

where the two-point functions are given by (3.54), (3.56), (3.58), and (3.59). For $j(\tau) = v(\tau) = 0$, Eq. (3.64) reduces to the well-known expression for the density matrix of the one-dimensional harmonic oscillator.

3.2.3 Expectation Values and Correlation Functions

We usually define expectation values as

$$\langle\cdots\rangle^{\mathbf{x}_b,\mathbf{x}_a} = \tilde{\varrho}_0^{-1}(\mathbf{x}_b,\mathbf{x}_a)\int\mathcal{D}'^d x\mathcal{D}^d p\,\cdots\,e^{-\mathcal{A}_0[\mathbf{p},\mathbf{x}]/\hbar}, \quad (3.65)$$

with the action (3.1) but vanishing currents,

$$\mathcal{A}_0[\mathbf{p},\mathbf{x}] \equiv \mathcal{A}_0[\mathbf{p},\mathbf{x};0,0]. \quad (3.66)$$

The expectation values are normalized with respect to the density matrix (3.36) with vanishing currents,

$$\tilde{\varrho}_0(\mathbf{x}_b, \mathbf{x}_a) \equiv \tilde{\varrho}_0(\mathbf{x}_b, \mathbf{x}_a)[0, 0], \tag{3.67}$$

which ensures $\langle 1 \rangle^{\mathbf{x}_b, \mathbf{x}_a} = 1$. For the following consideration, however, it is useful to reintroduce the currents as artificial quantities. If the expectation value of a polynomial function consisting of powers of x and p shall be evaluated, one can apply functional derivatives with respect to these currents. Such derivatives act as follows:

$$\frac{\delta}{\delta z(\tau)} \int d\tau' \, f(z(\tau'), u(\tau')) = \int d\tau' \, \frac{\partial f(z(\tau'), u(\tau'))}{\partial z(\tau')} \delta(\tau - \tau') = \frac{\partial f(z(\tau), u(\tau))}{\partial z(\tau)}. \tag{3.68}$$

Applying, for example, to the action (3.1) a functional derivative with respect to $\mathbf{j}(\tau)$ yields:

$$\frac{\delta}{\delta \mathbf{j}^T(\tau)} \mathcal{A}_0[\mathbf{p}, \mathbf{x}; \mathbf{j}, \mathbf{v}] = \mathbf{x}(\tau). \tag{3.69}$$

Analogously, one obtains when differentiating with respect to $\mathbf{v}(\tau)$:

$$\frac{\delta}{\delta \mathbf{v}^T(\tau)} \mathcal{A}_0[\mathbf{p}, \mathbf{x}; \mathbf{j}, \mathbf{v}] = \mathbf{p}(\tau). \tag{3.70}$$

We can use this recovery of $\mathbf{x}$ and $\mathbf{p}$ to formulate a redefinition of expectation values for polynomial quantities, e.g.

$$\langle x_k^n(\tau) p_l^m(\tau') \rangle^{\mathbf{x}_b, \mathbf{x}_a} = \tilde{\varrho}_0^{-1}(\mathbf{x}_b, \mathbf{x}_a)(-\hbar)^{n+m} \prod_{i=1}^{n} \left[\frac{\delta}{\delta j_k(\tau)} \right] \prod_{i=1}^{m} \left[\frac{\delta}{\delta v_l(\tau')} \right] \tilde{\varrho}_0(\mathbf{x}_b, \mathbf{x}_a)[\mathbf{j}, \mathbf{v}] \Bigg|_{\mathbf{j}=\mathbf{v}=0}. \tag{3.71}$$

In the following, we specify some values for (n, m), where n denotes the overall power of x and m that of p, to obtain the lowest-order correlations. For $(1, 0)$, we obtain the expectation value of $\mathbf{x}(\tau)$ by applying to the density matrix functional (3.36) a single functional derivative with respect to $\mathbf{j}(\tau)$ and setting the currents to zero thereafter:

$$\langle \mathbf{x}(\tau) \rangle^{\mathbf{x}_b, \mathbf{x}_a} = -\hbar \tilde{\varrho}_0^{-1}(\mathbf{x}_b, \mathbf{x}_a) \frac{\delta}{\delta \mathbf{j}^T(\tau)} \tilde{\varrho}_0(\mathbf{x}_b, \mathbf{x}_a)[\mathbf{j}, \mathbf{v}] \Bigg|_{\mathbf{j}=\mathbf{v}=0} = \mathbf{x}_{\mathrm{cl}}(\tau). \tag{3.72}$$

Thus, the expectation value of $\mathbf{x}(\tau)$ is simply identical with the classical path. Evaluating the case $(0, 1)$, we obtain the expectation value of the momentum $\mathbf{p}(\tau)$:

$$\langle \mathbf{p}(\tau) \rangle^{\mathbf{x}_b, \mathbf{x}_a} = -\hbar \tilde{\varrho}_0^{-1}(\mathbf{x}_b, \mathbf{x}_a) \frac{\delta}{\delta \mathbf{v}^T(\tau)} \tilde{\varrho}_0(\mathbf{x}_b, \mathbf{x}_a)[\mathbf{j}, \mathbf{v}] \Bigg|_{\mathbf{j}=\mathbf{v}=0} = \mathbf{p}_{\mathrm{cl}}(\tau). \tag{3.73}$$

Calculating $(2, 0)$, $(0, 2)$, and $(1, 1)$ yields the two-point correlation functions

$$\begin{aligned}
\langle x_k(\tau) x_l(\tau') \rangle^{\mathbf{x}_b, \mathbf{x}_a} &= \hbar^2 \tilde{\varrho}_0^{-1}(\mathbf{x}_b, \mathbf{x}_a) \frac{\delta^2}{\delta j_k(\tau) \delta j_l(\tau')} \tilde{\varrho}_0(\mathbf{x}_b, \mathbf{x}_a)[\mathbf{j}, \mathbf{v}] \Bigg|_{\mathbf{j}=\mathbf{v}=0} \\
&= G^{\mathrm{D}}_{x_k x_l}(\tau, \tau') + x_{\mathrm{cl},k}(\tau) x_{\mathrm{cl},l}(\tau'), \qquad (3.74) \\
\langle p_k(\tau) p_l(\tau') \rangle^{\mathbf{x}_b, \mathbf{x}_a} &= \hbar^2 \tilde{\varrho}_0^{-1}(\mathbf{x}_b, \mathbf{x}_a) \frac{\delta^2}{\delta v_k(\tau) \delta v_l(\tau')} \tilde{\varrho}_0(\mathbf{x}_b, \mathbf{x}_a)[\mathbf{j}, \mathbf{v}] \Bigg|_{\mathbf{j}=\mathbf{v}=0} \\
&= G^{\mathrm{D}}_{p_k p_l}(\tau, \tau') + p_{\mathrm{cl},k}(\tau) p_{\mathrm{cl},l}(\tau'), \\
\langle x_k(\tau) p_l(\tau') \rangle^{\mathbf{x}_b, \mathbf{x}_a} &= \hbar^2 \tilde{\varrho}_0^{-1}(\mathbf{x}_b, \mathbf{x}_a) \frac{\delta^2}{\delta j_k(\tau) \delta v_l(\tau')} \tilde{\varrho}_0(\mathbf{x}_b, \mathbf{x}_a)[\mathbf{j}, \mathbf{v}] \Bigg|_{\mathbf{j}=\mathbf{v}=0} \\
&= G^{\mathrm{D}}_{x_k p_l}(\tau, \tau') + x_{\mathrm{cl},k}(\tau) p_{\mathrm{cl},l}(\tau'). \qquad (3.75)
\end{aligned}$$

From Eq. (3.39) follows that the latter expectation value can be used to identify

$$\begin{aligned}\langle p_k(\tau)x_l(\tau')\rangle^{\mathbf{x}_b,\mathbf{x}_a} &= \hbar^2\,\tilde\varrho_0^{-1}(\mathbf{x}_b,\mathbf{x}_a)\frac{\delta^2}{\delta v_k(\tau)\delta j_l(\tau')}\tilde\varrho_0(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}]\Bigg|_{\mathbf{j}=\mathbf{v}=0}\\ &= G^{\rm D}_{p_kx_l}(\tau,\tau')+p_{{\rm cl},k}(\tau)x_{{\rm cl},l}(\tau').\end{aligned}\tag{3.76}$$

Re-expressing the two-point functions with the help of Eqs. (3.72) and (3.73), we obtain

$$\begin{aligned}G^{\rm D}_{x_kx_l}(\tau,\tau') &= \langle\tilde x_k(\tau)\tilde x_l(\tau')\rangle^{\mathbf{x}_b,\mathbf{x}_a}\,, \quad G^{\rm D}_{p_kp_l}(\tau,\tau') = \langle\tilde p_k(\tau)\tilde p_l(\tau')\rangle^{\mathbf{x}_b,\mathbf{x}_a}\,,\\ G^{\rm D}_{x_kp_l}(\tau,\tau') &= \langle\tilde x_k(\tau)\tilde p_l(\tau')\rangle^{\mathbf{x}_b,\mathbf{x}_a}\,, \quad G^{\rm D}_{p_kx_l}(\tau,\tau') = \langle\tilde p_k(\tau)\tilde x_l(\tau')\rangle^{\mathbf{x}_b,\mathbf{x}_a}\,,\end{aligned}\tag{3.77}$$

with abbreviations

$$\tilde{\mathbf{x}}(\tau)=\mathbf{x}(\tau)-\mathbf{x}_{\rm cl}(\tau),\qquad \tilde{\mathbf{p}}(\tau)=\mathbf{p}(\tau)-\mathbf{p}_{\rm cl}(\tau).\tag{3.78}$$

Thus, we have identified the elements of the $d\times d$ matrices $G^{\rm D}_{\mathbf{xx}}(\tau,\tau')$, $G^{\rm D}_{\mathbf{xp}}(\tau,\tau')$, $G^{\rm D}_{\mathbf{px}}(\tau,\tau')$, and $G^{\rm D}_{\mathbf{pp}}(\tau,\tau')$, introduced in Eq. (3.36), with appropriate two-point correlation functions.

3.3 Smearing Formula for Density Matrices

In the previous sections we have investigated the exactly solvable density matrix for systems governed by a Gaussian action (3.1) with external sources. We will now use the results to set up a perturbative treatment of density matrices for systems with nontrivial interaction. In order to calculate the expectation values, which appear in the perturbation expansion, we derive the *smearing formula*, which is useful, in particular, for nonpolynomial potentials.

3.3.1 Perturbative Expansion for the Density Matrix of a System with Interaction

The exact calculation of the density matrix

$$\tilde\varrho(\mathbf{x}_b,\mathbf{x}_a)=\int\limits_{\mathbf{x}(0)=\mathbf{x}_a}^{\mathbf{x}(\hbar\beta)=\mathbf{x}_b}\mathcal{D}'^d x\mathcal{D}^d p\,e^{-\mathcal{A}[\mathbf{p},\mathbf{x}]/\hbar}\tag{3.79}$$

with an action which contains a potential,

$$\mathcal{A}[\mathbf{p},\mathbf{x}]=\mathcal{A}_0[\mathbf{p},\mathbf{x}]+\int_0^{\hbar\beta}d\tau\,V(\mathbf{p}(\tau),\mathbf{x}(\tau)),\tag{3.80}$$

is impossible for most systems. The potential $V(\mathbf{p}(\tau),\mathbf{x}(\tau))$ shall be as general as possible, and thus it may depend on momentum and position. The potential is considered as a perturbation of the exactly calculable system with the action (3.66). A Taylor expansion of the exponential in (3.79) with respect to V yields a perturbation expansion around the density matrix $\tilde\varrho_0(x_b,x_a)$ of the unperturbed system, defined in (3.67):

$$\begin{aligned}\tilde\varrho(\mathbf{x}_b,\mathbf{x}_a) &= \int\limits_{\mathbf{x}(0)=\mathbf{x}_a}^{\mathbf{x}(\hbar\beta)=\mathbf{x}_b}\mathcal{D}'^d x\mathcal{D}^d p\,e^{-\mathcal{A}_0[\mathbf{p},\mathbf{x}]/\hbar}\Bigg[1-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\,V(\mathbf{p}(\tau),\mathbf{x}(\tau))\\ &\quad+\frac{1}{2!\hbar^2}\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2 V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))V(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))-\ldots\Bigg].\end{aligned}\tag{3.81}$$

Using the definition (3.65) of the expectation values, the perturbation expansion can be written as

$$\tilde\varrho(\mathbf{x}_b,\mathbf{x}_a)=\tilde\varrho_0(\mathbf{x}_b,\mathbf{x}_a)\left[1+\sum_{n=1}^{\infty}\frac{(-1)^n}{n!\hbar^n}\int_0^{\hbar\beta}d\tau_1\cdots\int_0^{\hbar\beta}d\tau_n\,\langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\cdots V(\mathbf{p}(\tau_n),\mathbf{x}(\tau_n))\rangle^{\mathbf{x}_b,\mathbf{x}_a}\right].\tag{3.82}$$

The introduction of cumulants, where the first two are given by

$$\begin{aligned}\langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle_c^{\mathbf{x}_b,\mathbf{x}_a} &= \langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle^{\mathbf{x}_b,\mathbf{x}_a}\,,\\ \langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))V(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle_c^{\mathbf{x}_b,\mathbf{x}_a} &= \langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))V(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle^{\mathbf{x}_b,\mathbf{x}_a}\\ &\quad -\langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle^{\mathbf{x}_b,\mathbf{x}_a}\,\langle V(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle^{\mathbf{x}_b,\mathbf{x}_a}\,,\end{aligned}$$

enables us to re-express the right-hand side of Eq. (3.82) by

$$\tilde{\varrho}(\mathbf{x}_b,\mathbf{x}_a)=\left(\frac{M}{2\pi\hbar^2\beta}\right)^{d/2}\exp\left[-\beta V_{\mathrm{eff,cl}}(\mathbf{x}_b,\mathbf{x}_a)\right]. \tag{3.83}$$

Here, we have used that, written in the form of a classical particle density

$$\tilde{\varrho}_{\mathrm{cl}}(\mathbf{x})=\left(\frac{M}{2\pi\hbar^2\beta}\right)^{d/2}\exp\left[-\beta V(\mathbf{x})\right], \tag{3.84}$$

the quantum statistical density matrix is governed by the *effective classical potential*

$$\begin{aligned}V_{\mathrm{eff,cl}}(\mathbf{x}_b,\mathbf{x}_a) &= -\frac{1}{\beta}\ln\left[\lambda_{\mathrm{th}}^{d/2}\tilde{\varrho}_0(\mathbf{x}_b,\mathbf{x}_a)\right]-\frac{1}{\beta}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!\hbar^n}\int_0^{\hbar\beta}d\tau_1\cdots\int_0^{\hbar\beta}d\tau_n\\ &\quad\times\langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\cdots V(\mathbf{p}(\tau_n),\mathbf{x}(\tau_n))\rangle_c^{\mathbf{x}_b,\mathbf{x}_a}\,,\end{aligned} \tag{3.85}$$

with the thermal wavelength

$$\lambda_{\mathrm{th}}=\sqrt{\frac{2\pi\hbar^2\beta}{M}}. \tag{3.86}$$

The calculation of the density matrix for any system reduces to the calculation of the effective classical potential (3.85) and thus to an evaluation of the respective cumulants.

3.3.2 Smearing Formula for Gaussian Fluctuations

As a first application of the generating functional (3.36) we derive a general rule for calculating correlation functions of polynomial or nonpolynomial functions of $\mathbf{x}(\tau)$ and $\mathbf{p}(\tau)$ [17]. The result will be expressed in the form of a *smearing formula*. This formula will represent an essential tool for calculating perturbation expansions with nonpolynomial interactions.

Consider the correlation functions of a product of local functions

$$\begin{aligned}&\langle F_1(\mathbf{x}(\tau_1))F_2(\mathbf{x}(\tau_2))\ldots F_N(\mathbf{x}(\tau_N))F_{N+1}(\mathbf{p}(\tau_{N+1}))F_{N+2}(\mathbf{p}(\tau_{N+2}))\ldots F_{N+M}(\mathbf{x}(\tau_{N+M}))\rangle^{\mathbf{x}_b,\mathbf{x}_a}\\ &=\tilde{\varrho}_0^{-1}(\mathbf{x}_b,\mathbf{x}_a)\int\limits_{\mathbf{x}(0)=\mathbf{x}_a}^{\mathbf{x}(\hbar\beta)=\mathbf{x}_b}\mathcal{D}'^d x\,\mathcal{D}p^d\prod_{n=1}^{N}\left[F_n(\mathbf{x}(\tau_n))\right]\prod_{m=1}^{M}\left[F_{N+m}(\mathbf{p}(\tau_{N+m}))\right]e^{-\mathcal{A}_0[\mathbf{p},\mathbf{x}]/\hbar}.\end{aligned} \tag{3.87}$$

By Fourier transforming the functions $F_n(\mathbf{x}(\tau_n))$ and $F_{N+m}(\mathbf{p}(\tau_{N+m}))$ according to

$$F_n(\mathbf{x}(\tau_n))=\int d^dx_n\,F_n(\mathbf{x}_n)\delta(\mathbf{x}_n-\mathbf{x}(\tau_n))=\int d^dx_n\,F(\mathbf{x}_n)\int\frac{d^d\xi_n}{(2\pi)^d}\exp\left\{i\boldsymbol{\xi}_n(\mathbf{x}_n-\mathbf{x}(\tau_n))\right\} \tag{3.88}$$

and

$$\begin{aligned}F_{N+m}(\mathbf{p}(\tau_{N+m})) &= \int\frac{d^dp_m}{(2\pi\hbar)^d}F_{N+m}(\mathbf{p}_m)\delta(\mathbf{p}_m-\mathbf{p}(\tau_{N+m}))\\ &= \int\frac{d^dp_m}{(2\pi\hbar)^d}F_{N+m}(\mathbf{p}_m)\int d^d\kappa_m\,\exp\left\{-\frac{i}{\hbar}\boldsymbol{\kappa}_m(\mathbf{p}_m-\mathbf{p}(\tau_{N+m}))\right\},\end{aligned} \tag{3.89}$$

the correlation functions (3.87) may be re-expressed as

$$\langle F_1(\mathbf{x}(\tau_1))\dots F_{N+M}(\mathbf{p}(\tau_{N+M}))\rangle^{\mathbf{x}_b,\mathbf{x}_a} = \tilde{\varrho}_0^{-1}(\mathbf{x}_b,\mathbf{x}_a)\prod_{n=1}^{N}\left[\int d^d x_n\, F_n(\mathbf{x}_n)\int\frac{d^d\xi_n}{(2\pi)^d}\,\exp\left(i\boldsymbol{\xi}_n\mathbf{x}_n\right)\right]$$
$$\times\prod_{m=1}^{M}\left[\int\frac{d^d p_m}{(2\pi\hbar)^d}\,F_{N+m}(\mathbf{p}_m)\int d^d\kappa_m\exp\left(-\frac{i}{\hbar}\boldsymbol{\kappa}_m\mathbf{p}_m\right)\right]\,\tilde{\varrho}_0(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}], \tag{3.90}$$

where the generating functional is given by (3.36). The currents $\mathbf{j}(\tau)$ and $\mathbf{v}(\tau)$ are specialized to

$$\mathbf{j}(\tau) = i\hbar\sum_{n=1}^{N}\boldsymbol{\xi}_n\delta(\tau-\tau_n), \qquad \mathbf{v}(\tau) = -i\sum_{m=1}^{M}\boldsymbol{\kappa}_m\delta(\tau-\tau_{N+m}). \tag{3.91}$$

Inserting these equations into the action of the functional (3.36) and the Green functions (3.26) and (3.38)–(3.40), we find the Fourier decomposition of the generating functional (3.36), so that the correlation functions (3.90) become

$$\langle F_1(\mathbf{x}(\tau_1))\dots F_{N+M}(\mathbf{p}(\tau_{N+M}))\rangle^{\mathbf{x}_b,\mathbf{x}_a} = \prod_{n=1}^{N}\left[\int d^d x_n\, F_n(\mathbf{x}_n)\int\frac{d^d\xi_n}{(2\pi)^d}\,\exp\left\{i\boldsymbol{\xi}_n[\mathbf{x}_n-\mathbf{x}_{\rm cl}(\tau_n)]\right\}\right]$$
$$\times\prod_{m=1}^{M}\left[\int\frac{d^d p_m}{(2\pi\hbar)^d}\,F_{N+m}(\mathbf{p}_m)\int d^d\kappa_m\exp\left\{-\frac{i}{\hbar}\boldsymbol{\kappa}_m[\mathbf{p}_m-\mathbf{p}_{\rm cl}(\tau_{N+m})]\right\}\right]$$
$$\times\exp\left\{-\frac{1}{2}\sum_{n,n'=1}^{N}\boldsymbol{\xi}_n G_{\mathbf{xx}}^{nn'}\boldsymbol{\xi}_{n'}+\frac{1}{\hbar}\sum_{n=1}^{N}\sum_{m=1}^{M}\boldsymbol{\xi}_n G_{\mathbf{xp}}^{nm}\boldsymbol{\kappa}_m-\frac{1}{2\hbar^2}\sum_{m,m'=1}^{M}\boldsymbol{\kappa}_m G_{\mathbf{pp}}^{mm'}\boldsymbol{\kappa}_{m'}\right\}, \tag{3.92}$$

where we used the abbreviations

$$G_{\mathbf{xx}}^{nn'} = G_{\mathbf{xx}}^{\rm D}(\tau_n,\tau_{n'}), \quad G_{\mathbf{xp}}^{nm} = G_{\mathbf{xp}}^{\rm D}(\tau_n,\tau_{N+m}), \quad G_{\mathbf{pp}}^{mm'} = G_{\mathbf{pp}}^{\rm D}(\tau_{N+m},\tau_{N+m'}). \tag{3.93}$$

To proceed, it is more convenient to write expression (3.92) as a convolution integral

$$\langle F_1(\mathbf{x}(\tau_1))\dots F_{N+M}(\mathbf{p}(\tau_{N+M}))\rangle^{\mathbf{x}_b,\mathbf{x}_a} = \prod_{n=1}^{N}\left[\int d^d x_n\, F_n(\mathbf{x}_n)\right]\prod_{m=1}^{M}\left[\frac{d^d p_m}{(2\pi\hbar)^d}\,F_{N+m}(\mathbf{p}_m)\right]$$
$$\times\hbar^{Md}\,P(\mathbf{x}_1,\dots,\mathbf{x}_N,\mathbf{p}_1,\dots,\mathbf{p}_M) \tag{3.94}$$

involving the Gaussian distribution

$$P(\mathbf{x}_1,\dots,\mathbf{p}_M) \equiv \frac{1}{(2\pi)^N}\int d^{N+M}w_1\,\exp\left\{i\mathbf{w}_1^T\mathbf{w}_2-\frac{1}{2}\mathbf{w}_1^T\,G\,\mathbf{w}_1\right\}. \tag{3.95}$$

The vectors $\mathbf{w}_1$ and $\mathbf{w}_2$ have $(N+M)d$ components and are defined as

$$\mathbf{w}_1^T = \left(\boldsymbol{\xi}_1,\dots,\boldsymbol{\xi}_N,\frac{1}{\hbar}\boldsymbol{\kappa}_1,\dots,\frac{1}{\hbar}\boldsymbol{\kappa}_M\right) \tag{3.96}$$

and

$$\mathbf{w}_2^T = \left(\mathbf{x}_1-\mathbf{x}_{\rm cl}(\tau_1),\dots,\mathbf{x}_N-\mathbf{x}_{\rm cl}(\tau_N),-\mathbf{p}_1+\mathbf{p}_{\rm cl}(\tau_{N+1}),\dots,-\mathbf{p}_M+\mathbf{p}_{\rm cl}(\tau_{N+M})\right). \tag{3.97}$$

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

$$G = \begin{pmatrix} A & B \\ B^T & C\end{pmatrix} \tag{3.98}$$

can be decomposed into block matrices A, B, and C. The $Nd\times Nd$-matrix A and the $Md\times Md$-matrix C are defined by

$$A = \begin{pmatrix} G_{\mathbf{xx}}^{11} & G_{\mathbf{xx}}^{12} & \cdots & G_{\mathbf{xx}}^{1N} \\ G_{\mathbf{xx}}^{12} & G_{\mathbf{xx}}^{11} & \cdots & G_{\mathbf{xx}}^{2N} \\ \vdots & \vdots & \ddots & \vdots \\ G_{\mathbf{xx}}^{1N} & G_{\mathbf{xx}}^{2N} & \cdots & G_{\mathbf{xx}}^{11} \end{pmatrix}, \quad C = \begin{pmatrix} G_{\mathbf{pp}}^{11} & G_{\mathbf{pp}}^{12} & \cdots & G_{\mathbf{pp}}^{1M} \\ G_{\mathbf{pp}}^{12} & G_{\mathbf{pp}}^{11} & \cdots & G_{\mathbf{pp}}^{2M} \\ \vdots & \vdots & \ddots & \vdots \\ G_{\mathbf{pp}}^{1M} & G_{\mathbf{pp}}^{2M} & \cdots & G_{\mathbf{pp}}^{11} \end{pmatrix} \tag{3.99}$$

and yield quadratic forms of the position and momentum variables, respectively. The $Nd\times Md$-matrix

$$B = \begin{pmatrix} -G_{\mathbf{xp}}^{11} & -G_{\mathbf{xp}}^{12} & \cdots & -G_{\mathbf{xp}}^{1M} \\ -G_{\mathbf{xp}}^{21} & -G_{\mathbf{xp}}^{11} & \cdots & -G_{\mathbf{xp}}^{2M} \\ \vdots & \vdots & \vdots & \vdots \\ -G_{\mathbf{xp}}^{N1} & -G_{\mathbf{xp}}^{N2} & \cdots & -G_{\mathbf{xp}}^{NM} \end{pmatrix} \tag{3.100}$$

gives rise to quadratic terms, which are linear in both position and momentum variables. The multidimensional integral in (3.95) is of Gaussian type and can easily be done, yielding an explicit expression for the Gaussian distribution (3.95)

$$P(\mathbf{x}_1, \ldots \mathbf{x}_N, \mathbf{p}_1, \ldots, \mathbf{p}_M) = \frac{1}{\sqrt{(2\pi)^{(N-M)d} \det G}} \exp\left\{-\frac{1}{2}\mathbf{w}_2^T\, G^{-1}\, \mathbf{w}_2\right\}, \tag{3.101}$$

where G^{-1} represents the matrix inverse of (3.98) whose block form is [see Appendix 3A for a direct derivation]

$$G^{-1} = \begin{pmatrix} X^{-1} & -X^{-1}BC^{-1} \\ -C^{-1}B^T X^{-1} & C^{-1} + C^{-1}B^T X^{-1}BC^{-1} \end{pmatrix} \tag{3.102}$$

with the abbreviation

$$X = A - BC^{-1}B^T. \tag{3.103}$$

The calculation of the determinant is presented in Appendix 3A and yields

$$\det G = \det C\, \det X, \tag{3.104}$$

when the matrix C is regular. For singular matrix C but A regular, we obtain

$$\det G = \det \tilde{X}\, \det A, \tag{3.105}$$

with $\tilde{X} = C - B^T A^{-1} B$.

With the Gaussian distribution (3.101), our result (3.94) constitutes a *smearing formula*, which describes the effect of harmonic fluctuations upon arbitrary products of functions of space and momentum variables at different times.

3.4 Generalized Wick Rules and Feynman Diagrams

In applications, there often occur correlation functions for mixtures of nonpolynomial functions $F(\tilde{x}_k)$ or $F(\tilde{p}_k)$ and powers according to

$$\begin{aligned} &\langle F(\tilde{x}_k(\tau_1))\, \tilde{x}_l^n(\tau_2)\rangle^{\mathbf{x}_b,\mathbf{x}_a}, \qquad \langle F(\tilde{x}_k(\tau_1))\, \tilde{p}_l^n(\tau_2)\rangle^{\mathbf{x}_b,\mathbf{x}_a}, \\ &\langle F(\tilde{p}_k(\tau_1))\, \tilde{x}_l^n(\tau_2)\rangle^{\mathbf{x}_b,\mathbf{x}_a}, \qquad \langle F(\tilde{p}_k(\tau_1))\, \tilde{p}_l^n(\tau_2)\rangle^{\mathbf{x}_b,\mathbf{x}_a}, \end{aligned} \tag{3.106}$$

where we consider functions of the shifted phase space coordinates (3.78). In order to evaluate such correlation functions, we derive in this section generalized Wick rules and Feynman diagrams on the basis of the smearing formula (3.94). For simplicity, we restrict ourselves to the calculation in one dimension, since it already involves the interesting features, which we want to discuss in the following.

3.4.1 Ordinary Wick Rules

It is well known that if one has to calculate expectation values of polynomials with even power, Wick's rule can be written as the sum over all possible permutations of products of two-point functions. We shortly recall to this expansion by considering the case of a position-dependent n-point correlation function in one dimension, n even, defined as

$$G^{(n)}(\tau_1, \dots, \tau_n) = \langle \tilde{x}(\tau_1) \cdots \tilde{x}(\tau_n) \rangle^{x_b, x_a} . \tag{3.107}$$

Note that it will be sufficient to study only the correlation functions involving the deviations from the classical path, respectively. This expectation value can be decomposed with the help of Wick's expansion

$$G^{(n)}(\tau_1, \dots, \tau_n) = \sum_{\text{pairs}} G^{(2)}(\tau_{P(1)}, \tau_{P(2)}) \cdots G^{(2)}(\tau_{P(n-1)}, \tau_{P(n)}), \tag{3.108}$$

where P denotes the operation of pairwise index permutation. Note that Eq. (3.108) may be considered as a consequence of a simple derivative rule

$$\langle F(\tilde{x}(\tau_1))\, \tilde{x}(\tau_2) \rangle^{x_b, x_a} = \langle \tilde{x}(\tau_1)\, \tilde{x}(\tau_2) \rangle^{x_b, x_a} \langle F'(\tilde{x}(\tau_1)) \rangle^{x_b, x_a} \tag{3.109}$$

with $F'(\tilde{x}) = \partial F(\tilde{x})/\partial x$. By applying this recursively, one eventually obtains (3.108). And conversely, the derivative rule (3.109) can be proved for *polynomial* functions $F(\tilde{x}(\tau))$, following directly from Wick's theorem (3.108).

The two-point Green function $G^{(2)}(\tau_1, \tau_2)$, occurring in (3.108), can be considered as a Wick contraction, which we introduce as follows:

$$\underbrace{\tilde{x}(\tau_1)\, \tilde{x}(\tau_2)} = \langle \tilde{x}(\tau_1)\, \tilde{x}(\tau_2) \rangle^{x_b, x_a} = G^{\mathrm{D}}_{xx}(\tau_1, \tau_2), \tag{3.110}$$

$$\underbrace{\tilde{x}(\tau_1)\, \tilde{p}(\tau_2)} = \langle \tilde{x}(\tau_1)\, \tilde{p}(\tau_2) \rangle^{x_b, x_a} = G^{\mathrm{D}}_{xp}(\tau_1, \tau_2), \tag{3.111}$$

$$\underbrace{\tilde{p}(\tau_1)\, \tilde{x}(\tau_2)} = \langle \tilde{p}(\tau_1)\, \tilde{x}(\tau_2) \rangle^{x_b, x_a} = G^{\mathrm{D}}_{px}(\tau_1, \tau_2) = G^{\mathrm{D}}_{xp}(\tau_2, \tau_1), \tag{3.112}$$

$$\underbrace{\tilde{p}(\tau_1)\, \tilde{p}(\tau_2)} = \langle \tilde{p}(\tau_1)\, \tilde{p}(\tau_2) \rangle^{x_b, x_a} = G^{\mathrm{D}}_{pp}(\tau_1, \tau_2). \tag{3.113}$$

Decomposing polynomial correlations of $\tilde{x}(\tau)$ and $\tilde{p}(\tau)$ with the help of these contractions corresponding to Eq. (3.108) or successively applying the derivative rule (3.109) leads to following results

$$\langle \tilde{x}^n(\tau_1)\, \tilde{x}^m(\tau_2) \rangle^{x_b, x_a} = \sum_{\substack{l=\alpha, \alpha+2, \\ \alpha+4, \dots}}^{\min(n,m)} c_l \left[G^{\mathrm{D}}_{xx}(\tau_1, \tau_1)\right]^{(n-l)/2} \left[G^{\mathrm{D}}_{xx}(\tau_1, \tau_2)\right]^{l} \left[G^{\mathrm{D}}_{xx}(\tau_2, \tau_2)\right]^{(m-l)/2}, \tag{3.114}$$

$$\langle \tilde{x}^n(\tau_1)\, \tilde{p}^m(\tau_2) \rangle^{x_b, x_a} = \sum_{\substack{l=\alpha, \alpha+2, \\ \alpha+4, \dots}}^{\min(n,m)} c_l \left[G^{\mathrm{D}}_{xx}(\tau_1, \tau_1)\right]^{(n-l)/2} [G^{\mathrm{D}}_{xp}(\tau_1, \tau_2)]^{l} \left[G^{\mathrm{D}}_{pp}(\tau_2, \tau_2)\right]^{(m-l)/2}, \tag{3.115}$$

$$\langle \tilde{p}^n(\tau_1)\, \tilde{x}^m(\tau_2) \rangle^{x_b, x_a} = \sum_{\substack{l=\alpha, \alpha+2, \\ \alpha+4, \dots}}^{\min(n,m)} c_l \left[G^{\mathrm{D}}_{pp}(\tau_1, \tau_1)\right]^{(n-l)/2} [G^{\mathrm{D}}_{xp}(\tau_2, \tau_1)]^{l} \left[G^{\mathrm{D}}_{xx}(\tau_2, \tau_2)\right]^{(m-l)/2}, \tag{3.116}$$

$$\langle \tilde{p}^n(\tau_1)\, \tilde{p}^m(\tau_2) \rangle^{x_b, x_a} = \sum_{\substack{l=\alpha, \alpha+2, \\ \alpha+4, \dots}}^{\min(n,m)} c_l \left[G^{\mathrm{D}}_{pp}(\tau_1, \tau_1)\right]^{(n-l)/2} \left[G^{\mathrm{D}}_{pp}(\tau_1, \tau_2)\right]^{l} \left[G^{\mathrm{D}}_{pp}(\tau_2, \tau_2)\right]^{(m-l)/2}, \tag{3.117}$$

with the multiplicity factor

$$c_l = \frac{(n-l-1)!!\, (m-l-1)!!\, n!\, m!}{l!\, (n-l)!\, (m-l)!} . \tag{3.118}$$

Note, that $(-k)!! \equiv 1$ for any positive integer k. For nonvanishing correlation, the sum $n+m$ must be even so that the regulation parameter α is defined as follows:

$$\alpha = \begin{cases} 0, & n, m \text{ even}, \\ 1, & n, m \text{ odd}. \end{cases} \tag{3.119}$$

The contractions defined in (3.110)–(3.113) can be used to treat Taylor-expandable functions $F(\tilde{x}(\tau))$ and $F(\tilde{p}(\tau))$ only. The desired derivative rules for such correlations read

$$\langle F(\tilde{x}(\tau_1))\, \tilde{x}^n(\tau_2)\rangle^{x_b,x_a} = \sum_{l=\alpha,\alpha+2,\alpha+4,\ldots}^{n} \frac{n!}{(n-l)!!\, l!} \left[G^{\mathrm{D}}_{xx}(\tau_2,\tau_2)\right]^{(n-l)/2} \left[G^{\mathrm{D}}_{xx}(\tau_1,\tau_2)\right]^{l} \left\langle F^{(l)}(\tilde{x}(\tau_1))\right\rangle^{x_b,x_a}, \tag{3.120}$$

$$\langle F(\tilde{x}(\tau_1))\, \tilde{p}^n(\tau_2)\rangle^{x_b,x_a} = \sum_{l=\alpha,\alpha+2,\alpha+4,\ldots}^{n} \frac{n!}{(n-l)!!\, l!} [G^{\mathrm{D}}_{pp}(\tau_2,\tau_2)]^{(n-l)/2}\; [G^{\mathrm{D}}_{xp}(\tau_1,\tau_2)]^{l} \left\langle F^{(l)}(\tilde{x}(\tau_1))\right\rangle^{x_b,x_a}, \tag{3.121}$$

$$\langle F(\tilde{p}(\tau_1))\, \tilde{p}^n(\tau_2)\rangle^{x_b,x_a} = \sum_{l=\alpha,\alpha+2,\alpha+4,\ldots}^{n} \frac{n!}{(n-l)!!\, l!} [G^{\mathrm{D}}_{pp}(\tau_2,\tau_2)]^{(n-l)/2} [G^{\mathrm{D}}_{pp}(\tau_1,\tau_2)]^{l} \left\langle F^{(l)}(\tilde{p}(\tau_1))\right\rangle^{x_b,x_a}, \tag{3.122}$$

$$\langle F(\tilde{p}(\tau_1))\, \tilde{x}^n(\tau_2)\rangle^{x_b,x_a} = \sum_{l=\alpha,\alpha+2,\alpha+4,\ldots}^{n} \frac{n!}{(n-l)!!\, l!} \left[G^{\mathrm{D}}_{xx}(\tau_2,\tau_2)\right]^{(n-l)/2} [G^{\mathrm{D}}_{xp}(\tau_2,\tau_1)]^{l} \left\langle F^{(l)}(\tilde{p}(\tau_1))\right\rangle^{x_b,x_a}. \tag{3.123}$$

The parameter α distinguishes between even and odd power n:

$$\alpha = \begin{cases} 0, & n \text{ even}, \\ 1, & n \text{ odd}, \end{cases} \tag{3.124}$$

since even (odd) powers of n lead to even (odd) derivatives of the function $F(\tilde{x}(\tau_1))$. The lth derivative $F^{(l)}(\tilde{x}(\tau_1))$ is formed with respect to $x(\tau_1)$, and $F^{(l)}(\tilde{p}(\tau_1))$ is the lth derivative with respect to $p(\tau_1)$. Note, that in (3.123) the Green function G^{D}_{xp} appears with exchanged time arguments, which in this case happens to be inessential due to the symmetry $G^{\mathrm{D}}_{xp}(\tau_2,\tau_1) = G^{\mathrm{D}}_{px}(\tau_1,\tau_2)$.

3.4.2 Generalized Wick Rule

According to their derivation, the contractions (3.120)–(3.123) are only applicable to functions $F(\tilde{x}(\tau))$ and $F(\tilde{p}(\tau))$ which can be Taylor-expanded. In the following, we will show with the help of the smearing formula (3.94) that these derivative rules remain valid for functions $F(\tilde{x}(\tau))$ and $F(\tilde{p}(\tau))$ with Laurent expansions. Expectations of this type appear in variational perturbation theory (see Ref. [20] for position-position coupling). Since the proceeding is similar in all the cases (3.120)–(3.123), we shall only discuss the expectation value

$$\langle F(\tilde{x}(\tau_1))\, \tilde{p}^n(\tau_2)\rangle^{x_b,x_a} \tag{3.125}$$

in detail. For this we consider the generating functional of all such expectation values following from (3.94)

$$\left\langle F(\tilde{x}(\tau_1))\, e^{j\tilde{p}(\tau_2)}\right\rangle^{x_b,x_a} = \frac{\hbar}{\sqrt{\det G}} \int_{-\infty}^{+\infty} dx\, F(x) \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar}\, e^{jp} \times \exp\left\{-\frac{1}{2\det G}\left[G^{\mathrm{D}}_{pp}(\tau_2,\tau_2)\, x^2 - 2G^{\mathrm{D}}_{xp}(\tau_1,\tau_2)\, xp + G^{\mathrm{D}}_{xx}(\tau_1,\tau_1)\, p^2\right]\right\}. \tag{3.126}$$

The p-integration can easily be done, leading to

$$
\begin{aligned}
\left\langle F(\tilde{x}(\tau_1))\, e^{j\tilde{p}^n(\tau_2)} \right\rangle^{x_b,x_a} &= e^{G^{\rm D}_{pp}(t_2,t_2)j^2/2} \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{2\pi G^{\rm D}_{xx}(t_1,t_1)}}\, F(x + j\, G^{\rm D}_{xp}(t_1,t_2))\, e^{-x^2/2G^{\rm D}_{xx}(t_1,t_1)} \\
&= e^{G^{\rm D}_{pp}(t_2,t_2)j^2/2} \sum_{l=0}^{\infty} \frac{1}{l!} \left[j\, G^{\rm D}_{xp}(t_1,t_2)\right]^l \left\langle F^{(l)}(\tilde{x}(t_1)) \right\rangle^{x_b,x_a} .
\end{aligned}
\tag{3.127}
$$

The correlation of two functions at different times has been reduced to a single-time expectation value of the lth derivative of the function $F(\tilde{x}(\tau_1))$ with respect to $x(\tau_1)$, denoted by $F^{(l)}(\tilde{x}(\tau_1))$, with Green functions describing the dependence on the second time. Expanding both sides in powers of j, we re-obtain (3.121).

Now we demonstrate that the derivative rules (3.120)–(3.123) for Laurent-expandable functions $F(\tilde{x}(\tau))$ and $F(\tilde{p}(\tau))$ also follow from generalized Wick rules. Without restriction of universality, we only consider the expectation value

$$
\langle F(\tilde{x}(\tau_1))\, \tilde{x}^n(\tau_2) \rangle^{x_b,x_a} . \tag{3.128}
$$

The proceeding to reduce the power of the polynomial at the expense of the function $F(\tilde{x}(\tau_1))$ is as follows:

1a. If possible ($n \geq 2$), contract $\tilde{x}(\tau_2)\,\tilde{x}(\tau_2)$ with multiplicity $(n-1)$, giving

$$
(n-1)\, \underbrace{\tilde{x}(\tau_2)\, \tilde{x}(\tau_2)}\, \left\langle F(\tilde{x}(\tau_1))\, \tilde{x}^{n-2}(\tau_2) \right\rangle^{x_b,x_a} , \tag{3.129}
$$

else jump to 1b. directly.

1b. Contract $F(\tilde{x}(\tau_1))\,\tilde{x}(\tau_2)$ and let the remaining polynomial invariant. We define this contraction by the symbol

$$
\underbrace{F(\tilde{x}(\tau_1))\, \tilde{x}(\tau_2)}\, \tilde{x}^{n-1}(\tau_2) = \underbrace{\tilde{x}(\tau_1)\, \tilde{x}(\tau_2)}\, \left\langle F'(\tilde{x}(\tau_1))\, \tilde{x}^{n-1}(\tau_2) \right\rangle^{x_b,x_a} . \tag{3.130}
$$

1c. Add the terms 1a. and 1b.

2. Repeat steps 1a.-1c. until only expectation values of $F(\tilde{x})$ or expectations of its derivatives remain.

Summarizing, we can express the first power reduction by the generalized Wick rule ($n \geq 2$)

$$
\begin{aligned}
\langle F(\tilde{x}(\tau_1))\, \tilde{x}^n(\tau_2) \rangle^{x_b,x_a} &= (n-1)\, \underbrace{\tilde{x}(\tau_2)\, \tilde{x}(\tau_2)}\, \left\langle F(\tilde{x}(\tau_1))\, \tilde{x}^{n-2}(\tau_2) \right\rangle^{x_b,x_a} \\
&\quad + \underbrace{F(\tilde{x}(\tau_1))\, \tilde{x}(\tau_2)}\, \tilde{x}^{n-1}(\tau_2)
\end{aligned}
\tag{3.131}
$$

with the contraction rules defined in (3.110) and (3.130). For $n = 1$, we obtain

$$
\langle F(\tilde{x}(\tau_1))\, \tilde{x}(\tau_2) \rangle^{x_b,x_a} = \underbrace{\tilde{x}(\tau_1)\, \tilde{x}(\tau_2)}\, \langle F'(x(\tau_1)) \rangle^{x_b,x_a} , \tag{3.132}
$$

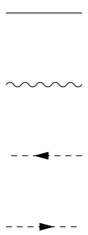
which is valid for *any* function $F(\tilde{x}(\tau))$ generalizing the rule (3.109) that was proved for polynomial functions only. Recursively applying this power reduction, we finally end up with the derivative rule (3.120). Note that the generalization of Wick's rule for mixed position-momentum or pure momentum couplings is done along similar lines, leading to the derivative rules (3.121)–(3.123).

3.4.3 New Feynman-Like Rules for Nonpolynomial Interactions

Higher-order perturbation expressions become usually complicated. For simple polynomial interactions, Feynman diagrams are a useful tool to classify perturbative contributions with the help of graphical rules. Here, we are going to set up analogous diagrammatic rules for perturbation expansions for nonpolynomial interactions $V(x(\tau), p(\tau))$, whose contributions may be expressed as expectations values

$$
\int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n \, \langle V(x(\tau_1), p(\tau_1)) \cdots V(x(\tau_n), p(\tau_n)) \rangle^{x_b,x_a} . \tag{3.133}
$$

From (3.110)–(3.113) follows that we have four basic propagators whose graphical representation may be defined as (setting $\hbar = M = \beta = 1$ from now on)



$$\tau_1 \;—\; \tau_2 \quad \equiv \langle \tilde{x}(\tau_1)\, \tilde{x}(\tau_2) \rangle^{x_b,x_a} = G^{\rm D}_{xx}(\tau_1,\tau_2),$$

$$\tau_1 \;\sim\; \tau_2 \quad \equiv \langle \tilde{p}(\tau_1)\, \tilde{p}(\tau_2) \rangle^{x_b,x_a} = G^{\rm D}_{pp}(\tau_1,\tau_2),$$

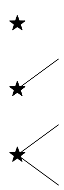
$$\tau_1 \;\text{-- -◄- --}\; \tau_2 \quad \equiv \langle \tilde{x}(\tau_1)\, \tilde{p}(\tau_2) \rangle^{x_b,x_a} = G^{\rm D}_{xp}(\tau_1,\tau_2),$$

$$\tau_1 \;\text{-- -►- --}\; \tau_2 \quad \equiv \langle \tilde{p}(\tau_1)\, \tilde{x}(\tau_2) \rangle^{x_b,x_a} = G^{\rm D}_{px}(\tau_1,\tau_2) = G^{\rm D}_{xp}(\tau_2,\tau_1).$$

A vertex is represented as usual by a small dot. The time variable is integrated over at a vertex in a perturbation expansion,

$$\bullet \quad \equiv \int_0^1 d\tau .$$

We now introduce the diagrammatic representations of the expectation value of arbitrary functions $F(\tilde{x}(\tau))$ or $F(\tilde{p}(\tau))$ and their derivatives as

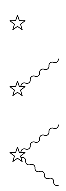


$$\equiv \int_0^1 d\tau\, \langle F(\tilde{x}(\tau)) \rangle^{x_b,x_a}, \qquad \equiv \int_0^1 d\tau\, \langle F(\tilde{p}(\tau)) \rangle^{x_b,x_a},$$

$$\equiv \int_0^1 d\tau\, \langle F'(\tilde{x}(\tau)) \rangle^{x_b,x_a}, \qquad \equiv \int_0^1 d\tau\, \langle F'(\tilde{p}(\tau)) \rangle^{x_b,x_a},$$

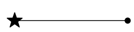
$$\equiv \int_0^1 d\tau\, \langle F''(\tilde{x}(\tau)) \rangle^{x_b,x_a}, \qquad \equiv \int_0^1 d\tau\, \langle F''(\tilde{p}(\tau)) \rangle^{x_b,x_a},$$

$$\vdots \qquad\qquad\qquad \vdots \quad .$$

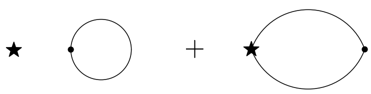


With these elements, we can compose Feynman graphs for two-point correlation functions of the type (3.106) for arbitrary n by successively applying the generalized Wick rule (3.131) or directly using the derivative relations (3.120)–(3.123). The general results become obvious by giving explicitly a graphical representation of the following four correlation functions

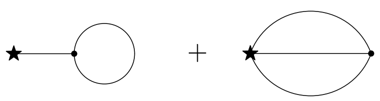
$$\int_0^1 d\tau_1 \int_0^1 d\tau_2\, \langle F(\tilde{x}(\tau_1))\, \tilde{x}(\tau_2) \rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2\, G^{\rm D}_{xx}(\tau_1,\tau_2)\, \langle F'(\tilde{x}(\tau_1)) \rangle^{x_b,x_a} \tag{3.134}$$

$\equiv$  ,

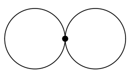
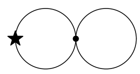
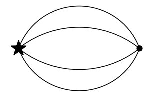
$$\int_0^1 d\tau_1 \int_0^1 d\tau_2\, \left\langle F(\tilde{x}(\tau_1))\, \tilde{x}^2(\tau_2) \right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \Big\{ G^{\rm D}_{xx}(\tau_2,\tau_2)\, \langle F(\tilde{x}(\tau_1)) \rangle^{x_b,x_a} + \left[G^{\rm D}_{xx}(\tau_1,\tau_2)\right]^2 \langle F''(\tilde{x}(\tau_1)) \rangle^{x_b,x_a} \Big\} \tag{3.135}$$

$\equiv$  ,

$$\int_0^1 d\tau_1 \int_0^1 d\tau_2\, \left\langle F(\tilde{x}(\tau_1))\, \tilde{x}^3(\tau_2) \right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \Big\{ 3\, G^{\rm D}_{xx}(\tau_1,\tau_2)\, G^{\rm D}_{xx}(\tau_2,\tau_2)\, \langle F'(\tilde{x}(\tau_1)) \rangle^{x_b,x_a} + \left[G^{\rm D}_{xx}(\tau_1,\tau_2)\right]^3 \langle F'''(\tilde{x}(\tau_1)) \rangle^{x_b,x_a} \Big\} \tag{3.136}$$

$\equiv 3$  ,

$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{x}(\tau_1))\, \tilde{x}^4(\tau_2)\right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \Big\{ \left[G^{\mathrm{D}}_{xx}(\tau_2,\tau_2)\right]^2 \left\langle F(\tilde{x}(\tau_1))\right\rangle^{x_b,x_a} + 6\left[G^{\mathrm{D}}_{xx}(\tau_1,\tau_2)\right]^2 G^{\mathrm{D}}_{xx}(\tau_2,\tau_2) \left\langle F''(\tilde{x}(\tau_1))\right\rangle^{x_b,x_a} + \left[G^{\mathrm{D}}_{xx}(\tau_1,\tau_2)\right]^4 \left\langle F^{(4)}(\tilde{x}(\tau_1))\right\rangle^{x_b,x_a} \Big\} \tag{3.137}$$

$\equiv \star$  $+\,6$  $+$  .

Mixed position-momentum and momentum-momentum correlations and their graphical representations are given in Appendix 3B.

The consideration of higher-order correlations with more than one function $F(\tilde{x}(\tau))$ or $F(\tilde{p}(\tau))$ can be reduced to the results (3.114)–(3.117) or (3.120)–(3.123) by expanding them with respect to the classical path or momentum, respectively. By expanding both functions in the expectation value, one obtains for example

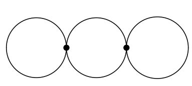
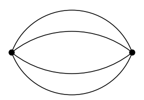
$$\left\langle F_1(\tilde{x}(\tau_1))\, F_2(\tilde{x}(\tau_2))\right\rangle^{x_b,x_a} = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{1}{m!\,n!}\, f_{1,m} f_{2,n} \left\langle \tilde{x}^m(\tau_1)\, \tilde{x}^n(\tau_2)\right\rangle^{x_b,x_a} \tag{3.138}$$

with

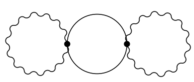
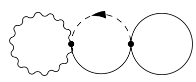
$$f_{i,m} = F_i^{(m)}(0), \quad i = 1,2. \tag{3.139}$$

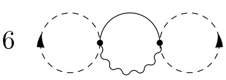
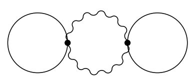
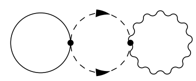
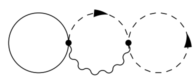
But constructing graphical rules for such general correlations is more involved due to the various summations over products of powers of propagators $G^{\mathrm{D}}_{xx}(\tau_i,\tau_j)$ with $i,j = 1,2$.

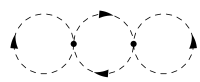
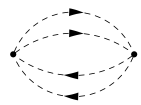
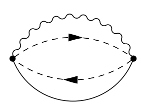
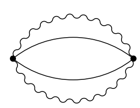
Finally, we apply the diagrammatic rules to the anharmonic oscillator with $\tilde{x}^4$-interaction, which is a powerful system being discussed in detail by the help of a perturbation expansion [4, Chap. 3]. With the Green functions given by (3.26) and (3.38)–(3.40), the two-point-correlation for the anharmonic system can then be expressed graphically, yielding the known decomposition for the second-order perturbative contribution

$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle \tilde{x}^4(\tau_1)\, \tilde{x}^4(\tau_2)\right\rangle_c^{x_b,x_a} \equiv 72$$  $+\,24$  , (3.140)

with subscript c indicating that we restrict ourselves to connected graphs only. Beyond this, our theory allows to describe nonstandard systems with polynomial interactions (3.133) depending on both, position and momentum, to higher order. Finally, we want to give the graphs for a four-interaction $\tilde{x}^2\,\tilde{p}^2$ to second order to see the variations of possible graphs in comparison with (3.140):

$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle \tilde{x}^2(\tau_1)\, \tilde{p}^2(\tau_1)\, \tilde{x}^2(\tau_2)\, \tilde{p}^2(\tau_2)\right\rangle_c^{x_b,x_a} \equiv 2$$  $+\,16$ 

$+\,16$  $+\,2$  $+\,4$  $+\,16$ 

$+\,16$  $+\,4$  $+\,16$  $+\,4$  . (3.141)

We see, that we have the same class of graphs already occurring in (3.140), however, with different propagators connecting the vertices. Thus, both classes decay into subclasses with different multiplicities, but the total numbers remain 72 and 24 for each type of class, respectively. Furthermore, all graphs are vacuum-like graphs. Eventually, it is easy to construct the Feynman graphs for polynomial correlations higher than second order by applying Wick's rule or the Feynman rules given in this section.

Due to its universality, the theory should serve as a basis for investigating physical systems with nonstandard Hamiltonian via perturbation theory and its variational extension.

3.5 Particle Density in the Presence of External Sources

The particle density for a quantum statistical system is given by the diagonal elements of the density matrix. This means, for an explicitly given system, that the knowledge of the density matrix implies the particle density and is obtained by

$$\varrho(\mathbf{x})[\mathbf{j},\mathbf{v}] \equiv \frac{\tilde{\varrho}(\mathbf{x},\mathbf{x})[\mathbf{j},\mathbf{v}]}{\mathrm{Tr}\,\tilde{\varrho}(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}]}. \tag{3.142}$$

The normalization ensures

$$\int d^dx\,\varrho(\mathbf{x})[\mathbf{j},\mathbf{v}] = \frac{\mathrm{Tr}\,\tilde{\varrho}(\mathbf{x},\mathbf{x})[\mathbf{j},\mathbf{v}]}{\mathrm{Tr}\,\tilde{\varrho}(\mathbf{x}_b,\mathbf{x}_a)[\mathbf{j},\mathbf{v}]} = 1. \tag{3.143}$$

In order to calculate the particle density for the general action (3.1), we follow, however, a different way, since extracting the diagonal elements of expression (3.36) requires the knowledge of the classical path with periodic boundary conditions $\mathbf{x}(0) = \mathbf{x}_a = \mathbf{x}(\hbar\beta) = \mathbf{x}_b \equiv \mathbf{x}$, which is determined by the solution (we assume that there is only one) of the general Hamiltonian equations (3.16) and (3.17). Rather, we utilize that the unnormalized particle density $\tilde{\varrho}(\mathbf{x})$ can also be obtained from a path integral over all periodic paths with an inserted δ function $\delta(\mathbf{x}(\tau') - \mathbf{x})$, which restricts the end points of the periodic paths to $\mathbf{x}$. This position is any point of the loop-like path $\mathbf{x}(\tau)$ at the time τ', but it is the same position in space for all loops we integrate over. Thus all periodic paths touch each other in this point. The unnormalized particle density for a system with an action (3.1) reads

$$\tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}] = \oint \mathcal{D}^dx\mathcal{D}^dp\,\delta(\mathbf{x}(\tau') - \mathbf{x})\,e^{-\mathcal{A}_0[\mathbf{p},\mathbf{x};\mathbf{j},\mathbf{v}]/\hbar}, \tag{3.144}$$

where the path integral measure is given by (3.3). Without any restriction of universality and as a consequence of the time-translation invariance of actions of periodic paths, one could also have chosen, for example, the points $\mathbf{x}(0) = \mathbf{x}_a$ or $\mathbf{x}(\hbar\beta) = \mathbf{x}_b$.

Similarly to (3.91), we rewrite the δ function in Eq. (3.144) as

$$\delta(\mathbf{x}(\tau') - \mathbf{x}) = \int \frac{d^dk}{(2\pi)^d} \exp\left[i\mathbf{k}^T\mathbf{x} - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\,\mathbf{j}_0^T(\tau)\mathbf{x}(\tau)\right], \tag{3.145}$$

with the artificial current

$$\mathbf{j}_0(\tau) = i\hbar\mathbf{k}\,\delta(\tau - \tau'). \tag{3.146}$$

After adding the second term in the brackets of the expression (3.145) to the action in the path integral of Eq. (3.144), the Gaussian phase space path integral is easily solved. Introducing $2d$-dimensional phase space coordinates and currents

$$\mathbf{w}^T(\tau) = \left(\mathbf{x}^T(\tau), \mathbf{p}^T(\tau)\right), \qquad \boldsymbol{\eta}^T = \left(\mathbf{j}^T(\tau) + \mathbf{j}_0(\tau), \mathbf{v}^T(\tau)\right), \tag{3.147}$$

and using the symmetric $2d \times 2d$-matrix (3.10), expression (3.144) can be written as

$$\tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}] = \int \frac{d^dk}{(2\pi)^d} e^{i\mathbf{k}^T\mathbf{x}} \oint \mathcal{D}^{2d}w$$

$$\times \exp\left[-\frac{1}{2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \mathbf{w}^T(\tau_1) S(\tau_1,\tau_2)\mathbf{w}(\tau_2) - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \boldsymbol{\eta}^T(\tau)\mathbf{w}(\tau)\right]. \quad (3.148)$$

The calculation is straightforward. After a quadratic completion and a rotation of the phase space vectors which makes S diagonal, the $2d$-dimensional path integral reduces to a $2d$-fold product of a single one. This yields

$$\tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}] = \frac{1}{\sqrt{\det S}} \int \frac{d^d k}{(2\pi)^d}\, e^{i\mathbf{k}^T\mathbf{x}} \exp\left[\frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, \boldsymbol{\eta}^T(\tau_1) S^{-1}(\tau_1,\tau_2)\boldsymbol{\eta}(\tau_2)\right]. \quad (3.149)$$

For further proceeding, it is practical to rewrite this expression with the help of the submatrices of S as defined in (3.10), (3.11), and (3.13). The calculation of the inverse of S and its determinant is done in Appendix 3A. We insert into Eq. (3.149) the components of

$$S^{-1}(\tau,\tau') = \begin{pmatrix} G^{\rm p}_{\mathbf{xx}}(\tau,\tau') & G^{\rm p}_{\mathbf{xp}}(\tau,\tau') \\ G^{\rm p}_{\mathbf{px}}(\tau,\tau') & G^{\rm p}_{\mathbf{pp}}(\tau,\tau') \end{pmatrix}, \quad (3.150)$$

which are two-point functions satisfying periodic boundary conditions,

$$G^{\rm p}_{\mathbf{rs}}(\tau,0) = G^{\rm p}_{\mathbf{rs}}(\tau,\hbar\beta), \qquad G^{\rm p}_{\mathbf{rs}}(0,\tau') = G^{\rm p}_{\mathbf{rs}}(\hbar\beta,\tau'), \qquad \mathbf{r},\mathbf{s} \in (\mathbf{x},\mathbf{p}). \quad (3.151)$$

These two-point functions have the same shape as those for Dirichlet boundary conditions defined in Eqs. (3.26) and (3.38)–(3.40). We will discuss the properties of Green functions with periodic boundary conditions later on. To proceed, we substitute $\mathbf{j}_0(\tau)$ by the right-hand side of Eq. (3.146), which enables us to perform the Fourier integral over k. This finally yields the general expression for the particle density:

$$\tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}] = \left(\frac{M}{2\pi\hbar^2\beta}\right)^{d/2} \frac{1}{\sqrt{\det D_{\mathbf{pp}} \det G^{\rm p\,-1}_{\mathbf{xx}} \det_{\rm s} G^{\rm p}_{\mathbf{xx}}(\tau',\tau')}} \exp\left\{-\frac{1}{2}\mathbf{x}^T G^{\rm p\,-1}_{\mathbf{xx}}(\tau',\tau')\mathbf{x}\right\}$$
$$\times \exp\Bigg\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \mathbf{J}^T(\tau) G^{\rm p\,-1}_{\mathbf{xx}}(\tau',\tau')\mathbf{x} + \frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \Big[\mathbf{j}^T(\tau_1) G^{\rm p}_{\mathbf{xx}}(\tau_1,\tau_2)\mathbf{j}(\tau_2)$$
$$+2\mathbf{j}^T(\tau_1) G^{\rm p}_{\mathbf{xp}}(\tau_1,\tau_2)\mathbf{v}(\tau_2) + \mathbf{v}^T(\tau_1) G^{\rm p}_{\mathbf{pp}}(\tau_1,\tau_2)\mathbf{v}(\tau_2)\Big]\Bigg\}, \quad (3.152)$$

where we have used the abbreviation

$$\mathbf{J}^T(\tau) = \mathbf{j}^T(\tau) G^{\rm p}_{\mathbf{xx}}(\tau,\tau') - \mathbf{v}^T(\tau)\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, G^{\rm p}_{\mathbf{pp}}(\tau,\tau_1) D_{\mathbf{px}}(\tau_1,\tau_2) G^{\rm p}_{\mathbf{xx}}(\tau_2,\tau'). \quad (3.153)$$

It is necessary to remark that, after discretizing the Euclidean time interval $[0,\hbar\beta]$ into $N+1$ pieces, the dimension of the matrix $G^{\rm p}_{\mathbf{xx}}(\tau',\tau')$ remains $d \times d$, since τ' is a fixed point of time within this interval. Thus, its determinant is calculated only over the space components. The determinant of the $(N+1)d \times (N+1)d$ matrices $G^{\rm p\,-1}_{\mathbf{xx}}$ and $D_{\mathbf{pp}}$ must be calculated, however, over all space-time components. We have marked the difference by attaching the subscript "s" to the determinant in the first case. For the evaluation of the determinants, it is useful to take into account, once more, the rules regarding the physical dimension given after Eq. (3.36).

3.6 Partition Function with Currents

The partition function is, beside the density matrix, another fundamental quantity of statistics. In the canonical ensemble of a closed thermodynamic system, it is related to the free energy F via

$$Z = e^{-\beta F}. \quad (3.154)$$

It is the free energy that we will devote considerable attention throughout this thesis. In a subsequent part, we are going to discuss its properties at finite and zero temperature, and in a different form, the role as effective classical potential.

Additionally, the partition function in the presence of external sources can also be used as a generating functional of the correlation functions, similar to the proceeding in Section 3.2.3.

3.6.1 Partition Function in the Presence of External Sources

The quantum statistical partition function is defined as the trace over the unnormalized density matrix. For a system governed by the action (3.1), this is the space integral of (3.152):

$$\begin{aligned} Z_0[\mathbf{j},\mathbf{v}] &= \operatorname{Tr}\tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}] = \int d^dx\,\tilde{\varrho}_0(\mathbf{x})[\mathbf{j},\mathbf{v}] \\ &= \frac{1}{\sqrt{\det S}}\exp\left[\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,\mathbf{C}^T(\tau)S^{-1}(\tau,\tau')\mathbf{C}(\tau')\right], \end{aligned} \tag{3.155}$$

with $\mathbf{C}^T(\tau)=\left(\mathbf{j}^T(\tau),\mathbf{v}^T(\tau)\right)$. Written in components of the matrix $S^{-1}(\tau,\tau')$, the functional (3.155) reads

$$\begin{aligned} Z_0[\mathbf{j},\mathbf{v}] = \frac{1}{\sqrt{\det D_{\mathbf{pp}}\det G_{\mathbf{xx}}^{\mathrm{p}-1}}}\exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\left[\mathbf{j}^T(\tau_1)G^{\mathrm{p}}_{\mathbf{xx}}(\tau_1,\tau_2)\mathbf{j}(\tau_2)\right.\right. \\ \left.\left.+\mathbf{j}^T(\tau_1)G^{\mathrm{p}}_{\mathbf{xp}}(\tau_1,\tau_2)\mathbf{v}(\tau_2)+\mathbf{v}^T(\tau_1)G^{\mathrm{p}}_{\mathbf{px}}(\tau_1,\tau_2)\mathbf{j}(\tau_2)+\mathbf{v}^T(\tau_1)G^{\mathrm{p}}_{\mathbf{pp}}(\tau_1,\tau_2)\mathbf{v}(\tau_2)\right]\right\}. \end{aligned} \tag{3.156}$$

The Green functions are obtained as the elements of the inverse matrix S^{-1}, which we investigate in detail in Appendix 3A. They look similar to those obeying Dirichlet boundary conditions defined in Eqs. (3.26) and (3.38)–(3.40), but they must satisfy periodic boundary conditions (3.151) now:

$$G^{\mathrm{p}}_{\mathbf{xx}}(\tau,\tau') = \left[D_{\mathbf{xx}}(\tau,\tau')-\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\,D_{\mathbf{xp}}(\tau,\tau_1)D^{-1}_{\mathbf{pp}}(\tau_1,\tau_2)D_{\mathbf{px}}(\tau_2,\tau')\right]^{-1}, \tag{3.157}$$

$$G^{\mathrm{p}}_{\mathbf{xp}}(\tau,\tau') = -\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\,G^{\mathrm{p}}_{\mathbf{xx}}(\tau,\tau_1)D_{\mathbf{xp}}(\tau_1,\tau_2)D^{-1}_{\mathbf{pp}}(\tau_2,\tau'), \tag{3.158}$$

$$G^{\mathrm{p}}_{\mathbf{px}}(\tau,\tau') = \left[G^{\mathrm{p}}_{\mathbf{xp}}\right]^T(\tau',\tau) = -\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\,D^{-1}_{\mathbf{pp}}(\tau,\tau_1)D_{\mathbf{px}}(\tau_1,\tau_2)G^{\mathrm{p}}_{\mathbf{xx}}(\tau_2,\tau'), \tag{3.159}$$

$$\begin{aligned} G^{\mathrm{p}}_{\mathbf{pp}}(\tau,\tau') &= D^{-1}_{\mathbf{pp}}(\tau,\tau')+\int_0^{\hbar\beta}d\tau_1\cdots\int_0^{\hbar\beta}d\tau_4 \\ &\quad\times D^{-1}_{\mathbf{pp}}(\tau,\tau_1)D_{\mathbf{px}}(\tau_1,\tau_2)G^{\mathrm{p}}_{\mathbf{xp}}(\tau_2,\tau_3)D_{\mathbf{xp}}(\tau_3,\tau_4)D^{-1}_{\mathbf{pp}}(\tau_4,\tau'). \end{aligned} \tag{3.160}$$

In the following, we specify these Green functions in the example of the one-dimensional harmonic oscillator.

3.6.2 The Harmonic Oscillator Revisited

As an illustration, we calculate the partition function and the periodic Green functions of the one-dimensional harmonic oscillator in the presence of external sources $\mathbf{j}$ and $\mathbf{v}$ (3.41). With the definitions (3.42), where we now omit the boundary terms for $D_{px}(\tau,\tau')$ due to the periodicity of the paths to be considered, the matrix S reads

$$S(\tau,\tau') = \frac{1}{\hbar}\begin{pmatrix} M\omega^2 & i\partial_\tau \\ -i\partial_\tau & M^{-1}\end{pmatrix}\delta(\tau-\tau'), \tag{3.161}$$

where $\partial_\tau \equiv \partial/\partial\tau$. Since only periodic paths must be considered, it is useful to transform the system to Fourier space. The completeness relation for the periodic eigenfunctions is

$$\delta(\tau-\tau') = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty} e^{-i\omega_m(\tau-\tau')}, \tag{3.162}$$

with Matsubara frequencies $\omega_m = 2\pi m/\hbar\beta$. Inserting this into (3.161), the Fourier representation of the matrix $S(\tau,\tau')$ becomes

$$S(\tau,\tau') = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty} S(\omega_m) e^{-i\omega_m(\tau-\tau')}, \tag{3.163}$$

where

$$S(\omega_m) = \begin{pmatrix} D_{xx} & D_{xp}(\omega_m) \\ D_{px}(\omega_m) & D_{pp} \end{pmatrix}. \tag{3.164}$$

Thus, the elements of this matrix are

$$D_{xx} = \frac{M\omega^2}{\hbar}, \qquad D_{xp}(\omega_m) = \frac{\omega_m}{\hbar} = -D_{px}(\omega_m), \qquad D_{pp} = \frac{1}{M\hbar}. \tag{3.165}$$

Combining these components according to the expressions (3.157)–(3.160), we obtain the periodic two-point correlation functions of the one-dimensional harmonic oscillator in Fourier space. Then, the back transformation in time space yields

$$G^{\rm p}_{xx,\omega}(\tau,\tau') = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\frac{\hbar}{M}\frac{1}{\omega_m^2+\omega^2}e^{-i\omega_m(\tau-\tau')} = \frac{\hbar}{2M\omega}\frac{\cosh\omega(|\tau-\tau'|-\hbar\beta/2)}{\sinh\hbar\beta\omega/2}, \tag{3.166}$$

$$\begin{aligned}
G^{\rm p}_{xp,\omega}(\tau,\tau') &= -\frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\frac{\hbar\omega_m}{\omega_m^2+\omega^2}e^{-i\omega_m(\tau-\tau')} = -iM\frac{\partial}{\partial\tau}G^{\rm p}_{xx,\omega}(\tau,\tau') \\
&= -\frac{i\hbar}{2}\left[\Theta(\tau-\tau')\frac{\sinh\omega(\tau-\tau'-\hbar\beta/2)}{\sinh\hbar\beta\omega/2} - \Theta(\tau'-\tau)\frac{\sinh\omega(\tau'-\tau-\hbar\beta/2)}{\sinh\hbar\beta\omega/2}\right] && (3.167) \\
&= -G^{\rm p}_{px,\omega}(\tau,\tau') = G^{\rm p}_{px,\omega}(\tau',\tau), && (3.168)
\end{aligned}$$

$$\begin{aligned}
G^{\rm p}_{pp,\omega}(\tau,\tau') &= \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\frac{\hbar M\omega^2}{\omega_m^2+\omega^2}e^{-i\omega_m(\tau-\tau')} = M^2\omega^2 G_{xx,\omega}(\tau,\tau') \\
&= \frac{1}{2}\hbar\omega M\frac{\cosh\omega(|\tau-\tau'|-\hbar\beta/2)}{\sinh\hbar\beta\omega/2}. && (3.169)
\end{aligned}$$

For the calculation of the prefactor in (3.155), we use the eigenvalue representation of the determinant of S

$$\begin{aligned}
[\det S]^{-1/2} &= \left[\prod_{m=-\infty}^{\infty}\prod_{k=+,-}\lambda_k(\omega_m)\right]^{-1/2} = \exp\left(-\frac{1}{2}{\rm Tr}\ln S\right) \\
&= \exp\left\{-\frac{1}{2}\sum_{m=-\infty}^{\infty}\left[\ln\lambda_+(\omega_m)+\ln\lambda_-(\omega_m)\right]\right\}. && (3.170)
\end{aligned}$$

The eigenvalues of $S(\omega_m)$ are determined from Eqs. (3.164) and (3.165). According to our rule to calculate determinants in units with $\hbar = \beta = M = 1$, this leads to

$$\lambda_\pm(\omega_m) = \frac{1}{2}\left(\omega^2+1\right) \pm \sqrt{\frac{1}{4}\left(\omega^2+1\right) - \left(\omega^2+\omega_m^2\right)}. \tag{3.171}$$

In (3.170), we have also utilized the definition of the logarithm of matrices via the diagonal representation of $S(\omega_m)$,

$$\ln S_{\rm diag}(\omega_m) = \begin{pmatrix} \ln \lambda_+(\omega_m) & 0 \\ 0 & \ln \lambda_-(\omega_m) \end{pmatrix}. \tag{3.172}$$

The use of the diagonal representation is possible, since the trace appearing in (3.170) is independent of the representation of S.

Inserting the eigenvalues (3.171) in (3.170), we find

$$[\det S]^{-1/2} = \exp\left\{ -\frac{1}{2} \ln \prod_{m=-\infty}^{\infty} \left[\omega^2 + \omega_m^2\right] \right\} = \exp\left\{ -\ln\omega - \ln \prod_{m=1}^{\infty} \left[\omega^2 + \omega_m^2\right] \right\}. \tag{3.173}$$

The product in the latter expression diverges, and we regularize it, similar to (3.62), with respect to the free particle. Thus, we obtain

$$[\det S]^{-1/2} = \frac{1}{\omega} \frac{\omega/2}{\sinh \omega/2}. \tag{3.174}$$

For vanishing currents, $j = v = 0$, this is just the partition function of the one-dimensional oscillator,

$$Z_\omega = Z_\omega[0,0] = [\det S]^{-1/2} = \frac{1}{2 \sinh \hbar\beta\omega/2}, \tag{3.175}$$

where we have chosen again physical units by demanding that the argument of sinh and the partition function itself must be dimensionless. Combining this result with the exponential containing the currents in Eq. (3.156), we obtain

$$\begin{aligned} Z_\omega[j,v] &= \frac{1}{2\sinh \hbar\beta\omega/2} \exp\left\{ \frac{1}{2\hbar^2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \Big[j(\tau) G^{\rm p}_{xx,\omega}(\tau,\tau') j(\tau') + j(\tau) G^{\rm p}_{xp,\omega}(\tau,\tau') v(\tau') \right. \\ &\quad \left. + v(\tau) G^{\rm p}_{px,\omega}(\tau,\tau') j(\tau') + v(\tau) G^{\rm p}_{pp,\omega}(\tau,\tau') v(\tau') \Big] \right\}, \end{aligned} \tag{3.176}$$

where the periodic Green functions of the harmonic oscillator are given in Eqs. (3.166)–(3.169).

3.7 Perturbative Expansion for the Free Energy

The free energy of a quantum statistical system is obtained as the logarithm of the partition function

$$F = -\frac{1}{\beta} \ln Z. \tag{3.177}$$

If we assume that the action of the system has the form (3.80), the partition function is given by the phase space path integral

$$Z = \oint \mathcal{D}^d p \mathcal{D}^d x \, e^{-\mathcal{A}[\mathbf{p},\mathbf{x}]/\hbar}, \tag{3.178}$$

and cannot exactly be solved in general. Considering the decomposition of the action ratio (3.80) into an unperturbed term and the interaction, and expanding the Boltzmann factor with respect to the potential $V(\mathbf{p}(\tau), \mathbf{x}(\tau))$ into a Taylor series, we obtain the perturbative expansion

$$Z = Z_0 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!\hbar^n} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n \, \langle V(\mathbf{p}(\tau_1), \mathbf{x}(\tau_1)) \cdots V(\mathbf{p}(\tau_n), \mathbf{x}(\tau_n)) \rangle_0 \,. \tag{3.179}$$

The expectation values are defined with the help of the unperturbed path integral

$$\langle \cdots \rangle_0 = Z_0^{-1} \oint \mathcal{D}^d p \mathcal{D}^d x \, \cdots \, e^{-\mathcal{A}_0[\mathbf{p},\mathbf{x}]/\hbar}, \tag{3.180}$$

where

$$Z_0 = Z_0[0,0] = \oint \mathcal{D}^d p \mathcal{D}^d x \, e^{-\mathcal{A}_0[\mathbf{p},\mathbf{x}]/\hbar} \tag{3.181}$$

is the partition function of the unperturbed system and its solution for vanishing currents is given by (3.156) with $\mathbf{j} = \mathbf{v} = 0$. With the definition of the expectation values (3.180), the periodic Green functions (3.157)–(3.160) can be expressed by the two-point correlation functions

$$G^{\mathrm{p}}_{x_k,x_l}(\tau,\tau') = \langle x_k(\tau) x_l(\tau')\rangle_0 \,, \tag{3.182}$$
$$G^{\mathrm{p}}_{x_k,p_l}(\tau,\tau') = \langle x_k(\tau) p_l(\tau')\rangle_0 \,, \tag{3.183}$$
$$G^{\mathrm{p}}_{p_k,x_l}(\tau,\tau') = \langle p_k(\tau) x_l(\tau')\rangle_0 \,, \tag{3.184}$$
$$G^{\mathrm{p}}_{p_k,p_l}(\tau,\tau') = \langle p_k(\tau) p_l(\tau')\rangle_0 \,. \tag{3.185}$$

We introduce cumulants, where the first two are

$$\langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle_{0,c} = \langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle_0 \,, \tag{3.186}$$
$$\begin{aligned}\langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))V(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle_{0,c} &= \langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))V(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle_0 \\ &\quad - \langle V(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle_0 \langle V(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle_0 \,,\end{aligned} \tag{3.187}$$

which enable us to find a suitable expression for the free energy from (3.179) by using (3.177). Thus, the perturbative expansion for the free energy reads

$$F = F_0 - \frac{1}{\beta}\sum_{n=1}^{\infty} \frac{(-1)^n}{n!\hbar^n} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n \, \langle V(\mathbf{p}(\tau_1)\mathbf{x}(\tau_1)) \cdots V(\mathbf{p}(\tau_n)\mathbf{x}(\tau_n))\rangle_{0,c} \,, \tag{3.188}$$

with the free energy of the unperturbed system

$$F_0 = -\frac{1}{\beta}\ln Z_0. \tag{3.189}$$

The free energy is the energy, which is available for a canonical thermodynamic system in a heat bath with volume V at temperature T to perform mechanical work. Thus, it is the portion of energy, which remains when the inner system energy U is reduced by the entropic energy TS. Assuming the system to be closed (T = const., V = const.), the entropy S ensures that the number of possible configurations of the system, expressed by the partition function Z, is maximal at equilibrium for a certain temperature T. Since Z is at maximum for an equilibrated system, the free energy is minimum. This is what Eq. (3.177) states. Thus, it is plausible that thermodynamics requires the relation

$$F = U - TS. \tag{3.190}$$

Since the inner energy U is identical with the entire system energy E, and the system goes over into its ground state for zero temperature, the quantum mechanical limit $T \to 0$ ($\beta \to \infty$) of the free energy is equal to the ground-state energy $E^{(0)}$ of the system:

$$\lim_{\beta\to\infty} F = E^{(0)}. \tag{3.191}$$

This is easily seen for the example of the harmonic oscillator, whose free energy is $F_\omega = (1/\beta)\ln 2\sinh \hbar\beta\omega/2$. For $\beta \to \infty$, $\sinh \hbar\beta\omega/2$ has the asymptotics $\exp(\hbar\beta\omega/2)/2$. Inserting this into the free energy yields $\lim_{\beta\to\infty} F_\omega = \hbar\omega/2 \equiv E^{(0)}_\omega$, which is the ground-state energy of the harmonic oscillator with one degree of freedom.

3A Algebraic Properties of Block Matrices

Consider a symmetric matrix consisting of block matrices A, B, and C,

$$S = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix} = S^T, \tag{3A.1}$$

where A and C are also symmetric matrices. In what follows we calculate the inverse of S. In a first step, we decompose the matrix into a product of triangular matrices. For regular matrix C, this means that C^{-1} exists, we choose

$$S = S_1\, S_2, \quad S_1 = \begin{pmatrix} I_A & B \\ 0 & C \end{pmatrix}, \quad S_2 = \begin{pmatrix} X & 0 \\ C^{-1}B^T & I_C \end{pmatrix}, \tag{3A.2}$$

with the abbreviation

$$X = A - BC^{-1}B^T. \tag{3A.3}$$

In (3A.2), we have also introduced the identity matrices I_A and I_C, which act in the same space as A and C, respectively. The inverse of S is determined by

$$S^{-1} = (S_1\, S_2)^{-1} = S_2^{-1} S_1^{-1}. \tag{3A.4}$$

Since $S_i S_i^{-1} = I_S$, $i = 1, 2$, we have to calculate

$$S_1 \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} = I_S, \quad S_2 \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} = I_S. \tag{3A.5}$$

The identity matrix

$$I_S = \begin{pmatrix} I_A & 0 \\ 0 & I_C \end{pmatrix} \tag{3A.6}$$

is composed of the identity matrices I_A and I_C. Thus, the determination of the elements of the inverse matrices S_1^{-1} and S_2^{-1} becomes simple and we obtain

$$S_1^{-1} = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} = \begin{pmatrix} X^{-1} & 0 \\ -C^{-1}B^T X^{-1} & I_C \end{pmatrix}, \quad S_2^{-1} = \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} = \begin{pmatrix} I_A & -BC^{-1} \\ 0 & C^{-1} \end{pmatrix}. \tag{3A.7}$$

Multiplying both in the order given in Eq. (3A.4) yields the desired inverse of S

$$S^{-1} = \begin{pmatrix} X^{-1} & -X^{-1}BC^{-1} \\ -C^{-1}B^T X^{-1} & C^{-1} + C^{-1}B^T X^{-1} BC^{-1} \end{pmatrix}. \tag{3A.8}$$

For the calculation of the determinant of S, we use again the decomposition (3A.2). Then, the determinant of S is given by the product rule for matrices

$$\det S = \det S_1 \det S_2 = \det C \det X. \tag{3A.9}$$

If C is singular but A regular, we can make use of another decomposition than (3A.2):

$$S = \begin{pmatrix} I_A & 0 \\ B^T A^{-1} & \tilde{X} \end{pmatrix} \begin{pmatrix} A & B \\ 0 & I_C \end{pmatrix}, \tag{3A.10}$$

with

$$\tilde{X} = C - B^T A^{-1} B. \tag{3A.11}$$

Then, the inverse of S turns out to be

$$S^{-1} = \begin{pmatrix} A^{-1} + A^{-1}BX^{-1}B^T A^{-1} & -A^{-1}B\tilde{X}^{-1} \\ -\tilde{X}^{-1}B^T A^{-1} & -\tilde{X}^{-1} \end{pmatrix} \tag{3A.12}$$

and the determinant is

$$\det S = \det \tilde{X} \det A. \tag{3A.13}$$

3B Generalized Correlation Functions

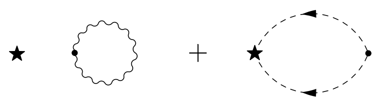
In this appendix we give the expectations for the correlation between a general position or momentum dependent function and a polynomial up to order $n = 4$:

Position-Momentum-Coupling:

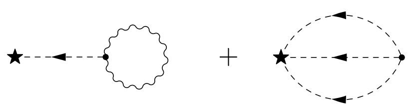
$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \langle F(\tilde{x}(\tau_1))\, \tilde{p}(\tau_2)\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \, G^{\mathrm{D}}_{xp}(\tau_1,\tau_2)\, \langle F'(\tilde{x}(\tau_1))\rangle^{x_b,x_a} \tag{3B.1}$$

$\equiv$  ,

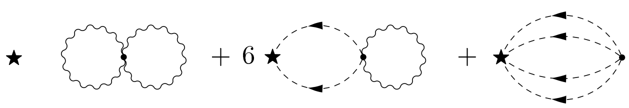
$$\begin{aligned}\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{x}(\tau_1))\, \tilde{p}^2(\tau_2)\right\rangle^{x_b,x_a} &= \int_0^1 d\tau_1 \int_0^1 d\tau_2 \left\{ G^{\mathrm{D}}_{pp}(\tau_2,\tau_2)\, \langle F(\tilde{x}(\tau_1))\rangle^{x_b,x_a} \right.\\ &\quad \left. + \left[G^{\mathrm{D}}_{xp}(\tau_1,\tau_2)\right]^2 \langle F''(\tilde{x}(\tau_1))\rangle^{x_b,x_a} \right\}\end{aligned} \tag{3B.2}$$

$\equiv$  ,

$$\begin{aligned}\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{x}(\tau_1))\, \tilde{p}^3(\tau_2)\right\rangle^{x_b,x_a} &= \int_0^1 d\tau_1 \int_0^1 d\tau_2 \left\{ 3\, G^{\mathrm{D}}_{xp}(\tau_1,\tau_2)\, G^{\mathrm{D}}_{pp}(\tau_2,\tau_2)\, \langle F'(\tilde{x}(\tau_1))\rangle^{x_b,x_a} \right.\\ &\quad \left. + \left[G^{\mathrm{D}}_{xp}(\tau_1,\tau_2)\right]^3 \langle F'''(\tilde{x}(\tau_1))\rangle^{x_b,x_a} \right\}\end{aligned} \tag{3B.3}$$

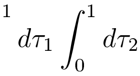
$\equiv$ 3  ,

$$\begin{aligned}\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{x}(\tau_1))\, \tilde{p}^4(\tau_2)\right\rangle^{x_b,x_a} &= \int_0^1 d\tau_1 \int_0^1 d\tau_2 \left\{ \left[G^{\mathrm{D}}_{pp}(\tau_2,\tau_2)\right]^2 \langle F(\tilde{x}(\tau_1))\rangle^{x_b,x_a} \right.\\ &\quad + 6\left[G^{\mathrm{D}}_{xp}(\tau_1,\tau_2)\right]^2 G^{\mathrm{D}}_{pp}(\tau_2,\tau_2)\, \langle F''(\tilde{x}(\tau_1))\rangle^{x_b,x_a}\\ &\quad \left. + \left[G^{\mathrm{D}}_{xp}(\tau_1,\tau_2)\right]^4 \left\langle F^{(4)}(\tilde{x}(\tau_1))\right\rangle^{x_b,x_a} \right\}\end{aligned} \tag{3B.4}$$

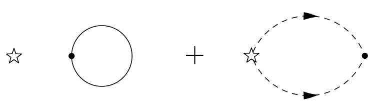
$\equiv$  ;

Momentum-Position-Coupling:

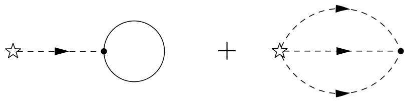
$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \langle F(\tilde{p}(\tau_1))\, \tilde{x}(\tau_2)\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \, G^{\mathrm{D}}_{px}(\tau_1,\tau_2)\, \langle F'(\tilde{p}(\tau_1))\rangle^{x_b,x_a} \tag{3B.5}$$

$\equiv$  ,

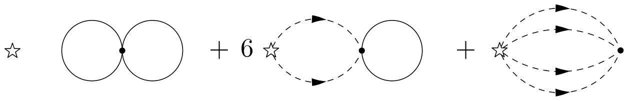
$$\begin{aligned}\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{p}(\tau_1))\, \tilde{x}^2(\tau_2)\right\rangle^{x_b,x_a} &= \int_0^1 d\tau_1 \int_0^1 d\tau_2 \left\{ G^{\mathrm{D}}_{xx}(\tau_2,\tau_2)\, \langle F(\tilde{p}(\tau_1))\rangle^{x_b,x_a} \right.\\ &\quad \left. + \left[G^{\mathrm{D}}_{px}(\tau_1,\tau_2)\right]^2 \langle F''(\tilde{p}(\tau_1))\rangle^{x_b,x_a} \right\}\end{aligned} \tag{3B.6}$$

$\equiv$  ,

$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{p}(\tau_1))\, \tilde{x}^3(\tau_2) \right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \Big\{ 3\, G^{\rm D}_{px}(\tau_1,\tau_2)\, G^{\rm D}_{xx}(\tau_2,\tau_2)\, \langle F'(\tilde{p}(\tau_1))\rangle^{x_b,x_a} + \left[G^{\rm D}_{px}(\tau_1,\tau_2)\right]^3 \langle F'''(\tilde{p}(\tau_1))\rangle^{x_b,x_a} \Big\} \tag{3B.7}$$

≡ 3  ,

$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{p}(\tau_1))\, \tilde{x}^4(\tau_2) \right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \Big\{ \left[G^{\rm D}_{xx}(\tau_2,\tau_2)\right]^2 \langle F(\tilde{p}(\tau_1))\rangle^{x_b,x_a} + 6 \left[G^{\rm D}_{px}(\tau_1,\tau_2)\right]^2 G^{\rm D}_{xx}(\tau_2,\tau_2) \, \langle F''(\tilde{p}(\tau_1))\rangle^{x_b,x_a} + \left[G^{\rm D}_{px}(\tau_1,\tau_2)\right]^4 \left\langle F^{(4)}(\tilde{p}(\tau_1))\right\rangle^{x_b,x_a} \Big\} \tag{3B.8}$$

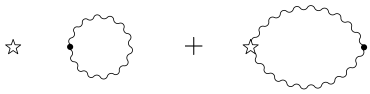
≡  ;

Momentum-Momentum-Coupling:

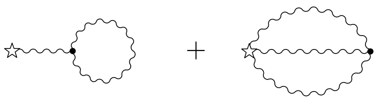
$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{p}(\tau_1))\, \tilde{p}(\tau_2) \right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \, G^{\rm D}_{pp}(\tau_1,\tau_2) \, \langle F'(\tilde{p}(\tau_1))\rangle^{x_b,x_a} \tag{3B.9}$$

≡  ,

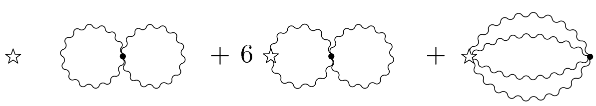
$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{p}(\tau_1))\, \tilde{p}^2(\tau_2) \right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \Big\{ G^{\rm D}_{pp}(\tau_2,\tau_2) \, \langle F(\tilde{p}(\tau_1))\rangle^{x_b,x_a} + \left[G^{\rm D}_{pp}(\tau_1,\tau_2)\right]^2 \langle F''(\tilde{p}(\tau_1))\rangle^{x_b,x_a} \Big\} \tag{3B.10}$$

≡  ,

$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{p}(\tau_1))\, \tilde{p}^3(\tau_2) \right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \Big\{ 3\, G^{\rm D}_{pp}(\tau_1,\tau_2)\, G^{\rm D}_{pp}(\tau_2,\tau_2)\, \langle F'(\tilde{p}(\tau_1))\rangle^{x_b,x_a} + \left[G^{\rm D}_{pp}(\tau_1,\tau_2)\right]^3 \langle F'''(\tilde{p}(\tau_1))\rangle^{x_b,x_a} \Big\} \tag{3B.11}$$

≡ 3  ,

$$\int_0^1 d\tau_1 \int_0^1 d\tau_2 \, \left\langle F(\tilde{p}(\tau_1))\, \tilde{p}^4(\tau_2) \right\rangle^{x_b,x_a} = \int_0^1 d\tau_1 \int_0^1 d\tau_2 \Big\{ \left[G^{\rm D}_{pp}(\tau_2,\tau_2)\right]^2 \langle F(\tilde{p}(\tau_1))\rangle^{x_b,x_a} + 6 \left[G^{\rm D}_{pp}(\tau_1,\tau_2)\right]^2 G^{\rm D}_{pp}(\tau_2,\tau_2) \, \langle F''(\tilde{p}(\tau_1))\rangle^{x_b,x_a} + \left[G^{\rm D}_{pp}(\tau_1,\tau_2)\right]^4 \left\langle F^{(4)}(\tilde{p}(\tau_1))\right\rangle^{x_b,x_a} \Big\} \tag{3B.12}$$

≡  .

The case of position-position-coupling has already been calculated in Section 3.4.3.