Part I

The Path Integral from a Perturbative Perspective

CHAPTER 2

Perturbatively Defined Path Integral in Phase Space

As an alternative to Feynman's time-sliced definition, we introduce a perturbative definition of path integrals in phase space [12]. This will be shown to lead naturally to a high-temperature expansion for the effective classical Hamiltonian of quantum statistical systems. In this definition, the unperturbed system is trivial and the calculation of Feynman diagrams is simple. As an application, we shall apply this formalism to find the effective classical Hamiltonian for the harmonic oscillator.

2.1 Introduction

The definition of path integrals by time-slicing [4] becomes ambiguous for physical systems with non-trivial metric, where operator quantum mechanics has an ordering problem and reparametrization invariance has been a problem for many years [13]. It was solved recently by a perturbative definition of path integrals in *configuration space* [14] using dimensional regularization methods, which successfully guarantees gauge invariance in the quantum theory of non-Abelian gauge fields [15]. Ultimately, rules were found for calculating integrals over products of distributions, which establish a unique procedure for a perturbative calculation of path integrals, which fully respects reparametrization invariance [16]. The path integral of any system is expanded around that of a free particle in powers of the coupling constant of the potential.

Here we extend the definition to path integrals in *phase space* and derive a short-time expansion of the Hamiltonian quantum mechanical time evolution amplitude. In Euclidean space, the density matrix is obtained as a high-temperature expansion. By a simple resummation, this series can be turned into an expansion in powers of the coupling constant of the potential described above. In the expansion to be derived the solution for an exactly known nontrivial path integral such as that of a free particle is *not* required. The perturbative definition presented here is completely general. The usual expansion around the free-particle system can always be reproduced by simply changing the order of summations.

In a first step, the method is used to calculate the *effective classical Hamiltonian* of the harmonic oscillator $H_{\omega,\text{eff}}(p_0, x_0)$ by exactly summing up the perturbation series. In terms of $H_{\omega,\text{eff}}(p_0, x_0)$, the quantum statistical partition function is given by the classically looking phase space integral

$$Z_\omega = \int \frac{dx_0 dp_0}{2\pi\hbar} \exp\left\{-\beta H_{\omega,\text{eff}}(p_0, x_0)\right\}, \tag{2.1}$$

where $\beta = 1/k_B T$ is the inverse thermal energy.

2.2 Perturbative Definition of the Path Integral for Density Matrices

Slicing the interval $[0, \hbar\beta]$ into $N+1$ pieces of width $\varepsilon = \hbar\beta/(N+1)$, the unnormalized density matrix can be expressed by the continuum limit of a product of integrals as [4]

$$\tilde{\varrho}(x_b, x_a) = \lim_{N\to\infty} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} dx_n\right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar}\, e^{ip_n(x_n - x_{n-1})/\hbar}\right] \exp\left\{-\varepsilon \sum_{n=1}^{N+1} H(p_n, x_n)/\hbar\right\}, \quad (2.2)$$

where $x_a = x_0$ and $x_b = x_{N+1}$ are the fixed end points of the path. Upon expanding the last exponential in powers of $\varepsilon/\hbar$, we recognize that the zeroth-order contribution to the density matrix (2.2) is an *infinite product of* δ *functions* due to the identity

$$\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar}\, e^{ip_n(x_n - x_{n-1})/\hbar} = \delta(x_n - x_{n-1}). \quad (2.3)$$

This infinite product simply reduces to

$$\lim_{N\to\infty} \int_{-\infty}^{\infty} dx_N \cdots dx_1\, \delta(x_{N+1} - x_N) \cdots \delta(x_2 - x_1)\delta(x_1 - x_0) = \delta(x_b - x_a), \quad (2.4)$$

which is the unperturbed contribution to the unnormalized density matrix (2.2) obtained here from a trivial path integral. Thus, the phase space path integral for the unnormalized density matrix (2.2) can be perturbatively defined as

$$\begin{aligned} \tilde{\varrho}(x_b, x_a) &= \delta(x_b - x_a) + \sum_{n=1}^{\infty} \frac{(-1)^n}{\hbar^n n!} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n \\ &\quad \times \langle H(p(\tau_1), x(\tau_1)) \cdots H(p(\tau_n), x(\tau_n))\rangle_0^{x_b, x_a}, \end{aligned} \quad (2.5)$$

with expectation values

$$\langle \cdots \rangle_0^{x_b, x_a} = \lim_{N\to\infty} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} dx_n\right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \cdots e^{ip_n(x_n - x_{n-1})/\hbar}\right]. \quad (2.6)$$

These expectation values may be pictured by Feynman diagrams. This is possible for polynomial as well as nonpolynomial functions of momentum and position [17]. We show this in detail in Section 3.4. Note that the exponent on the right-hand side of Eq. (2.6) is the time-sliced version of the eikonal $S = -i \int d\tau\, p(\tau) dx(\tau)/d\tau$.

2.3 Restricted Partition Function and Two-Point Correlations

The trace over the unnormalized density matrix (2.5) of our unperturbed system with vanishing Hamiltonian $H(p, x) = 0$ yields the partition function, which diverges with the phase space volume. This divergence is the same as in the classical partition function. The regularization of these divergences is possible by excluding from the phase space path integral the zero-frequency fluctuations x_0 and p_0 of the Fourier decomposition of the periodic path $x(\tau)$ and momentum $p(\tau)$, respectively [4,18,19]. At the end, we may calculate the quantum statistical partition function from the classical phase space integral

$$Z = \int \frac{dx_0 dp_0}{2\pi\hbar}\, Z^{p_0 x_0}. \quad (2.7)$$

The restricted partition function in the integrand contains the Boltzmann factor of the effective classical Hamiltonian defined by the path integral

$$Z^{p_0x_0} \equiv \exp\{-\beta H_{\rm eff}(p_0,x_0)\} = 2\pi\hbar \oint \mathcal{D}x\mathcal{D}p\, \delta(x_0-\overline{x})\delta(p_0-\overline{p}) \times \exp\left(-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left\{-i[p(\tau)-p_0]\frac{d}{d\tau}[x(\tau)-x_0] + H(p(\tau),x(\tau))\right\}\right), \tag{2.8}$$

with the measure

$$\oint \mathcal{D}x\mathcal{D}p = \lim_{N\to\infty}\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dx_n dp_n}{2\pi\hbar}\right]. \tag{2.9}$$

The quantities $\overline{x}$ and $\overline{p}$ are the temporal mean values $\overline{x}=\int_0^{\hbar\beta} d\tau\, x(\tau)/\hbar\beta$ and $\overline{p}=\int_0^{\hbar\beta} d\tau\, p(\tau)/\hbar\beta$.

As illustrated in the preceding section, the unperturbed system can be assumed to have a vanishing Hamiltonian. The calculation of the restricted partition function $Z^{p_0x_0}$ of this system, denoted by $Z_0^{p_0x_0}$, is then as trivial as for its unnormalized density matrix in (2.4). A cancellation of δ functions yields $Z_0^{p_0x_0}=1$.

In what follows, we want to find the correlation functions of position- and momentum-dependent quantities. For this purpose it is convenient to introduce the generating functional

$$Z_0^{p_0x_0}[j,v] = 2\pi\hbar \oint \mathcal{D}x\mathcal{D}p\, \delta(x_0-\overline{x})\delta(p_0-\overline{p}) \times \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[-i[p(\tau)-p_0]\frac{d}{d\tau}[x(\tau)-x_0] + j(\tau)[x(\tau)-x_0] + v(\tau)[p(\tau)-p_0]\right]\right\}, \tag{2.10}$$

with currents $j(\tau)$ and $v(\tau)$. The action in the exponent contains only the trivial Euclidean eikonal $S=-i\int d\tau\,(p-p_0)d(x-x_0)/d\tau$. The calculation yields

$$Z_0^{p_0x_0}[j,v] = \exp\left\{\frac{1}{\hbar^2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, j(\tau)G^{p_0x_0}(\tau,\tau')v(\tau')\right\}, \tag{2.11}$$

where the periodic Green function has the Fourier representation

$$G^{p_0x_0}(\tau,\tau') = \frac{2i}{\beta}\sum_{m=1}^{\infty}\frac{\sin\omega_m(\tau-\tau')}{\omega_m} \tag{2.12}$$

with Matsubara frequencies

$$\omega_m = \frac{2\pi m}{\hbar\beta}, \tag{2.13}$$

omitting the zero-mode. Evaluating the sum in Eq. (2.12) yields

$$G^{p_0x_0}(\tau,\tau') = -\frac{i}{2\beta}\left\{2(\tau-\tau') - \hbar\beta\left[\Theta(\tau-\tau')-\Theta(\tau'-\tau)\right]\right\}. \tag{2.14}$$

Observe the antisymmetry $G^{p_0x_0}(\tau,\tau')=-G^{p_0x_0}(\tau',\tau)$. As a consequence of reparametrization invariance of the eikonal $S=-i\int d\tau\,(p-p_0)d(x-x_0)/d\tau$, the Green function depends only on the reduced variables

$$\overline{\tau} \equiv \frac{\tau}{\beta} \tag{2.15}$$

and can thus be written as

$$G^{p_0x_0}(\overline{\tau},\overline{\tau}') = -\frac{i}{2}\left\{2(\overline{\tau}-\overline{\tau}') - \hbar\left[\Theta(\overline{\tau}-\overline{\tau}')-\Theta(\overline{\tau}'-\overline{\tau})\right]\right\}. \tag{2.16}$$

Introducing expectation values as

$$\langle \cdots \rangle_0^{p_0 x_0} = 2\pi\hbar \oint \mathcal{D}x\mathcal{D}p\, \delta(x_0 - \overline{x})\delta(p_0 - \overline{p}) \cdots \exp\left\{ \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau\, i[p(\tau) - p_0] \frac{d}{d\tau}[x(\tau) - x_0] \right\}, \quad (2.17)$$

the two-point functions are obtained from the generating functional (2.10) by performing appropriate functional derivatives with respect to $j(\tau)$ and $v(\tau)$, respectively:

$$\langle \tilde{x}(\tau)\tilde{x}(\tau')\rangle_0^{p_0 x_0} = 0, \quad (2.18)$$

$$\langle \tilde{x}(\tau)\tilde{p}(\tau')\rangle_0^{p_0 x_0} = G^{p_0 x_0}(\tau, \tau'), \quad (2.19)$$

$$\langle \tilde{p}(\tau)\tilde{p}(\tau')\rangle_0^{p_0 x_0} = 0. \quad (2.20)$$

The off-diagonal nature of the trivial action in (2.17) entails that only *mixed* position-momentum correlations do not vanish.

2.4 Perturbative Expansion for the Effective Classical Hamiltonian

Expanding the restricted partition function (2.8) in powers of the Hamiltonian,

$$Z^{p_0 x_0} = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{\hbar^n n!} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n\, \langle H(p(\tau_1), x(\tau_1)) \cdots H(p(\tau_n), x(\tau_n))\rangle_0^{p_0 x_0}, \quad (2.21)$$

rewriting this into a cumulant expansion, and utilizing the relation (2.8) between restricted partition function and effective classical Hamiltonian, we obtain

$$H_{\text{eff}}(p_0, x_0) = \frac{1}{\beta} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{\hbar^n n!} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n\, \langle H(p(\tau_1), x(\tau_1)) \cdots H(p(\tau_n), x(\tau_n))\rangle_{0,c}^{p_0 x_0}. \quad (2.22)$$

Using Wick's rule, all correlation functions can be expressed in terms of products of two-point functions. Since only mixed two-point functions (2.14) can lead to nonvanishing contributions to the effective classical Hamiltonian, we use the rescaled version (2.16) of the Green function. The scaling transformation gives a factor β from each of the n integral measures. Thus the expansion (2.22) is a *high-temperature* expansion of the effective classical Hamiltonian:

$$H_{\text{eff}}(p_0, x_0) = \sum_{n=1}^{\infty} \beta^{n-1} \frac{(-1)^{n+1}}{\hbar^n n!} \int_0^{\hbar} d\overline{\tau}_1 \cdots \int_0^{\hbar} d\overline{\tau}_n\, \langle H(p(\overline{\tau}_1), x(\overline{\tau}_1)) \cdots H(p(\overline{\tau}_n), x(\overline{\tau}_n))\rangle_{0,c}^{p_0 x_0}. \quad (2.23)$$

For the following considerations it is useful to assume the Hamilton function to be of standard form

$$H(p(\overline{\tau}), x(\overline{\tau})) = \frac{p^2(\overline{\tau})}{2M} + gV(x(\overline{\tau})), \quad (2.24)$$

where we have introduced the coupling constant g of the potential. Defining the functionals

$$a[p] = \int_0^{\hbar} d\overline{\tau}\, \frac{p^2(\overline{\tau})}{2M}, \qquad b[x] = \int_0^{\hbar} d\overline{\tau}\, V(x(\overline{\tau})), \quad (2.25)$$

the high-temperature expansion (2.23) is expressed as

$$H_{\text{eff}}(p_0, x_0) = \sum_{n=1}^{\infty} \beta^{n-1} \frac{(-1)^{n+1}}{n!\hbar^n} \sum_{k=0}^{n} g^k \binom{n}{k} \langle a^{n-k}[p] b^k[x]\rangle_{0,c}^{p_0 x_0}. \quad (2.26)$$

Before pointing out how this high-temperature expansion is connected with an expansion in powers of the coupling constant g of the potential, we calculate the exact effective classical Hamiltonian of the harmonic oscillator.

2.5 Effective Classical Hamiltonian of Harmonic Oscillator

In this section, we calculate the effective classical Hamiltonian for the harmonic oscillator

$$H_\omega(p,x) = \frac{p^2}{2M} + \frac{1}{2}M\omega^2 x^2 \tag{2.27}$$

by an exact resummation of the high-temperature expansion (2.26). For systematically expressing the terms of this expansion, it is useful to introduce the following Feynman rules:

$\overline{\tau}_1$ $\overline{\tau}_2 \equiv \langle p(\overline{\tau}_1)p(\overline{\tau}_2)\rangle_0^{p_0x_0} = p_0^2,$ (2.28)

$\overline{\tau}_1$ $\overline{\tau}_2 \equiv \langle x(\overline{\tau}_1)x(\overline{\tau}_2)\rangle_0^{p_0x_0} = x_0^2,$ (2.29)

$\overline{\tau}_1$ $\overline{\tau}_2 \equiv \langle x(\overline{\tau}_1)p(\overline{\tau}_2)\rangle_0^{p_0x_0} = G^{p_0x_0}(\overline{\tau}_1,\overline{\tau}_2) + x_0p_0,$ (2.30)

$\overline{\tau}_1$ $\overline{\tau}_2 \equiv \langle p(\overline{\tau}_1)x(\overline{\tau}_2)\rangle_0^{p_0x_0} = -G^{p_0x_0}(\overline{\tau}_1,\overline{\tau}_2) + p_0x_0,$ (2.31)

$\overline{\tau}$ $\equiv \langle p(\overline{\tau})\rangle_0^{p_0x_0} = p_0,$ (2.32)

$\overline{\tau}$ $\equiv \langle x(\overline{\tau})\rangle_0^{p_0x_0} = x_0,$ (2.33)

 $\equiv \int_0^\hbar d\overline{\tau},$ (2.34)

where the current-like expectations in (2.32) and (2.33) arise from $\langle \tilde{p}(\overline{\tau})\rangle_0^{p_0x_0} = 0$ and $\langle \tilde{x}(\overline{\tau})\rangle_0^{p_0x_0} = 0$, respectively. In order to simplify the calculation of the expectation values in the high-temperature expansion of the effective classical Hamiltonian (2.26), we also define operational subgraphs

 $\equiv \frac{1}{2M\hbar}\int_0^\hbar d\overline{\tau}\, p^2(\overline{\tau}),$ (2.35)

 $\equiv \frac{1}{2\hbar}M\omega^2\int_0^\hbar d\overline{\tau}\, x^2(\overline{\tau}),$ (2.36)

which are useful for the systematic construction of the Feynman diagrams. These diagrams are composed by attaching the legs of such subgraphs to one another or by connecting legs with suitable currents. Note that only combinations of different types of subgraphs lead to nonvanishing contributions, since the connection of subgraphs of same type,

 , , (2.37)

leads to a new subgraph, which contains a propagator (2.28) or (2.29), respectively. These propagators are, however, independent of $\overline{\tau}$, such that the $\overline{\tau}$-integrals related to the vertices in these subgraphs are trivial. Thus, there does not really exist a connection between these vertices and the propagators (2.28) and (2.29) can be expressed by the currents (2.32) and (2.33):

$\overline{\tau}_1$ $\overline{\tau}_2 = \overline{\tau}_1$ $\overline{\tau}_2$, (2.38)

$\overline{\tau}_1$ $\overline{\tau}_2 = \overline{\tau}_1$ $\overline{\tau}_2$. (2.39)

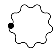
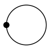
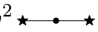
As a consequence, connected diagrams for $n > 1$ containing propagators of type (2.28) or (2.29) *must* break up into disconnected parts. Analytically, this is seen by considering for example

$$\langle x(\overline{\tau}_1)x(\overline{\tau}_2)\rangle_0^{p_0x_0} = \langle \tilde{x}(\overline{\tau}_1)\tilde{x}(\overline{\tau}_2)\rangle_0^{p_0x_0} + \langle x(\overline{\tau}_1)\rangle_0^{p_0x_0}\,\langle x(\overline{\tau}_2)\rangle_0^{p_0x_0}\,. \tag{2.40}$$

The first term on the right-hand side vanishes due to Eq. (2.18), while the second simply yields x_0^2, which proves Eq. (2.29). This means that only Feynman diagrams, which consist of a mixture of subgraphs (2.35) and (2.36) contribute to the effective classical Hamiltonian. To illustrate this, we discuss the first and second order of expansion (2.23) in more detail.

The Feynman diagrams of the first-order contribution to the effective classical Hamiltonian are simply constructed from the subgraphs

$H^{(1)}_{\omega,\text{eff}}(p_0,x_0) \propto$ $+$

$= \frac{1}{2M\hbar}$  $+ \frac{1}{2\hbar} M\omega^2$  $= \frac{1}{2M\hbar}$ $+ \frac{1}{2\hbar} M\omega^2$ 

$$= \frac{p_0^2}{2M} + \frac{1}{2} M\omega^2 x_0^2, \qquad (2.41)$$

where we have used the identities (2.38) and (2.39) in the second expression of the second line. Note that the first-order term (2.41) obviously reproduces the classical Hamiltonian. This is the consequence of the high-temperature expansion (2.26), since only the first-order contribution is nonzero in the limit $\beta = 1/k_B T \to 0$. The second-order contribution reads

$H^{(2)}_{\omega,\mathrm{eff}}(p_0, x_0) \propto$ (+)(+)

$= -\frac{\omega^2}{8\hbar^2\beta}\Big(8$ $+4$  $\Big)$. (2.42)

The chain diagram is zero, while the loop diagram has the value $-\hbar^4\zeta(2)/2\pi^2$, where

$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z} \qquad (2.43)$$

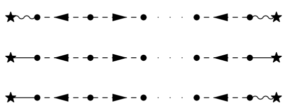
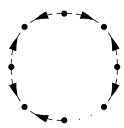
is the Riemann ζ function. Thus we obtain

$$H^{(2)}_{\omega,\mathrm{eff}}(p_0, x_0) = \beta\hbar^2\omega^2\zeta(2)/4\pi^2. \qquad (2.44)$$

This second-order contribution (2.42) shows the characteristic types of Feynman diagrams appearing in each order $n > 1$ of the expansion (2.23) for the harmonic oscillator: chain and loop diagrams. In order to calculate the nth-order contribution, we must evaluate these diagrams more general. By constructing Feynman diagrams from the product of n sums of subgraphs,

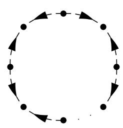
$H^{(n)}_{\omega,\mathrm{eff}}(p_0, x_0) \propto \underbrace{(\ \ldots\ )(\ \ldots\ )\cdots(\ \ldots\ )}_{n\ \text{times}}$: (+)(+) $\cdots$ (+), (2.45)

it turns out that only following chain and loop diagrams contribute:

  . (2.46)

The evaluation of the chain diagrams is easily done and yields zero. An explicit calculation in Fourier space shows that there occur Kronecker symbols $\delta_{m\,0}$. Since the Matsubara sum of the Green function (2.12) does not contain the zero mode $m = 0$, all chain diagrams are zero.

Determining the values of loop diagrams is more involved. It is obvious that loop diagrams can only be constructed in *even* order ($n = 2, 4, 6, \ldots$), since for a loop diagram with mixed propagators (2.30) or (2.31) pairs of different subgraphs (2.35) and (2.36) are necessary. Thus we have found the result that *odd* orders of expansion (2.26) *vanish*, and only loop diagrams for $n \in \{2, 4, 6, \ldots\}$ must be calculated. Evaluating loop diagrams of nth order in Fourier space is straightforward and entails

 $= 2\,(-1)^k \left(\frac{\hbar^2}{2\pi}\right)^{2k} \zeta(2k)$, (2.47)

where $k = n/2$. The multiplicity of such a diagram with $2k$ vertices is easily determined, yielding

$$\mu_k = \frac{2^{2k}(2k)!}{2k}. \qquad (2.48)$$

Thus the high-temperature expansion for the effective Hamiltonian of the harmonic oscillator can be written as

$$H_{\omega,\text{eff}}(p_0,x_0)=\frac{p_0^2}{2M}+\frac{1}{2}M\omega^2x_0^2+\sum_{k=1}^{\infty}\beta^{2k-1}\frac{(-1)^{k+1}}{k}\left(\frac{\hbar\omega}{2\pi}\right)^{2k}\zeta(2k). \tag{2.49}$$

Substituting the ζ function by its definition (2.43) and exchanging the summations, the last term in Eq. (2.49) can be expressed as a logarithm

$$\sum_{k=1}^{\infty}\beta^{2k-1}\frac{(-1)^{k+1}}{k}\left(\frac{\hbar\omega}{2\pi}\right)^{2k}\zeta(2k)=\frac{1}{\beta}\ln\left(\prod_{n=1}^{\infty}\left[1+\frac{\hbar^2\beta^2\omega^2}{4\pi^2n^2}\right]\right). \tag{2.50}$$

Applying the relation

$$\frac{1}{z}\sinh z=\prod_{n=1}^{\infty}\left(1+\frac{z^2}{n^2\pi^2}\right), \tag{2.51}$$

we find the more familiar form of the effective classical Hamiltonian for a harmonic oscillator

$$H_{\omega,\text{eff}}(p_0,x_0)=\frac{p_0^2}{2M}+\frac{1}{2}M\omega^2x_0^2-\frac{1}{\beta}\ln\frac{\hbar\omega\beta}{2\sinh\hbar\omega\beta/2}. \tag{2.52}$$

Performing the x_0- and p_0-integrations in Eq. (2.1), we obtain the well-known form of the partition function of the harmonic oscillator $Z_\omega=1/2\sinh\hbar\omega\beta/2$.

2.6 High-Temperature Versus Weak-Coupling Expansion

In Section 2.4 we have shown that the perturbative expansion around a vanishing Hamiltonian leads to a perturbative series in powers of the inverse temperature in a natural manner. Now we elaborate its relation to more customary perturbative expansions in powers of the coupling constant g of the potential. Changing the order of summation in Eq. (2.26), we obtain

$$H_{\text{eff}}(p_0,x_0)=\sum_{k=0}^{\infty}g^k\sum_{n=0}^{\infty}\beta^{n+k-1}\binom{n+k}{k}\frac{(-1)^{n+k+1}}{(n+k)!\hbar^{n+k}}\left\langle a^n[p]b^k[x]\right\rangle_{0,c}^{p_0x_0}+\frac{1}{\beta}, \tag{2.53}$$

which is rewritten, after explicitly evaluating the $(n=0)$- and $(k=0)$-contributions, as

$$\begin{aligned}H_{\text{eff}}(p_0,x_0) &= \frac{p_0^2}{2M}+gV(x_0)+\frac{1}{\beta}\sum_{k=1}^{\infty}g^k\sum_{n=1}^{\infty}\frac{(-1)^{n+k+1}}{n!k!\hbar^{n+k}(2M)^n}\\ &\quad\times\int_0^{\hbar\beta}d\tau_1\cdots\int_0^{\hbar\beta}d\tau_k\int_0^{\hbar\beta}d\tau_{k+1}\cdots\int_0^{\hbar\beta}d\tau_{k+n}\\ &\quad\times\left\langle V(x(\tau_1))\cdots V(x(\tau_k))p^2(\tau_{k+1})\cdots p^2(\tau_{k+n})\right\rangle_{0,c}^{p_0x_0}.\end{aligned} \tag{2.54}$$

In this expression, we have inverted the scaling transformation in Eq. (2.15), and used the expectation values

$$\int_0^{\hbar\beta}d\tau\,\left\langle p^2(\tau)\right\rangle_{0,c}^{p_0x_0}=\hbar\beta p_0^2,\qquad\int_0^{\hbar\beta}d\tau\,\left\langle V(x(\tau))\right\rangle_{0,c}^{p_0x_0}=\hbar\beta V(x_0). \tag{2.55}$$

All higher-order expectations of functions, which only depend on x *or* p are zero, due to the vanishing of expectations of functions of $\tilde{x}$ or $\tilde{p}$ in a Wick expansion into products of two-point functions (2.18) and (2.20). All other possible contributions are disconnected.

We now observe that the expansion (2.54) is equal to a perturbation expansion around a free-particle theory

$$\begin{aligned} H_{\text{eff}}(p_0, x_0) \;&=\; \frac{p_0^2}{2M} + gV(x_0) + \frac{1}{\beta}\sum_{k=1}^{\infty} g^k \frac{(-1)^{k+1}}{k!\hbar^k} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_k \\ &\times \langle V(x(\tau_1)) \cdots V(x(\tau_k)) \rangle_{\text{free},c}^{x_0} , \end{aligned} \tag{2.56}$$

in which cumulants are formed from position-dependent expectation values

$$\begin{aligned} \langle \cdots \rangle_{\text{free}}^{x_0} \;&=\; 2\pi\hbar e^{\beta p_0^2/2M} \oint \mathcal{D}x\mathcal{D}p\, \delta(x_0 - \overline{x})\delta(p_0 - \overline{p}) \cdots \\ &\times \exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \, \left[-i(p(\tau) - p_0)\frac{\partial}{\partial\tau}(x(\tau) - x_0) + \frac{1}{2M}p^2(\tau) \right] \right\}. \end{aligned} \tag{2.57}$$

This expression is identical with

$$\langle \cdots \rangle_{\text{free}}^{x_0} = \sqrt{\frac{2\pi\hbar^2\beta}{M}} \oint \mathcal{D}'x \, \delta(x_0 - \overline{x}) \cdots \exp\left\{ -\frac{M}{2\hbar}\int_0^{\hbar\beta} d\tau \, \dot{x}^2(\tau) \right\}, \tag{2.58}$$

with the dot denoting the derivative with respect to τ. The new measure is

$$\oint \mathcal{D}'x = \lim_{N\to\infty} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{2\pi\hbar\varepsilon/M}} \right]. \tag{2.59}$$

In the following section we will consider how the expectation values appearing in the high-temperature expansion (2.54) of the effective classical Hamiltonian go over into the cumulants in the weak-coupling expansion (2.56). We thus study the relation between both expansions and we are led to the so-called *smearing formula* for arbitrary expectation values of functions depending on position or/and momentum. Being a Gaussian convolution of these functions, its application will be in particular useful for calculating expectation values of nonpolynomial expressions.

2.7 Free-Particle Smearing Formula

Consider a general correlation function appearing in the expansion (2.54) of the effective classical Hamiltonian, which can be written as

$$M_{kn} = \prod_{m=1}^{k+n} \left[\int_0^{\hbar\beta} d\tau_m \right] \left\langle \prod_{l=1}^{k} [V(x(\tau_l))] \prod_{s=1}^{n} [p^2(\tau_{k+s})] \right\rangle_0^{p_0 x_0} . \tag{2.60}$$

In order to reduce the expectation value to an expression, which has already been calculated we split off the time dependences by Fourier transformations. This yields

$$\begin{aligned} M_{kn} \;&=\; \prod_{m=1}^{k+n} \left[\int_0^{\hbar\beta} d\tau_m \right] \prod_{l=1}^{k} \left[\int_{-\infty}^{\infty} \frac{d\kappa_l}{2\pi} V(\kappa_l) e^{i\kappa_l x_0} \right] \prod_{s=1}^{n} \left[\int_{-\infty}^{\infty} \frac{d\overline{p}_s}{2\pi\hbar} \overline{p}_s^2 \int_{-\infty}^{\infty} d\xi_s \, e^{i(\overline{p}_s - p_0)\xi_s/\hbar} \right] \\ &\times \left\langle \exp\left\{ i\sum_{l=1}^{k} \kappa_l [x(\tau_l) - x_0] - \frac{i}{\hbar}\sum_{s=1}^{n} \xi_s [p(\tau_{k+s}) - p_0] \right\} \right\rangle_0^{p_0 x_0} . \end{aligned} \tag{2.61}$$

By introducing currents

$$j(\tau) = -i\hbar\sum_{l=1}^{k} \delta(\tau - \tau_l)\kappa_l, \quad v(\tau) = i\sum_{s=1}^{n} \delta(\tau - \tau_{k+s})\xi_s, \tag{2.62}$$

the expectation value in Eq. (2.61) can be rewritten as the generating functional (2.10) with the result (2.11). We reinsert now the expressions (2.62) for the currents into the functional (2.11) and perform the τ-integrations. This leads to

$$Z_0^{p_0 x_0}[\kappa, \xi] = \exp\left[\frac{1}{\hbar}\sum_{l=1}^{k}\sum_{s=1}^{n}\kappa_l G^{p_0 x_0}(\tau_l, \tau_{k+s})\xi_s\right]. \tag{2.63}$$

Using this result in Eq. (2.61), the ξ_s-integration can be done and yields

$$\int_{-\infty}^{\infty}\frac{d\xi_s}{2\pi\hbar}\exp\left\{\frac{i}{\hbar}\left[\overline{p}_s - p_0 - i\sum_{l=1}^{k}\kappa_l G^{p_0 x_0}(\tau_l, \tau_{k+s})\right]\xi_s\right\} = \delta\left(\overline{p}_s - p_0 - i\sum_{l=1}^{k}\kappa_l G^{p_0 x_0}(\tau_l, \tau_{k+s})\right), \tag{2.64}$$

leaving us with

$$M_{kn} = \prod_{l=1}^{k}\left[\int_0^{\hbar\beta} d\tau_l \int_{-\infty}^{\infty}\frac{d\kappa_l}{2\pi}V(\kappa_l)e^{i\kappa_l x_0}\right]\prod_{s=1}^{n}\left[\int_0^{\hbar\beta} d\tau_{k+s}\left(p_0 + i\sum_{l=1}^{k}\kappa_l G^{p_0 x_0}(\tau_l, \tau_{k+s})\right)^2\right]. \tag{2.65}$$

After expanding the squared parentheses, terms like

$$\int_0^{\hbar\beta} d\tau_{P(k+1)} p_0^2 \int_0^{\hbar\beta} d\tau_{P(k+2)} \cdots \int_0^{\hbar\beta} d\tau_{P(k+s)}\, f_1(\tau_{P(k+2)}, \ldots, \tau_{P(k+s)}) \tag{2.66}$$

and

$$\int_0^{\hbar\beta} d\tau_{P(k+1)}\, G^{p_0 x_0}(\tau_{P(k+1)}, \tau_l) \int_0^{\hbar\beta} d\tau_{P(k+2)} \cdots \int_0^{\hbar\beta} d\tau_{P(k+s)}\, f_2(\tau_{P(k+2)}, \ldots, \tau_{P(k+s)}) \tag{2.67}$$

occur, where $f_1(\tau_{P(k+2)}, \ldots, \tau_{P(k+s)})$ and $f_2(\tau_{P(k+2)}, \ldots, \tau_{P(k+s)})$ are functions independent of τ_{k+1}. Due to the separate time integration, expressions of the form (2.66) correspond to disconnected diagrams and may be omitted in the following. Since $\int_0^{\hbar\beta} d\tau\, G^{p_0,x_0}(\tau, \tau')$ vanishes, terms like (2.67) do not contribute. The permutation operator P exhibits that this is also right for any permutation of the τ_i's ($i \in \{1, \ldots, s\}$). Since we shall omit disconnected contributions (2.66), we are left with the cumulant

$$\begin{aligned} M_{c,kn} &= \prod_{l=1}^{k}\left[\int_0^{\hbar\beta} d\tau_l \int_{-\infty}^{\infty}\frac{d\kappa_l}{2\pi}V(\kappa_l)e^{i\kappa_l x_0}\right] \\ &\times \prod_{s=1}^{n}\left[(-1)\sum_{l_1,l_2=1}^{k}\kappa_{l_1}\kappa_{l_2}\int_0^{\hbar\beta} d\tau_{k+s} G^{p_0 x_0}(\tau_{l_1}, \tau_{k+s}) G^{p_0 x_0}(\tau_{k+s}, \tau_{l_2})\right]. \end{aligned} \tag{2.68}$$

Using the Fourier decomposition of the Green function (2.12) with Matsubara frequencies (2.13), the time integration in the second product is easily done yielding

$$\begin{aligned} \int_0^{\hbar\beta} d\tau_{k+s} G^{p_0 x_0}(\tau_{l_1}, \tau_{k+s}) G^{p_0 x_0}(\tau_{k+s}, \tau_{l_2}) &= -\frac{2\hbar}{\beta}\sum_{m=1}^{\infty}\frac{1}{\omega_m^2}\cos\omega_m(\tau_{l_1} - \tau_{l_2}) \\ &= -\frac{M}{\hbar}\, G_{\text{free}}^{p_0 x_0}(\tau_{l_1}, \tau_{l_2}), \end{aligned} \tag{2.69}$$

where

$$G_{\text{free}}^{p_0 x_0}(\tau, \tau') = \frac{1}{2M\beta}\left(|\tau - \tau'|^2 - \hbar\beta|\tau - \tau'| + \frac{1}{6}\hbar^2\beta^2\right) \tag{2.70}$$

is the Green function for a free particle with periodic boundary conditions and the zero-frequency mode excluded. It satisfies the equation of motion

$$\frac{M}{2\hbar}\frac{\partial^2}{\partial\tau^2}\, G^{p_0x_0}_{\text{free}}(\tau,\tau') = \delta(\tau-\tau'), \qquad \tau,\tau'\in[0,\hbar\beta]. \tag{2.71}$$

with periodic boundary conditions $G^{p_0x_0}_{\text{free}}(\tau,\tau') \equiv G^{p_0x_0}_{\text{free}}(\tau-\tau') = G^{p_0x_0}_{\text{free}}(\tau-\tau'+\hbar\beta)$. Thus the cumulant (2.68) can be written as

$$M_{c,kn} = \prod_{l=1}^{k}\left[\int_0^{\hbar\beta} d\tau_l \int_{-\infty}^{\infty}\frac{d\kappa_l}{2\pi}\, V(\kappa_l)e^{i\kappa_l x_0}\right]\left[\frac{M}{\hbar}\sum_{l_1,l_2=1}^{k}\kappa_{l_1}G^{p_0x_0}_{\text{free}}(\tau_{l_1},\tau_{l_2})\kappa_{l_2}\right]^n . \tag{2.72}$$

The expansion (2.54) can now be expressed as

$$H_{\text{eff}}(p_0,x_0) = \frac{p_0^2}{2M} + gV(x_0) + \frac{1}{\beta}\sum_{k=1}^{\infty} g^k\frac{(-1)^{k+1}}{k!\hbar^k}\sum_{n=1}^{\infty}\frac{(-1)^n}{2^n n!}\, M_{c,kn}. \tag{2.73}$$

It is useful to move the classical potential term $gV(x_0)$ into the last sum. This is done by extending the second sum in (2.73) by the $n=0$-term:

$$\sum_{k=1}^{\infty} g^k\frac{(-1)^{k+1}}{k!\hbar^k}\prod_{l=1}^{k}\left[\int_0^{\hbar\beta} d\tau_l\int_{-\infty}^{\infty}\frac{d\kappa_l}{2\pi}\, V(\kappa_l)e^{i\kappa_l x_0}\right]$$
$$= \sum_{k=1}^{\infty} g^k\frac{(-1)^{k+1}}{k!\hbar^k}\int_0^{\hbar\beta} d\tau_1\dots\int_0^{\hbar\beta} d\tau_k\, [V(x_0)]^k = gV(x_0). \tag{2.74}$$

In the second expression we have utilized that terms with $k>1$ lead to disconnected contributions, which do not appear in $M_{c,kn}$. Thus expansion (2.73) reads

$$\begin{aligned} H_{\text{eff}}(p_0,x_0) &= \frac{p_0^2}{2M} + \frac{1}{\beta}\sum_{k=1}^{\infty} g^k\frac{(-1)^{k+1}}{k!\hbar^k}\prod_{l=1}^{k}\left[\int_0^{\hbar\beta} d\tau_l\int_{-\infty}^{\infty} dx_l\, V(x_l)\int_{-\infty}^{\infty}\frac{d\kappa_l}{2\pi}\right] \\ &\quad\times \exp\left\{ i\boldsymbol{\kappa}(\mathbf{x}_0-\mathbf{x}) - \frac{1}{2}\boldsymbol{\kappa}^T\mathbf{G}^{p_0x_0}_{\text{free}}\boldsymbol{\kappa}\right\}, \end{aligned} \tag{2.75}$$

where we have introduced the n-dimensional vectors $\boldsymbol{\kappa} = (\kappa_1,\dots,\kappa_n)$ and the symmetric $n\times n$ matrix of Green functions

$$\mathbf{G}^{p_0x_0}_{\text{free}} = \begin{pmatrix} G^{p_0x_0}_{\text{free}}(\tau_1,\tau_1) & \cdots & G^{p_0x_0}_{\text{free}}(\tau_1,\tau_n) \\ \vdots & \ddots & \vdots \\ G^{p_0x_0}_{\text{free}}(\tau_1,\tau_n) & \cdots & G^{p_0x_0}_{\text{free}}(\tau_n,\tau_n)\end{pmatrix}. \tag{2.76}$$

After diagonalizing this matrix, the κ_l-integrals in Eq. (2.75) are easily calculated. The effective classical Hamiltonian can then be expressed with the help of a Gaussian convolution integral, which smears out products of the potential $V(x)$:

$$\begin{aligned} H_{\text{eff}}(p_0,x_0) &= \frac{p_0^2}{2M} + \frac{1}{\beta}\sum_{k=1}^{\infty} g^k\frac{(-1)^{k+1}}{k!\hbar^k}\prod_{l=1}^{k}\left[\int_0^{\hbar\beta} d\tau_l\int_{-\infty}^{\infty} dx_l\, V(x_l)\right] \\ &\quad\times\frac{1}{\sqrt{2\pi\det\mathbf{G}^{p_0x_0}_{\text{free}}}}\exp\left\{-\frac{1}{2}\sum_{l_1,l_2=1}^{k}(x_{l_1}-x_0)[G^{p_0x_0}_{\text{free}}(\tau_{l_1},\tau_{l_2})]^{-1}(x_{l_2}-x_0)\right\}. \end{aligned} \tag{2.77}$$

The extension of this result to higher spatial dimensions is straightforward.