Ακίνητα κινεῖς
You stir what should not be stirred
HERODOTUS (484 BC–425 BC)

3

External Sources, Correlations, and Perturbation Theory

Important information on every quantum-mechanical system is carried by the correlation functions of the path $x(t)$. They are defined as the expectation values of products of path positions at different times, $x(t_1)\cdots x(t_n)$, to be calculated as functional averages. Quantities of this type are observable in simple scattering experiments. The most efficient extraction of correlation functions from a path integral proceeds by adding to the Lagrangian an external time-dependent mechanical force term disturbing the system linearly, and by studying the response to the disturbance. A similar linear term is used extensively in quantum field theory, for instance in quantum electrodynamics where it is no longer a mechanical force, but a source of fields, i.e., a charge or a current density. For this reason we shall call this term generically source or current term.

In this chapter, the procedure is developed for the harmonic action, where a linear source term does not destroy the solvability of the path integral. The resulting amplitude is a simple functional of the current. Its functional derivatives will supply all correlation functions of the system, and for this reason it is called the *generating functional* of the theory. It serves to derive the celebrated *Wick rule* for calculating the correlation functions of an arbitrary number of $x(t)$. This forms the basis for perturbation expansions of anharmonic theories.

3.1 External Sources

Consider a harmonic oscillator with an action

$$\mathcal{A}_\omega = \int_{t_a}^{t_b} dt\, \frac{M}{2}(\dot{x}^2 - \omega^2 x^2). \tag{3.1}$$

Let it be disturbed by an external *source* or *current* $j(t)$ coupled linearly to the particle coordinate $x(t)$. The source action is

$$\mathcal{A}_j = \int_{t_a}^{t_b} dt\; x(t)j(t). \tag{3.2}$$

The total action

$$\mathcal{A} = \mathcal{A}_\omega + \mathcal{A}_j \tag{3.3}$$

is still harmonic in x and $\dot{x}$, which makes it is easy to solve the path integral in the presence of a source term. In particular, the source term does not destroy the factorization property (2.153) of the time evolution amplitude into a classical amplitude $e^{i\mathcal{A}_{j,\mathrm{cl}}/\hbar}$ and a fluctuation factor $F_{\omega,j}(t_b,t_a)$,

$$(x_bt_b|x_at_a)^j_\omega = e^{(i/\hbar)\mathcal{A}_{j,\mathrm{cl}}}F_{\omega,j}(t_b,t_a). \tag{3.4}$$

Here $\mathcal{A}_{j,\mathrm{cl}}$ is the action for the classical orbit $x_{j,\mathrm{cl}}(t)$ which minimizes the total action $\mathcal{A}$ in the presence of the source term and which obeys the equation of motion

$$\ddot{x}_{j,\mathrm{cl}}(t) + \omega^2 x_{j,\mathrm{cl}}(t) = j(t). \tag{3.5}$$

In the sequel, we shall first work with the classical orbit $x_{\mathrm{cl}}(t)$ extremizing the action *without* the source term:

$$x_{\mathrm{cl}}(t) = \frac{x_b\sin\omega(t-t_a) + x_a\sin\omega(t_b-t)}{\sin\omega(t_b-t_a)}. \tag{3.6}$$

All paths will be written as a sum of the classical orbit $x_{\mathrm{cl}}(t)$ and a fluctuation $\delta x(t)$:

$$x(t) = x_{\mathrm{cl}}(t) + \delta x(t). \tag{3.7}$$

Then the action separates into a classical and a fluctuating part, each of which contains a source-free and a source term:

$$\begin{aligned}\mathcal{A} = \mathcal{A}_\omega + \mathcal{A}_j &\equiv \mathcal{A}_{\mathrm{cl}} + \mathcal{A}_{\mathrm{fl}}\\ &= (\mathcal{A}_{\omega,\mathrm{cl}} + \mathcal{A}_{j,\mathrm{cl}}) + (\mathcal{A}_{\omega,\mathrm{fl}} + \mathcal{A}_{j,\mathrm{fl}}).\end{aligned} \tag{3.8}$$

The time evolution amplitude can be expressed as

$$\begin{aligned}(x_bt_b|x_at_a)^j_\omega &= e^{(i/\hbar)\mathcal{A}_{\mathrm{cl}}}\int\mathcal{D}x\exp\left(\frac{i}{\hbar}\mathcal{A}_{\mathrm{fl}}\right)\\ &= e^{(i/\hbar)(\mathcal{A}_{\omega,\mathrm{cl}}+\mathcal{A}_{j,\mathrm{cl}})}\int\mathcal{D}x\exp\left[\frac{i}{\hbar}(\mathcal{A}_{\omega,\mathrm{fl}}+\mathcal{A}_{j,\mathrm{fl}})\right].\end{aligned} \tag{3.9}$$

The classical action $\mathcal{A}_{\omega,\mathrm{cl}}$ is known from Eq. (2.159):

$$\mathcal{A}_{\omega,\mathrm{cl}} = \frac{M\omega}{2\sin\omega(t_b-t_a)}\left[(x_b^2+x_a^2)\cos\omega(t_b-t_a) - 2x_bx_a\right]. \tag{3.10}$$

The classical source term is known from (3.6):

$$\begin{aligned}\mathcal{A}_{j,\mathrm{cl}} &= \int_{t_a}^{t_b}dt\; x_{\mathrm{cl}}(t)j(t) \qquad (3.11)\\ &= \frac{1}{\sin\omega(t_b-t_a)}\int_{t_a}^{t_b}dt[x_a\sin\omega(t_b-t) + x_b\sin\omega(t-t_a)]j(t).\end{aligned}$$

Consider now the fluctuating part of the action, $\mathcal{A}_{\rm fl} = \mathcal{A}_{\omega,\rm fl} + \mathcal{A}_{j,\rm fl}$. Since $x_{\rm cl}(t)$ extremizes the action without the source, $\mathcal{A}_{\rm fl}$ contains a term linear in $\delta x(t)$. After a partial integration [making use of the vanishing of $\delta x(t)$ at the ends] it can be written as

$$\mathcal{A}_{\rm fl} = \frac{M}{2}\int_{t_a}^{t_b} dt dt'\, \delta x(t) D_{\omega^2}(t,t')\delta x(t') + \int_{t_a}^{t_b} dt\, \delta x(t) j(t), \tag{3.12}$$

where $D_{\omega^2}(t,t')$ is the differential operator

$$D_{\omega^2}(t,t') = (-\partial_t^2 - \omega^2)\delta(t-t') = \delta(t-t')(-\partial_{t'}^2 - \omega^2), \quad t,t' \in (t_a,t_b). \tag{3.13}$$

It may be considered as a functional matrix in the space of the t-dependent functions vanishing at t_a, t_b. The equality of the two expressions is seen as follows. By partial integrations one has

$$\int_{t_a}^{t_b} dt\, f(t)\partial_t^2 g(t) = \int_{t_a}^{t_b} dt\, \partial_t^2 f(t) g(t), \tag{3.14}$$

for any $f(t)$ and $g(t)$ vanishing at the boundaries (or for periodic functions in the interval). The left-hand side can directly be rewritten as $\int_{t_a}^{t_b} dt dt'\, f(t)\delta(t-t')\partial_{t'}^2 g(t')$, the right-hand side as $\int_{t_a}^{t_b} dt dt'\, \partial_t^2 f(t)\delta(t-t')g(t')$, and after further partial integrations, as $\int dt dt'\, f(t)\partial_t^2\delta(t-t')g(t)$.

The inverse $D_{\omega^2}^{-1}(t,t')$ of the functional matrix (3.13) is formally defined by the relation

$$\int_{t_a}^{t_b} dt' D_{\omega^2}(t'',t') D_{\omega^2}^{-1}(t',t) = \delta(t''-t), \quad t'',t \in (t_a,t_b), \tag{3.15}$$

which shows that it is the standard classical Green function of the harmonic oscillator of frequency ω:

$$G_{\omega^2}(t,t') \equiv D_{\omega^2}^{-1}(t,t') = (-\partial_t^2 - \omega^2)^{-1}\delta(t-t'), \quad t,t' \in (t_a,t_b). \tag{3.16}$$

This definition is not unique since it leaves room for an additional arbitrary solution $H(t,t')$ of the homogeneous equation $\int_{t_a}^{t_b} dt' D_{\omega^2}(t'',t')H(t',t) = 0$. This freedom will be removed below by imposing appropriate boundary conditions.

In the fluctuation action (3.12), we now perform a *quadratic completion* by a shift of $\delta x(t)$ to

$$\delta\tilde{x}(t) \equiv \delta x(t) + \frac{1}{M}\int_{t_a}^{t_b} dt' G_{\omega^2}(t,t')j(t'). \tag{3.17}$$

Then the action becomes quadratic in both $\delta\tilde{x}$ and j:

$$\mathcal{A}_{\rm fl} = \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' \left[\frac{M}{2}\delta\tilde{x}(t) D_{\omega^2}(t,t')\delta\tilde{x}(t') - \frac{1}{2M} j(t) G_{\omega^2}(t,t') j(t')\right]. \tag{3.18}$$

The Green function obeys the same boundary condition as the fluctuations $\delta x(t)$:

$$G_{\omega^2}(t,t') = 0 \quad \text{for} \quad \begin{cases} t = t_b\,, & t' \text{ arbitrary,} \\ t \text{ arbitrary,} & t' = t_a\,. \end{cases} \tag{3.19}$$

Thus, the shifted fluctuations $\delta\tilde{x}(t)$ of (3.17) also vanish at the ends and run through the same functional space as the original $\delta x(t)$. The measure of path integration $\int \mathcal{D}\delta x(t)$ is obviously unchanged by the simple shift (3.17). Hence the path integral $\int \mathcal{D}\delta\tilde{x}$ over $e^{i\mathcal{A}_{\rm fl}/\hbar}$ with the action (3.18) gives, via the first term in $\mathcal{A}_{\rm fl}$, the harmonic fluctuation factor $F_\omega(t_b - t_a)$ calculated in (2.171):

$$F_\omega(t_b - t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}}\sqrt{\frac{\omega}{\sin\omega(t_b - t_a)}}. \tag{3.20}$$

The source part in (3.18) contributes only a trivial exponential factor

$$F_{j,\rm fl} = \exp\left\{\frac{i}{\hbar}\mathcal{A}_{j,\rm fl}\right\}, \tag{3.21}$$

whose exponent is quadratic in $j(t)$:

$$\mathcal{A}_{j,\rm fl} = -\frac{1}{2M}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' j(t) G_{\omega^2}(t,t') j(t'). \tag{3.22}$$

The total time evolution amplitude in the presence of a source term can therefore be written as the product

$$(x_b t_b|x_a t_a)_\omega^j = (x_b t_b|x_a t_a)_\omega F_{j,\rm cl} F_{j,\rm fl}, \tag{3.23}$$

where $(x_b t_b|x_a t)_\omega$ is the source-free time evolution amplitude

$$\begin{aligned}(x_b t_b|x_a t_a)_\omega = e^{(i/\hbar)\mathcal{A}_{\omega,\rm cl}} F_\omega(t_b - t_a) &= \frac{1}{\sqrt{2\pi i\hbar/M}}\sqrt{\frac{\omega}{\sin\omega(t_b - t_a)}} \\ &\times \exp\left\{\frac{i}{2\hbar}\frac{M\omega}{\sin\omega(t_b - t_a)}[(x_b^2 + x_a^2)\cos\omega(t_b - t_a) - 2x_b x_a]\right\},\end{aligned} \tag{3.24}$$

and $F_{j,\rm cl}$ is an amplitude containing the classical action (3.11):

$$\begin{aligned}F_{j,\rm cl} &= e^{(i/\hbar)\mathcal{A}_{j,\rm cl}} \\ &= \exp\left\{\frac{i}{\hbar}\frac{1}{\sin\omega(t_b - t_a)}\int_{t_a}^{t_b} dt[x_a \sin\omega(t_b - t) + x_b \sin\omega(t - t_a)]\, j(t)\right\}.\end{aligned} \tag{3.25}$$

To complete the result we need to know the Green function $G_{\omega^2}(t,t')$ explicitly, which will be calculated in the next section.

3.2 Green Function of Harmonic Oscillator

According to Eq. (3.16), the Green function in Eq. (3.22) is obtained by inverting the second-order differential operator $-\partial_t^2 - \omega^2$:

$$G_{\omega^2}(t,t') = (-\partial_t^2 - \omega^2)^{-1}\delta(t-t'), \quad t,t' \in (t_a,t_b). \tag{3.26}$$

As remarked above, this function is defined only up to solutions of the homogeneous differential equation associated with the operator $-\partial_t^2 - \omega^2$. The boundary conditions removing this ambiguity are the same as for the fluctuations $\delta x(t)$, i.e., $G_{\omega^2}(t,t')$ vanishes if either t or t' or both hit an endpoint t_a or t_b (Dirichlet boundary condition). The Green function is symmetric in t and t'. For the sake of generality, we shall find the Green function also for the more general differential equation with time-dependent frequency,

$$[-\partial_t^2 - \Omega^2(t)]G_{\Omega^2}(t,t') = \delta(t-t'), \tag{3.27}$$

with the same boundary conditions.

There are several ways of calculating this explicitly.

3.2.1 Wronski Construction

The simplest way proceeds via the so-called *Wronski construction*, which is based on the following observation. For different time arguments, $t > t'$ or $t < t'$, the Green function $G_{\Omega^2}(t,t')$ has to solve the homogeneous differential equations

$$(-\partial_t^2 - \omega^2)G_{\Omega^2}(t,t') = 0, \qquad (-\partial_{t'}^2 - \omega^2)G_{\Omega^2}(t,t') = 0. \tag{3.28}$$

It must therefore be a linear combination of two independent solutions of the homogeneous differential equation in t as well as in t', and it must satisfy the Dirichlet boundary condition of vanishing at the respective endpoints.

Constant Frequency

If $\Omega^2(t) \equiv \omega^2$, this implies that for $t > t'$, $G_{\omega^2}(t,t')$ must be proportional to $\sin\omega(t_b - t)$ as well as to $\sin\omega(t'-t_a)$, leaving only the solution

$$G_{\omega^2}(t,t') = C\sin\omega(t_b-t)\sin\omega(t'-t_a), \qquad t > t'. \tag{3.29}$$

For $t < t'$, we obtain similarly

$$G_{\omega^2}(t,t') = C\sin\omega(t_b-t')\sin\omega(t-t_a), \qquad t < t'. \tag{3.30}$$

The two cases can be written as a single expression

$$G_{\omega^2}(t,t') = C\sin\omega(t_b-t_>)\sin\omega(t_<-t_a), \tag{3.31}$$

where the symbols $t_>$ and $t_<$ denote the larger and the smaller of the times t and t', respectively. The unknown constant C is fixed by considering coincident times $t = t'$. There, the time derivative of $G_{\omega^2}(t,t')$ must have a discontinuity which gives rise to the δ-function in (3.15). For $t > t'$, the derivative of (3.29) is

$$\partial_t G_{\omega^2}(t,t') = -C\omega \cos\omega(t_b - t)\sin\omega(t' - t_a), \tag{3.32}$$

whereas for $t < t'$

$$\partial_t G_{\omega^2}(t,t') = C\omega \sin\omega(t_b - t')\cos\omega(t - t_a). \tag{3.33}$$

At $t = t'$ we find the discontinuity

$$\partial_t G_{\omega^2}(t,t')|_{t=t'+\epsilon} - \partial_t G_{\omega^2}(t,t')|_{t=t'-\epsilon} = -C\omega \sin\omega(t_b - t_a). \tag{3.34}$$

Hence $-\partial_t^2 G_{\omega^2}(t,t')$ is proportional to a δ-function:

$$-\partial_t^2 G_{\omega^2}(t,t') = C\omega \sin\omega(t_b - t_a)\delta(t - t'). \tag{3.35}$$

By normalizing the prefactor to unity, we fix C and find the desired Green function:

$$G_{\omega^2}(t,t') = \frac{\sin\omega(t_b - t_>)\sin\omega(t_< - t_a)}{\omega\sin\omega(t_b - t_a)}. \tag{3.36}$$

It exists only if $t_b - t_a$ is not equal to an integer multiple of π/ω. This restriction was encountered before in the amplitude without external sources; its meaning was discussed in the two paragraphs following Eq. (2.168).

The constant in the denominator of (3.36) is the Wronski determinant (or *Wronskian*) of the two solutions $\xi(t) = \sin\omega(t_b - t)$ and $\eta(t) = \sin\omega(t - t_a)$ which was introduced in (2.222):

$$W[\xi(t), \eta(t)] \equiv \xi(t)\dot\eta(t) - \dot\xi(t)\eta(t). \tag{3.37}$$

An alternative expression for (3.36) is

$$G_{\omega^2}(t,t') = \frac{-\cos\omega(t_b - t_a - |t - t'|) + \cos\omega(t_b + t_a - t - t')}{2\omega\sin\omega(t_b - t_a)}. \tag{3.38}$$

In the limit $\omega \to 0$ we obtain the free-particle Green function

$$\begin{aligned} G_0(t,t') &= \frac{1}{(t_b - t_a)}(t_b - t_>)(t_< - t_a) \\ &= \frac{1}{t_b - t_a}\left[-tt' - \frac{1}{2}(t_b - t_a)|t - t'| + \frac{1}{2}(t_a + t_b)(t + t') - t_a t_b\right]. \end{aligned} \tag{3.39}$$

Time-Dependent Frequency

It is just as easy to find the Green functions of the more general differential equation (3.27) with a time-dependent oscillator frequency $\Omega(t)$. We construct first a so-called *retarded Green function* (compare page 38) as a product of a Heaviside function with a smooth function

$$G_{\Omega^2}(t,t') = \Theta(t-t')\Delta(t,t'). \tag{3.40}$$

Inserting this into the differential equation (3.27) we find

$$\begin{aligned}[-\partial_t^2 - \Omega^2(t)]G_{\Omega^2}(t,t') &= \Theta(t-t')\,[-\partial_t^2 - \Omega^2(t)]\Delta(t,t') \\ &- \dot{\delta}(t-t') - 2\partial_t\Delta(t,t')\delta(t-t').\end{aligned} \tag{3.41}$$

Expanding

$$\Delta(t,t') = \Delta(t,t) + [\partial_t\Delta(t,t')]_{t=t'}(t-t') + \frac{1}{2}[\partial_t^2\Delta(t,t')]_{t=t'}(t-t')^2 + \dots\ , \tag{3.42}$$

and using the fact that

$$(t-t')\dot{\delta}(t-t') = -\delta(t-t'), \quad (t-t')^n\dot{\delta}(t-t') = 0 \quad \text{for} \quad n>1, \tag{3.43}$$

the second line in (3.41) can be rewritten as

$$-\dot{\delta}(t-t')\Delta(t,t') - \delta(t-t')\partial_t\Delta(t,t'). \tag{3.44}$$

By choosing the initial conditions

$$\Delta(t,t) = 0, \quad \dot{\Delta}(t,t')|_{t'=t} = -1, \tag{3.45}$$

we satisfy the inhomogeneous differential equation (3.27) provided $\Delta(t,t')$ obeys the homogeneous differential equation

$$[-\partial_t^2 - \Omega^2(t)]\Delta(t,t') = 0, \quad \text{for} \ \ t>t'\ . \tag{3.46}$$

This equation is solved by a linear combination

$$\Delta(t,t') = \alpha(t')\xi(t) + \beta(t')\eta(t) \tag{3.47}$$

of any two independent solutions $\eta(t)$ and $\xi(t)$ of the homogeneous equation

$$[-\partial_t^2 - \Omega^2(t)]\xi(t) = 0, \qquad [-\partial_t^2 - \Omega^2(t)]\eta(t) = 0. \tag{3.48}$$

Their Wronski determinant $W = \xi(t)\dot{\eta}(t) - \dot{\xi}(t)\eta(t)$ is nonzero and, of course, time-independent, so that we can determine the coefficients in the linear combination (3.47) from (3.45) and find

$$\Delta(t,t') = \frac{1}{W}\left[\xi(t)\eta(t') - \xi(t')\eta(t)\right]. \tag{3.49}$$

The right-hand side contains the so-called Jacobi commutator of the two functions $\xi(t)$ and $\eta(t)$. Here we list a few useful algebraic properties of $\Delta(t,t')$:

$$\Delta(t,t') = \frac{\Delta(t_b,t)\Delta(t',t_a) - \Delta(t,t_a)\Delta(t_b,t')}{\Delta(t_b,t_a)}, \tag{3.50}$$

$$\Delta(t_b,t)\partial_{t_b}\,\Delta(t_b,t_a) - \Delta(t,t_a) = \Delta(t_b,t_a)\partial_t\Delta(t_b,t), \tag{3.51}$$

$$\Delta(t,t_a)\partial_{t_b}\Delta(t_b,t_a) - \Delta(t_b,t) = \Delta(t_b,t_a)\partial_t\Delta(t,t_a). \tag{3.52}$$

The retarded Green function (3.40) is so far not the unique solution of the differential equation (3.27), since one may always add a general solution of the homogeneous differential equation (3.48):

$$G_{\Omega^2}(t,t') = \Theta(t-t')\Delta(t,t') + a(t')\xi(t) + b(t')\eta(t), \tag{3.53}$$

with arbitrary coefficients $a(t')$ and $b(t')$. This ambiguity is removed by the Dirichlet boundary conditions

$$\begin{aligned} G_{\Omega^2}(t_b,t) &= 0, \quad t_b \neq t, \\ G_{\Omega^2}(t,t_a) &= 0, \quad t \neq t_a. \end{aligned} \tag{3.54}$$

Imposing these upon (3.53) leads to a simple algebraic pair of equations

$$a(t)\xi(t_a) + b(t)\eta(t_a) = 0, \tag{3.55}$$

$$a(t)\xi(t_b) + b(t)\eta(t_b) = \Delta(t,t_b). \tag{3.56}$$

Denoting the 2×2 -coefficient matrix by

$$\Lambda = \begin{pmatrix} \xi(t_a) & \eta(t_a) \\ \xi(t_b) & \eta(t_b) \end{pmatrix}, \tag{3.57}$$

we observe that under the condition

$$\det\Lambda = W\Delta(t_a,t_b) \neq 0, \tag{3.58}$$

the system (3.56) has a unique solution for the coefficients $a(t)$ and $b(t)$ in the Green function (3.53). Inserting this into (3.54) and using the identity (3.50), we obtain from this Wronski's general formula corresponding to (3.36)

$$G_{\Omega^2}(t,t') = \frac{\Theta(t-t')\Delta(t_b,t)\Delta(t',t_a) + \Theta(t'-t)\Delta(t,t_a)\Delta(t_b,t')}{\Delta(t_a,t_b)}. \tag{3.59}$$

At this point it is useful to realize that the functions in the numerator coincide with the two specific linearly independent solutions $D_a(t)$ and $D_b(t)$ of the homogenous differential equations (3.48) which were introduced in Eqs. (2.228) and (2.229). Comparing the initial conditions of $D_a(t)$ and $D_b(t)$ with that of the function $\Delta(t,t')$ in Eq. (3.45), we readily identify

$$D_a(t) \equiv \Delta(t,t_a), \qquad D_b(t) \equiv \Delta(t_b,t), \tag{3.60}$$

and formula (3.59) can be rewritten as

$$G_{\Omega^2}(t,t') = \frac{\Theta(t-t')D_b(t)D_a(t') + \Theta(t'-t)D_a(t)D_b(t')}{D_a(t_b)}. \tag{3.61}$$

It should be pointed out that this equation renders a unique and well-defined Green function if the differential equation $[-\partial_t^2 - \Omega^2(t)]y(t) = 0$ has no solutions with Dirichlet boundary conditions $y(t_a) = y(t_b) = 0$, generally called *zero-modes*. A zero mode would cause problems since it would certainly be one of the independent solutions of (3.49), say $\eta(t)$. Due to the property $\eta(t_a) = \eta(t_b) = 0$, however, the determinant of Λ would vanish, thus destroying the condition (3.58) which was necessary to find (3.59). Indeed, the function $\Delta(t,t')$ in (3.49) would remain undetermined since the boundary condition $\eta(t_a) = 0$ together with (3.55) implies that also $\xi(t_a) = 0$, making $W = \xi(t)\dot\eta(t) - \dot\xi(t)\eta(t)$ vanish at the initial time t_a, and thus for all times.

3.2.2 Spectral Representation

A second way of specifying the Green function explicitly is via its *spectral representation*.

Constant Frequency

For constant frequency $\Omega(t) \equiv \omega$, the fluctuations $\delta x(t)$ which satisfy the differential equation

$$(-\partial_t^2 - \omega^2)\,\delta x(t) = 0, \tag{3.62}$$

and vanish at the ends $t = t_a$ and $t = t_b$, are expanded into a complete set of orthonormal functions:

$$x_n(t) = \sqrt{\frac{2}{t_b - t_a}}\sin\nu_n(t - t_a), \tag{3.63}$$

with the frequencies [compare (2.115)]

$$\nu_n = \frac{\pi n}{t_b - t_a}. \tag{3.64}$$

These functions satisfy the orthonormality relations

$$\int_{t_a}^{t_b} dt\, x_n(t) x_{n'}(t) = \delta_{nn'}. \tag{3.65}$$

Since the operator $-\partial_t^2 - \omega^2$ is diagonal on $x_n(t)$, this is also true for the Green function $G_{\omega^2}(t,t') = (-\partial_t^2 - \omega^2)^{-1}\delta(t-t')$. Let G_n be its eigenvalues defined by

$$\int_{t_a}^{t_b} dt\, G_{\omega^2}(t,t') x_n(t') = G_n x_n(t). \tag{3.66}$$

Then we expand $G_{\omega^2}(t,t')$ as follows:

$$G_{\omega^2}(t,t') = \sum_{n=1}^{\infty} G_n x_n(t) x_n(t'). \tag{3.67}$$

By definition, the eigenvalues of $G_{\omega^2}(t,t')$ are the inverse eigenvalues of the differential operator $(-\partial_t^2 - \omega^2)$, which are $\nu_n^2 - \omega^2$. Thus

$$G_n = (\nu_n^2 - \omega^2)^{-1}, \tag{3.68}$$

and we arrive at the spectral representation of $G_{\omega^2}(t,t')$:

$$G_{\omega^2}(t,t') = \frac{2}{t_b - t_a} \sum_{n=1}^{\infty} \frac{\sin \nu_n(t-t_a) \sin \nu_n(t'-t_a)}{\nu_n^2 - \omega^2}. \tag{3.69}$$

We may use the trigonometric relation

$$\sin \nu_n(t_b - t) = -\sin \nu_n[(t-t_a) - (t_b - t_a)] = -(-1)^n \sin \nu_n(t-t_a)$$

to rewrite (3.69) as

$$G_{\omega^2}(t,t') = \frac{2}{t_b - t_a} \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\sin \nu_n(t_b - t) \sin \nu_n(t'-t_a)}{\nu_n^2 - \omega^2}. \tag{3.70}$$

These expressions make sense only if $t_b - t_a$ is not equal to an integer multiple of π/ω, where one of the denominators in the sums vanishes. This is the same range of $t_b - t_a$ as in the Wronski expression (3.36).

Time-Dependent Frequency

The spectral representation can also be written down for the more general Green function with a time-dependent frequency defined by the differential equation (3.27). If $y_n(t)$ are the eigenfunctions solving the differential equation with eigenvalue λ_n

$$K(t) y_n(t) = \lambda_n y_n(t), \tag{3.71}$$

and if these eigenfunctions satisfy the orthogonality and completeness relations

$$\int_{t_a}^{t_b} dt\, y_n(t) y_{n'}(t) = \delta_{nn'}, \tag{3.72}$$

$$\sum_n y_n(t) y_n(t') = \delta(t-t'), \tag{3.73}$$

and if, moreover, there exists no zero-mode for which $\lambda_n = 0$, then $G_{\Omega^2}(t,t')$ has the spectral representation

$$G_{\Omega^2}(t,t') = \sum_n \frac{y_n(t) y_n(t')}{\lambda_n}. \tag{3.74}$$

This is easily verified by multiplication with $K(t)$ using (3.71) and (3.73).

It is instructive to prove the equality between the Wronskian construction and the spectral representations (3.36) and (3.70). It will be useful to do this in several steps. In the present context, some of these may appear redundant. They will, however, yield intermediate results which will be needed in Chapters 7 and 18 when discussing path integrals occurring in quantum field theories.

3.3 Green Functions of First-Order Differential Equation

An important quantity of statistical mechanics are the Green functions $G^{\rm p}_{\Omega}(t,t')$ which solve the *first-order* differential equation

$$[i\partial_t - \Omega(t)]\, G_{\Omega}(t,t') = i\delta(t-t'), \quad t-t' \in [0, t_b - t_a), \tag{3.75}$$

or its Euclidean version $G^{\rm p}_{\Omega,{\rm e}}(\tau,\tau'')$ which solves the differential equation, obtained from (3.75) for $t=-i\tau$:

$$[\partial_\tau - \Omega(\tau)]\, G_{\Omega,{\rm e}}(\tau,\tau') = \delta(\tau-\tau'), \quad \tau-\tau' \in [0, \hbar\beta). \tag{3.76}$$

These can be calculated for an arbitrary function $\Omega(t)$.

3.3.1 Time-Independent Frequency

Consider first the simplest case of a Green function $G^{\rm p}_{\omega}(t,t')$ with fixed frequency ω which solves the *first-order* differential equation

$$(i\partial_t - \omega)G^{\rm p}_{\omega}(t,t') = i\delta(t-t'), \quad t-t' \in [0, t_b - t_a). \tag{3.77}$$

The equation determines $G^{\rm p}_{\omega}(t,t')$ only up to a solution $H(t,t')$ of the homogeneous differential equation $(i\partial_t - \omega)H(t,t') = 0$. The ambiguity is removed by imposing the *periodic* boundary condition

$$G^{\rm p}_{\omega}(t,t') \equiv G^{\rm p}_{\omega}(t-t') = G^{\rm p}_{\omega}(t-t'+t_b-t_a), \tag{3.78}$$

indicated by the superscript p. With this boundary condition, the Green function $G^{\rm p}_{\omega}(t,t')$ is translationally invariant in time. It depends only on the difference between t and t' and is periodic in it.

The spectral representation of $G^{\rm p}_{\omega}(t,t')$ can immediately be written down, assuming that $t_b - t_a$ does not coincide with an even multiple of π/ω:

$$G^{\rm p}_{\omega}(t-t') = \frac{1}{t_b-t_a}\sum_{m=-\infty}^{\infty} e^{-i\omega_m(t-t')}\frac{i}{\omega_m - \omega}. \tag{3.79}$$

The frequencies ω_m are twice as large as the previous ν_m's in (3.64):

$$\omega_m \equiv \frac{2\pi m}{t_b - t_a}, \qquad m = 0, \pm 1, \pm 2, \pm 3, \ldots\ . \tag{3.80}$$

As for the periodic orbits in Section 2.9, there are "about as many" ω_m as ν_m, since there is an ω_m for each positive *and* negative integer m, whereas the ν_m are all positive (see the last paragraph in that section). The frequencies (3.80) are the real-time analogs of the Matsubara frequencies (2.381) of quantum statistics with the usual correspondence $t_b - t_a = -i\hbar/k_BT$ of Eq. (2.330).

To calculate the spectral sum, we use the Poisson summation formula in the form (1.197):

$$\sum_{m=-\infty}^{\infty} f(m) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} e^{2\pi i\mu n} f(\mu). \tag{3.81}$$

Accordingly, we rewrite the sum over ω_m as an integral over ω', followed by an auxiliary sum over n which squeezes the variable ω' onto the proper discrete values $\omega_m = 2\pi m/(t_b - t_a)$:

$$G^{\rm p}_\omega(t) = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega'[t-(t_b-t_a)n]} \frac{i}{\omega' - \omega}. \tag{3.82}$$

At this point it is useful to introduce another Green function $G_\omega(t-t')$ associated with the first-order differential equation (3.77) on an *infinite* time interval:

$$G_\omega(t) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega' t} \frac{i}{\omega' - \omega}. \tag{3.83}$$

In terms of this function, the periodic Green function (3.82) can be written as a sum which exhibits in a most obvious way the periodicity under $t \to t + (t_b - t_a)$:

$$G^{\rm p}_\omega(t) = \sum_{n=-\infty}^{\infty} G_\omega(t - (t_b - t_a)n). \tag{3.84}$$

The advantage of using $G_\omega(t - t')$ is that the integral over ω' in (3.83) can easily be done. We merely have to prescribe how to treat the singularity at $\omega' = \omega$. This also removes the freedom of adding a homogeneous solution $H(t, t')$. To make the integral unique, we replace ω by $\omega - i\eta$ where η is a very small positive number, i.e., by the $i\eta$-prescription introduced after Eq. (2.168). This moves the pole in the integrand of (3.83) into the lower half of the complex ω'-plane, making the integral over ω' in $G_\omega(t)$ fundamentally different for $t < 0$ and for $t > 0$. For $t < 0$, the contour of integration can be closed in the complex ω'-plane by a semicircle in the *upper* half-plane at no extra cost, since $e^{-i\omega' t}$ is exponentially small there (see Fig. 3.1). With the integrand being analytic in the upper half-plane we can contract the contour to zero and find that the integral vanishes. For $t > 0$, on the other hand, the contour is closed in the lower half-plane containing a pole at $\omega' = \omega - i\eta$. When contracting the contour to zero, the integral picks up the residue at this pole and yields a factor $-2\pi i$. At the point $t = 0$, finally, we can close the contour either way. The integral over the semicircles is now nonzero, $\mp 1/2$, which has to be subtracted from the residues 0 and 1, respectively, yielding 1/2. Hence we find

$$\begin{aligned} G_\omega(t) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega' t} \frac{i}{\omega' - \omega + i\eta} \\ &= e^{-i\omega t} \times \begin{cases} 1 & \text{for} \quad t > 0, \\ \frac{1}{2} & \text{for} \quad t = 0, \\ 0 & \text{for} \quad t < 0. \end{cases} \end{aligned} \tag{3.85}$$

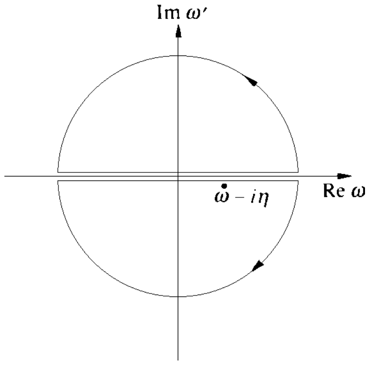

Figure 3.1 Pole in Fourier transform of Green functions $G_\omega^{\mathrm{p,a}}(t)$, and infinite semicircles in the upper (lower) half-plane which extend the integrals to a closed contour for $t < 0$ $(t > 0)$.

The vanishing of the Green function for $t < 0$ is the *causality property* of $G_\omega(t)$ discussed in (1.310) and (1.311). It is a general property of functions whose Fourier transforms are analytic in the upper half-plane.

The three cases in (3.85) can be collected into a single formula using the Heaviside function $\Theta(t)$ of Eq. (1.313):

$$G_\omega(t) = e^{-i\omega t}\bar{\Theta}(t). \tag{3.86}$$

The periodic Green function (3.84) can then be written as

$$G_\omega^{\mathrm{p}}(t) = \sum_{n=-\infty}^{\infty} e^{-i\omega[t-(t_b-t_a)n]}\bar{\Theta}(t-(t_b-t_a)n). \tag{3.87}$$

Being periodic in $t_b - t_a$, its explicit evaluation can be restricted to the basic interval

$$t \in [0, t_b - t_a). \tag{3.88}$$

Inside the interval $(0, t_b - t_a)$, the sum can be performed as follows:

$$\begin{aligned} G_\omega^{\mathrm{p}}(t) &= \sum_{n=-\infty}^{0} e^{-i\omega[t-(t_b-t_a)n]} = \frac{e^{-i\omega t}}{1-e^{-i\omega(t_b-t_a)}} \\ &= -i\frac{e^{-i\omega[t-(t_b-t_a)/2]}}{2\sin[\omega(t_b-t_a)/2]}, \quad t \in (0, t_b - t_a). \end{aligned} \tag{3.89}$$

At the point $t = 0$, the initial term with $\bar{\Theta}(0)$ contributes only $1/2$ so that

$$G_\omega^{\mathrm{p}}(0) = G_\omega^{\mathrm{p}}(0+) - \frac{1}{2}. \tag{3.90}$$

Outside the basic interval (3.88), the Green function is determined by its periodicity. For instance,

$$G_\omega^{\mathrm{p}}(t) = -i\frac{e^{-i\omega[t+(t_b-t_a)/2]}}{2\sin[\omega(t_b-t_a)/2]}, \quad t \in (-(t_b - t_a), 0). \tag{3.91}$$

Note that as t crosses the upper end of the interval $[0, t_b - t_a)$, the sum in (3.87) picks up an additional term (the term with $n = 1$). This causes a jump in $G^{\rm p}_\omega(t)$ which enforces the periodicity. At the upper point $t = t_b - t_a$, there is again a reduction by $1/2$ so that $G^{\rm p}_\omega(t_b - t_a)$ lies in the middle of the jump, just as the value $1/2$ lies in the middle of the jump of the Heaviside function $\bar\Theta(t)$.

The periodic Green function is of great importance in the quantum statistics of Bose particles (see Chapter 7). After a continuation of the time to imaginary values, $t \to -i\tau$, $t_b - t_a \to -i\hbar/k_BT$, it takes the form

$$G^{\rm p}_{\omega,{\rm e}}(\tau) = \frac{1}{1 - e^{-\hbar\omega/k_BT}} e^{-\omega\tau}, \qquad \tau \in (0, \hbar\beta), \tag{3.92}$$

where the subscript e records the Euclidean character of the time. The prefactor is related to the average boson occupation number of a particle state of energy $\hbar\omega$, given by the *Bose-Einstein distribution function*

$$n^{\rm b}_\omega = \frac{1}{e^{\hbar\omega/k_BT} - 1}. \tag{3.93}$$

In terms of it,

$$G^{\rm p}_{\omega,{\rm e}}(\tau) = (1 + n^{\rm b}_\omega) e^{-\omega\tau}, \qquad \tau \in (0, \hbar\beta). \tag{3.94}$$

The τ-behavior of the subtracted periodic Green function $G^{\rm p\prime}_{\omega,{\rm e}}(\tau) \equiv G^{\rm p}_{\omega,{\rm e}}(\tau) - 1/\hbar\beta\omega$ is shown in Fig. 3.2.

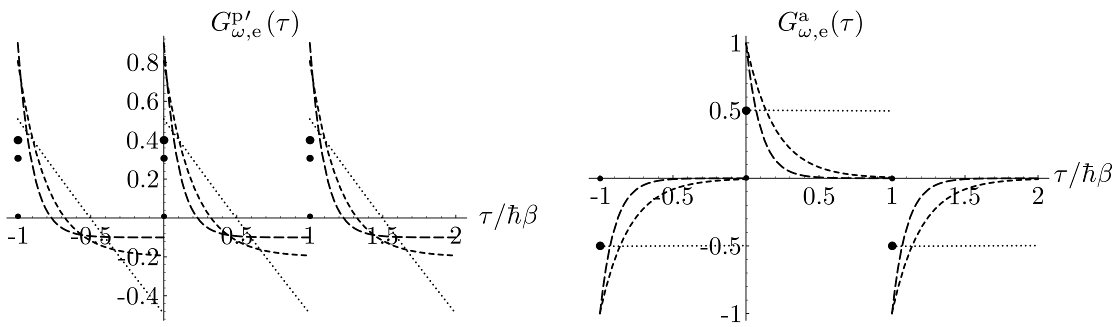

Figure 3.2 Subtracted periodic Green function $G^{\rm p\prime}_{\omega,{\rm e}} \equiv G^{\rm p}_{\omega,{\rm e}}(\tau) - 1/\hbar\beta\omega$ and antiperiodic Green function $G^{\rm a}_{\omega,{\rm e}}(\tau)$ for frequencies $\omega = (0,\, 5,\, 10)/\hbar\beta$ (with increasing dash length). The points show the values at the jumps of the three functions (with increasing point size) corresponding to the relation (3.90).

As a next step, we consider a Green function $G^{\rm p}_{\omega^2}(t)$ associated with the second-order differential operator $-\partial_t^2 - \omega^2$,

$$G^{\rm p}_{\omega^2}(t, t') = (-\partial_t^2 - \omega^2)^{-1} \delta(t - t'), \quad t - t' \in [t_a, t_b), \tag{3.95}$$

which satisfies the periodic boundary condition:

$$G^{\rm p}_{\omega^2}(t, t') \equiv G^{\rm p}_{\omega^2}(t - t') = G^{\rm p}_{\omega^2}(t - t' + t_b - t_a). \tag{3.96}$$

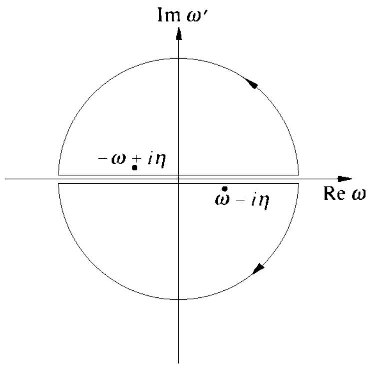

Figure 3.3 Two poles in Fourier transform of Green function $G^{\mathrm{p,a}}_{\omega^2}(t)$.

Just like $G^{\mathrm{p}}_{\omega}(t,t')$, this periodic Green function depends only on the time difference $t-t'$. It obviously has the spectral representation

$$G^{\mathrm{p}}_{\omega^2}(t) = \frac{1}{t_b - t_a} \sum_{m=-\infty}^{\infty} e^{-i\omega_m t} \frac{1}{\omega_m^2 - \omega^2}, \tag{3.97}$$

which makes sense as long as $t_b - t_a$ is not equal to an even multiple of π/ω. At infinite $t_b - t_a$, the sum becomes an integral over ω_m with singularities at $\pm\omega$ which must be avoided by an $i\eta$-prescription, which adds a negative imaginary part to the frequency ω [compare the discussion after Eq. (2.168)]. This fixes also the continuation from small $t_b - t_a$ beyond the multiple values of π/ω. By decomposing

$$\frac{1}{\omega'^2 - \omega^2 + i\eta} = \frac{1}{2i\omega}\left(\frac{i}{\omega' - \omega + i\eta} - \frac{i}{\omega' + \omega - i\eta}\right), \tag{3.98}$$

the calculation of the Green function (3.97) can be reduced to the previous case. The positions of the two poles of (3.98) in the complex ω'-plane are illustrated in Fig. 3.3. In this way we find, using (3.89),

$$\begin{aligned} G^{\mathrm{p}}_{\omega^2}(t) &= \frac{1}{2\omega i}\left[G^{\mathrm{p}}_{\omega}(t) - G^{\mathrm{p}}_{-\omega}(t)\right] \\ &= -\frac{1}{2\omega}\frac{\cos\omega[t-(t_b-t_a)/2]}{\sin[\omega(t_b-t_a)/2]}, \quad t \in [0, t_b - t_a). \end{aligned} \tag{3.99}$$

In $G^{\mathrm{p}}_{-\omega}(t)$ one must keep the small negative imaginary part attached to the frequency ω. For an infinite time interval $t_b - t_a$, this leads to a Green function $G^{\mathrm{p}}_{\omega^2}(t-t')$: also

$$G_{-\omega}(t) = -e^{-i\omega t}\bar{\Theta}(-t). \tag{3.100}$$

The directional change in encircling the pole in the ω' -integral leads to the exchange $\bar{\Theta}(t) \to -\bar{\Theta}(-t)$.

Outside the basic interval $t \in [0, t_b - t_a)$, the function is determined by its periodicity. For $t \in [-(t_b - t_a), 0)$, we may simply replace t by $|t|$.

As a further step we consider another Green function $G^{\rm a}_\omega(t,t')$. It fulfills the same first-order differential equation $i\partial_t-\omega$ as $G^{\rm p}_\omega(t,t')$:

$$(i\partial_t-\omega)G^{\rm a}_\omega(t,t')=i\delta(t-t'),\quad t-t'\in[0,t_b-t_a),\tag{3.101}$$

but in contrast to $G^{\rm p}_\omega(t,t')$ it satisfies the antiperiodic boundary condition

$$G^{\rm a}_\omega(t,t')\equiv G^{\rm a}_\omega(t-t')=-G^{\rm a}_\omega(t-t'+t_b-t_a).\tag{3.102}$$

As for periodic boundary conditions, the Green function $G^{\rm a}_\omega(t,t')$ depends only on the time difference $t-t'$. In contrast to $G^{\rm p}_\omega(t,t')$, however, $G^{\rm a}_\omega(t,t')$ changes sign under a shift $t\to t+(t_b-t_a)$. The Fourier expansion of $G^{\rm a}_\omega(t-t')$ is

$$G^{\rm a}_\omega(t)=\frac{1}{t_b-t_a}\sum_{m=-\infty}^{\infty}e^{-i\omega^{\rm f}_m t}\frac{i}{\omega^{\rm f}_m-\omega},\tag{3.103}$$

where the frequency sum covers the *odd* Matsubara-like frequencies

$$\omega^{\rm f}_m=\frac{\pi(2m+1)}{t_b-t_a}.\tag{3.104}$$

The superscript f stands for *fermionic* since these frequencies play an important role in the statistical mechanics of particles with Fermi statistics to be explained in Section 7.10 [see Eq. (7.414)].

The antiperiodic Green functions are obtained from a sum similar to (3.82), but modified by an additional phase factor $e^{i\pi n}=(-)^n$. When inserted into the Poisson summation formula (3.81), such a phase is seen to select the half-integer numbers in the integral instead of the integer ones:

$$\sum_{m=-\infty}^{\infty}f(m+1/2)=\int_{-\infty}^{\infty}d\mu\sum_{n=-\infty}^{\infty}(-)^n e^{2\pi i\mu n}f(\mu).\tag{3.105}$$

Using this formula, we can expand

$$\begin{aligned}G^{\rm a}_\omega(t)&=\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}(-)^n e^{-i\omega'[t-(t_b-t_a)n]}\frac{i}{\omega'-\omega+i\eta}\\&=\sum_{n=-\infty}^{\infty}(-)^n G_\omega(t-(t_b-t_a)n),\end{aligned}\tag{3.106}$$

or, more explicitly,

$$G^{\rm a}_\omega(t)=\sum_{n=-\infty}^{\infty}e^{-i\omega[t-(t_b-t_a)n]}(-)^n\bar\Theta(t-(t_b-t_a)n).\tag{3.107}$$

For $t\in[0,t_b-t_a)$, this gives

$$\begin{aligned}G^{\rm a}_\omega(t)&=\sum_{n=-\infty}^{0}e^{-i\omega[t-(t_b-t_a)n]}(-)^n=\frac{e^{i\omega t}}{1+e^{-i\omega(t_b-t_a)}}\\&=\frac{e^{-i\omega[t-(t_b-t_a)/2]}}{2\cos[\omega(t_b-t_a)/2]},\quad t\in[0,t_b-t_a).\end{aligned}\tag{3.108}$$

Outside the interval $t \in [0, t_b - t_a)$, the function is defined by its antiperiodicity. The τ-behavior of the antiperiodic Green function $G^{\rm a}_{\omega,{\rm e}}(\tau)$ is also shown in Fig. 3.2.

In the limit $\omega \to 0$, the right-hand side of (3.108) is equal to 1/2, and the antiperiodicity implies that

$$G^{\rm a}_0(t) = \frac{1}{2}\,\epsilon(t), \qquad t \in [-(t_b - t_a), (t_b - t_a)]. \tag{3.109}$$

Antiperiodic Green functions play an important role in the quantum statistics of Fermi particles. After analytically continuing t to the imaginary time $-i\tau$ with $t_b - t_a \to -i\hbar/k_BT$, the expression (3.108) takes the form

$$G^{\rm a}_{\omega,{\rm e}}(\tau) = \frac{1}{1 + e^{-\hbar\omega/k_BT}} e^{-\omega\tau}, \quad \tau \in [0, \hbar\beta). \tag{3.110}$$

The prefactor is related to the average Fermi occupation number of a state of energy $\hbar\omega$, given by the *Fermi-Dirac distribution function*

$$n^{\rm f}_\omega = \frac{1}{e^{\hbar\omega/k_BT} + 1}. \tag{3.111}$$

In terms of it,

$$G^{\rm a}_{\omega,{\rm e}}(\tau) = (1 - n^{\rm f}_\omega) e^{-\omega\tau}, \quad \tau \in [0, \hbar\beta). \tag{3.112}$$

With the help of $G^{\rm a}_\omega(t)$, we form the antiperiodic analog of (3.97), (3.99), i.e., the antiperiodic Green function associated with the second-order differential operator $-\partial_t^2 - \omega^2$:

$$\begin{aligned} G^{\rm a}_{\omega^2}(t) &= \frac{1}{t_b - t_a} \sum_{m=0}^{\infty} e^{-i\omega^{\rm f}_m t} \frac{1}{\omega^{{\rm f}\,2}_m - \omega^2} \\ &= \frac{1}{2\omega i}[G^{\rm a}_\omega(t) - G^{\rm a}_{-\omega}(t)] \\ &= -\frac{1}{2\omega} \frac{\sin\omega[t - (t_b - t_a)/2]}{\cos[\omega(t_b - t_a)/2]}, \quad t \in [0, t_b - t_a]. \end{aligned} \tag{3.113}$$

Outside the basic interval $t \in [0, t_b - t_a]$, the Green function is determined by its antiperiodicity. If, for example, $t \in [-(t_b - t_a), 0]$, one merely has to replace t by $|t|$.

Note that the Matsubara sums

$$G^{\rm p}_{\omega^2,{\rm e}}(0) = \frac{1}{\hbar\beta} \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + \omega^2}, \qquad G^{\rm p}_{\omega,{\rm e}}(0) = \frac{1}{\hbar\beta} \sum_{m=-\infty}^{\infty} \frac{1}{\omega^{{\rm f}\,2}_m + \omega^2}, \tag{3.114}$$

can also be calculated from the combinations of the simple Green functions (3.79) and (3.103):

$$\frac{1}{2\omega}\left[G^{\rm p}_{\omega,{\rm e}}(\eta) + G^{\rm p}_{\omega,{\rm e}}(-\eta)\right] = \frac{1}{2\omega}\left[G^{\rm p}_{\omega,{\rm e}}(\eta) + G^{\rm p}_{\omega,{\rm e}}(\hbar\beta - \eta)\right] = \frac{1}{2\omega}\left(1 + n^{\rm b}_\omega\right)\left(1 + e^{-\beta\omega}\right)$$

$$= \frac{1}{2\omega}\coth\frac{\hbar\omega\beta}{2}, \tag{3.115}$$

$$\frac{1}{2\omega}\left[G^{\rm a}_{\omega,{\rm e}}(\eta)+G^{\rm a}_{\omega,{\rm e}}(-\eta)\right] = \frac{1}{2\omega}\left[G^{\rm a}_{\omega,{\rm e}}(\eta)-G^{\rm a}_{\omega,{\rm e}}(\hbar\beta-\eta)\right] = \frac{1}{2\omega}\left(1-n^{\rm f}_\omega\right)\left(1-e^{-\beta\omega}\right)$$

$$= \frac{1}{2\omega}\tanh\frac{\hbar\omega\beta}{2}, \tag{3.116}$$

where η is an infinitesimal positive number needed to specify on which side of the jump the Green functions $G^{\rm p,a}_{\omega,{\rm e}}(\tau)$ at $\tau=0$ have to be evaluated (see Fig. 3.2).

3.3.2 Time-Dependent Frequency

The above results (3.89) and (3.108) for the periodic and antiperiodic Green functions of the first-order differential operator $(i\partial_t-\omega)$ can easily be found also for arbitrary time-dependent frequencies $\Omega(t)$, thus solving (3.75). We shall look for the retarded version which vanishes for $t<t'$. This property is guaranteed by the ansatz containing the Heaviside function (1.313):

$$G_\Omega(t,t') = \bar\Theta(t-t')g(t,t'). \tag{3.117}$$

Using the property (1.307) of the Heaviside function, that its time derivative yields the δ-function, and normalizing $g(t,t)$ to be equal to 1, we see that $g(t,t')$ must solve the homogenous differential equation

$$\left[i\partial_t-\Omega(t)\right]g(t,t') = 0. \tag{3.118}$$

The solution is

$$g(t,t') = K(t')e^{-i\int_c^t dt''\,\Omega(t'')}. \tag{3.119}$$

The condition $g(t,t)=1$ fixes $K(t)=e^{i\int_c^t dt''\,\Omega(t'')}$, so that we obtain

$$G_\Omega(t,t') = \bar\Theta(t-t')e^{-i\int_{t'}^t dt''\,\Omega(t'')}. \tag{3.120}$$

The most general Green function is a sum of this and an arbitrary solution of the homogeneous equation (3.118):

$$G_\Omega(t,t') = \left[\bar\Theta(t-t')+C(t')\right]e^{-i\int_{t'}^t dt''\,\Omega(t'')}. \tag{3.121}$$

For a periodic frequency $\Omega(t)$ we impose periodic boundary conditions upon the Green function, setting $G_\Omega(t_a,t')=G_\Omega(t_b,t')$. This is ensured if for $t_b>t>t'>t_a$:

$$C(t')e^{-i\int_{t'}^{t_a} dt''\,\Omega(t'')} = \left[1+C(t')\right]e^{-i\int_{t'}^{t_b} dt''\,\Omega(t'')}. \tag{3.122}$$

This equation is solved by a t'-independent $C(t')$:

$$C = n^{\rm p}_\Omega \equiv \frac{1}{e^{i\int_{t_a}^{t_b} dt''\,\Omega(t'')}-1}. \tag{3.123}$$

Hence we obtain the periodic Green function

$$G_\Omega^{\rm p}(t,t') = \left[\bar\Theta(t-t') + n_\Omega^{\rm p}\right] e^{-i\int_{t'}^{t} dt''\,\Omega(t'')}. \tag{3.124}$$

For antiperiodic boundary conditions we obtain the same equation with $n_\Omega^{\rm p}$ replaced by $-n_\Omega^{\rm a}$ where

$$n_\Omega^{\rm a} \equiv \frac{1}{e^{i\int_{t_a}^{t_b} dt\,\Omega(t)} + 1}. \tag{3.125}$$

Note that a sign change in the time derivative of the first-order differential equation (3.75) to

$$\left[-i\partial_t - \Omega(t)\right] G_\Omega(t,t') = i\delta(t-t') \tag{3.126}$$

has the effect of interchanging in the time variable t and t' of the Green function Eq. (3.120).

If the frequency $\Omega(t)$ is a matrix, all exponentials have to be replaced by time-ordered exponentials [recall (1.252)]

$$e^{i\int_{t_a}^{t_b} dt\,\Omega(t)} \to \hat T e^{i\int_{t_a}^{t_b} dt\,\Omega(t)}. \tag{3.127}$$

As remarked in Subsection 2.15.4, this integral cannot, in general, be calculated explicitly. A simple formula is obtained only if the matrix $\Omega(t)$ varies only little around a fixed matrix Ω_0.

For imaginary times $\tau = it$ we generalize the results (3.92) and (3.110) for the periodic and antiperiodic imaginary-time Green functions of the first-order differential equation (3.76) to time-dependent periodic frequencies $\Omega(\tau)$. Here the Green function (3.120) becomes

$$G_\Omega(\tau,\tau') = \bar\Theta(\tau-\tau') e^{-\int_{\tau'}^{\tau} d\tau''\,\Omega(\tau'')}, \tag{3.128}$$

and the periodic Green function (3.124):

$$G_\Omega(\tau,\tau') = \left[\bar\Theta(\tau-\tau') + n^{\rm b}\right] e^{-\int_{\tau'}^{\tau} d\tau''\,\Omega(\tau'')}, \tag{3.129}$$

where

$$n^{\rm b} \equiv \frac{1}{e^{\int_0^{\hbar\beta} d\tau''\,\Omega(\tau'')} - 1} \tag{3.130}$$

is the generalization of the Bose distribution function in Eq. (3.93). For antiperiodic boundary conditions we obtain the same equation, except that the generalized Bose distribution function is replaced by the negative of the generalized Fermi distribution function in Eq. (3.111):

$$n^{\rm f} \equiv \frac{1}{e^{\int_0^{\hbar\beta} d\tau''\,\Omega(\tau'')} + 1}. \tag{3.131}$$

For the opposite sign of the time derivative in (3.128), the arguments τ and τ' are interchanged.

From the Green functions (3.124) or (3.128) we may find directly the trace of the logarithm of the operators $[-i\partial_t + \Omega(t)]$ or $[\partial_\tau + \Omega(\tau)]$. At imaginary time, we multiply $\Omega(\tau)$ with a strength parameter g, and use the formula

$$\mathrm{Tr}\log\left[\partial_\tau + g\Omega(\tau)\right] = \int_0^g dg'\, G_{g'\Omega}(\tau,\tau). \tag{3.132}$$

Inserting on the right-hand side of Eq. (3.129), we find for $g = 1$:

$$\begin{aligned}\mathrm{Tr}\log\left[\partial_\tau + \Omega(\tau)\right] &= \log\left\{2\sinh\left[\frac{1}{2}\int_0^{\hbar\beta} d\tau''\,\Omega(\tau'')\right]\right\}\\ &= \frac{1}{2}\int_0^{\hbar\beta} d\tau''\,\Omega(\tau'') + \log\left[1 - e^{-\int_0^{\hbar\beta} d\tau''\,\Omega(\tau'')}\right],\end{aligned} \tag{3.133}$$

which reduces at low temperature to

$$\mathrm{Tr}\log\left[\partial_\tau + \Omega(\tau)\right] = \frac{1}{2}\int_0^{\hbar\beta} d\tau''\,\Omega(\tau''). \tag{3.134}$$

The result is the same for the opposite sign of the time derivative and the trace of the logarithm is sensitive only to $\bar\Theta(\tau - \tau')$ at $\tau = \tau'$, where it is equal to $1/2$.

As an exercise for dealing with distributions it is instructive to rederive this result in the following perturbative way. For a positive $\Omega(\tau)$, we introduce an infinitesimal positive quantity η and decompose

$$\begin{aligned}\mathrm{Tr}\log\left[\pm\partial_\tau + \Omega(\tau)\right] &= \mathrm{Tr}\log\left[\pm\partial_\tau + \eta\right] + \mathrm{Tr}\log\left[1 + (\pm\partial_\tau + \eta)^{-1}\,\Omega(\tau)\right]\\ &= \mathrm{Tr}\log\left[\pm\partial_\tau + \eta\right] + \mathrm{Tr}\log\left[1 + (\pm\partial_\tau + \eta)^{-1}\,\Omega(\tau)\right].\end{aligned} \tag{3.135}$$

The first term $\mathrm{Tr}\log\left[\pm\partial_\tau + \eta\right] = \mathrm{Tr}\log\left[\pm\partial_\tau + \eta\right] = \int_{-\infty}^{\infty} d\omega\log\omega$ vanishes since $\int_{-\infty}^{\infty} d\omega\log\omega = 0$ in dimensional regularization by Veltman's rule [see (2.508)]. Using the Green functions

$$\left[\pm\partial_\tau + \eta\right]^{-1}(\tau,\tau') = \left\{\begin{matrix}\bar\Theta(\tau - \tau')\\ \bar\Theta(\tau' - \tau)\end{matrix}\right\}, \tag{3.136}$$

the second term can be expanded in a Taylor series

$$\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\int d\tau_1\cdots \mathrm{d}\tau_n\,\Omega(\tau_1)\bar\Theta(\tau_1-\tau_2)\Omega(\tau_2)\bar\Theta(\tau_2-\tau_3)\cdots\Omega(\tau_n)\bar\Theta(\tau_n-\tau_1). \tag{3.137}$$

For the lower sign of $\pm\partial_\tau$, the Heaviside functions have reversed arguments $\tau_2 - \tau_1, \tau_3 - \tau_2, \ldots, \tau_1 - \tau_n$. The integrals over a cyclic product of Heaviside functions in (3.137) are zero since the arguments $\tau_1, \ldots, \tau_n$ are time-ordered which makes the argument of the last factor $\bar\Theta(\tau_n - \tau_1)$ [or $\bar\Theta(\tau_1 - \tau_n)$] negative and thus $\bar\Theta(\tau_n - \tau_1) = 0$ [or $\bar\Theta(\tau_1 - \tau_n)$]. Only the first term survives yielding

$$\int d\tau_1\,\Omega(\tau_1)\bar\Theta(\tau_1 - \tau_1) = \frac{1}{2}\int d\tau\,\Omega(\tau), \tag{3.138}$$

such that we re-obtain the result (3.134).

This expansion (3.133) can easily be generalized to an arbitrary matrix $\Omega(\tau)$ or a time-dependent operator, $\hat{H}(\tau)$. Since $\hat{H}(\tau)$ and $\hat{H}(\tau')$ do not necessarily commute, the generalization is

$$\mathrm{Tr}\log[\hbar\partial_\tau + \hat{H}(\tau)] = \frac{1}{2\hbar}\mathrm{Tr}\left[\int_0^{\hbar\beta} d\tau\, \hat{H}(\tau)\right] - \sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Tr}\left[\hat{T}e^{-n\int_0^{\hbar\beta} d\tau''\, \hat{H}(\tau'')/\hbar}\right], \tag{3.139}$$

where $\hat{T}$ is the time ordering operator (1.241). Each term in the sum contains a power of the time evolution operator (1.255).

3.4 Summing Spectral Representation of Green Function

After these preparations we are ready to perform the spectral sum (3.70) for the Green function of the differential equation of second order with Dirichlet boundary conditions. Setting $t_2 \equiv t_b - t,\ t_1 \equiv t' - t_a$, we rewrite (3.70) as

$$\begin{aligned} G_{\omega^2}(t,t') &= \frac{2}{t_b - t_a}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(2i)^2}\frac{(e^{i\nu_n t_2} - e^{-i\nu_n t_2})(e^{i\nu_n t_1} - e^{-i\nu_n t_1})}{\nu_n^2 - \omega^2} \\ &= \frac{1}{2}\frac{1}{t_b - t_a}\sum_{n=1}^{\infty}(-1)^n\frac{[(e^{-i\nu_n(t_2+t_1)} - e^{-i\nu_n(t_2-t_1)}) + \text{c.c.}]}{\nu_n^2 - \omega^2} \\ &= \frac{1}{2}\frac{1}{t_b - t_a}\sum_{n=-\infty}^{\infty}(-1)^n\frac{e^{-i\nu_n(t_2+t_1)} - e^{-i\nu_n(t_2-t_1)}}{\nu_n^2 - \omega^2}. \end{aligned} \tag{3.140}$$

We now separate even and odd frequencies ν_n and write these as bosonic and fermionic Matsubara frequencies $\omega_m = \nu_{2m}$ and $\omega_m^{\mathrm{f}} = \nu_{2m+1}$, respectively, recalling the definitions (3.80) and (3.104). In this way we obtain

$$\begin{aligned} G_{\omega^2}(t,t') = \frac{1}{2}\Bigg\{ &\frac{1}{t_b - t_a}\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m(t_2+t_1)}}{\omega_m^2 - \omega^2} - \frac{1}{t_b - t_a}\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m^{\mathrm{f}}(t_2+t_1)}}{\omega_m^{\mathrm{f}\,2} - \omega^2} \\ &- \frac{1}{t_b - t_a}\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m(t_2-t_1)}}{\omega_m^2 - \omega^2} + \frac{1}{t_b - t_a}\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m^{\mathrm{f}}(t_2-t_1)}}{\omega_m^{\mathrm{f}\,2} - \omega^2}\Bigg\}. \end{aligned} \tag{3.141}$$

Inserting on the right-hand side the periodic and antiperiodic Green functions (3.99) and (3.108), we obtain the decomposition

$$G_{\omega^2}(t,t') = \frac{1}{2}\left[G_\omega^{\mathrm{p}}(t_2+t_1) - G_\omega^{\mathrm{a}}(t_2+t_1) - G_\omega^{\mathrm{p}}(t_2-t_1) + G_\omega^{\mathrm{a}}(t_2-t_1)\right]. \tag{3.142}$$

Using (3.99) and (3.113) we find that

$$G_\omega^{\mathrm{p}}(t_2+t_1) - G_\omega^{\mathrm{p}}(t_2-t_1) = \frac{\sin\omega[t_2 - (t_b - t_a)/2]\sin\omega t_1}{\omega\sin[\omega(t_b - t_a)/2]}, \tag{3.143}$$

$$G_\omega^{\mathrm{a}}(t_2+t_1) - G_\omega^{\mathrm{a}}(t_2-t_1) = -\frac{\cos\omega[t_2 - (t_b - t_a)/2]\sin\omega t_1}{\omega\cos[\omega(t_b - t_a)/2]}, \tag{3.144}$$

such that (3.142) becomes

$$G_{\omega^2}(t,t') = \frac{1}{\omega \sin \omega(t_b - t_a)} \sin \omega t_2 \sin \omega t_1, \tag{3.145}$$

in agreement with the earlier result (3.36).

An important limiting case is

$$t_a \to -\infty, \quad t_b \to \infty. \tag{3.146}$$

Then the boundary conditions become irrelevant and the Green function reduces to

$$G_{\omega^2}(t,t') = -\frac{i}{2\omega} e^{-i\omega|t-t'|}, \tag{3.147}$$

which obviously satisfies the second-order differential equation

$$(-\partial_t^2 - \omega^2) G_{\omega^2}(t,t') = \delta(t-t'). \tag{3.148}$$

The periodic and antiperiodic Green functions $G^{\rm p}_{\omega^2}(t,t')$ and $G^{\rm a}_{\omega^2}(t,t')$ at finite $t_b - t_a$ in Eqs. (3.99) and (3.113) are obtained from $G_{\omega^2}(t,t')$ by summing over all periodic repetitions [compare (3.106)]

$$\begin{aligned} G^{\rm p}_{\omega^2}(t,t') &= \sum_{n=-\infty}^{\infty} G(t+n(t_b-t_a),t'), \\ G^{\rm a}_{\omega^2}(t,t') &= \sum_{n=-\infty}^{\infty} (-1)^n G_{\omega^2}(t+n(t_b-t_a),t'). \end{aligned} \tag{3.149}$$

For completeness let us also sum the spectral representation with the normalized wave functions [compare (3.98)–(3.69)]

$$x_0(t) = \sqrt{\frac{1}{t_b - t_a}}, \qquad x_n(t) = \sqrt{\frac{2}{t_b - t_a}} \cos \nu_n (t - t_a), \tag{3.150}$$

which reads:

$$G^{\rm N}_{\omega^2}(t,t') = \frac{2}{t_b - t_a} \left[-\frac{1}{2\omega^2} + \sum_{n=1}^{\infty} \frac{\cos \nu_n(t-t_a) \cos \nu_n(t'-t_a)}{\nu_n^2 - \omega^2} \right]. \tag{3.151}$$

It satisfies the *Neumann boundary conditions*

$$\partial_t G^{\rm N}_{\omega^2}(t,t')\Big|_{t=t_b} = 0, \qquad \partial_{t'} G^{\rm N}_{\omega^2}(t,t')\Big|_{t'=t_a} = 0. \tag{3.152}$$

The spectral representation (3.151) can be summed by a decomposition (3.140), if that the lowest line has a plus sign between the exponentials, and (3.142) becomes

$$G^{\rm N}_{\omega^2}(t,t') = \frac{1}{2} \left[G^{\rm p}_{\omega}(t_2+t_1) - G^{\rm a}_{\omega}(t_2+t_1) + G^{\rm p}_{\omega}(t_2-t_1) - G^{\rm a}_{\omega}(t_2-t_1) \right]. \tag{3.153}$$

Using now (3.99) and (3.113) we find that

$$G^{\rm p}_{\omega}(t_2+t_1)+G^{\rm p}_{\omega}(t_2-t_1)=-\frac{\cos\omega[t_2-(t_b-t_a)/2]\cos\omega t_1}{\omega\sin[\omega(t_b-t_a)/2]}, \tag{3.154}$$

$$G^{\rm a}_{\omega}(t_2+t_1)+G^{\rm a}_{\omega}(t_2-t_1)=-\frac{\sin\omega[t_2-(t_b-t_a)/2]\cos\omega t_1}{\omega\cos[\omega(t_b-t_a)/2]}, \tag{3.155}$$

and we obtain instead of (3.145):

$$G^{\rm N}_{\omega^2}(t,t')=-\frac{1}{\omega\sin\omega(t_b-t_a)}\cos\omega(t_b-t_>)\,\cos\omega(t_<-t_a), \tag{3.156}$$

which has the small-ω expansion

$$G^{\rm N}_{\omega^2}(t,t')\underset{\omega^2\approx 0}{\approx}-\frac{1}{(t_b-t_a)\omega^2}+\frac{t_b-t_a}{3}-\frac{1}{2}|t-t'|-\frac{1}{2}(t+t')+\frac{1}{2(t_b-t_a)}\left(t^2+t'^2\right). \tag{3.157}$$

3.5 Wronski Construction for Periodic and Antiperiodic Green Functions

The Wronski construction in Subsection 3.2.1 of Green functions with time-dependent frequency $\Omega(t)$ satisfying the differential equation (3.27)

$$[-\partial_t^2-\Omega^2(t)]G_{\Omega^2}(t,t')=\delta(t-t') \tag{3.158}$$

can easily be carried over to the Green functions $G^{\rm p,a}_{\Omega^2}(t,t')$ with periodic and antiperiodic boundary conditions. As in Eq. (3.53) we decompose

$$G^{\rm p,a}_{\Omega^2}(t,t')=\bar\Theta(t-t')\Delta(t,t')+a(t')\xi(t)+b(t')\eta(t), \tag{3.159}$$

with independent solutions of the homogenous equations $\xi(t)$ and $\eta(t)$, and insert this into (3.27), where $\delta^{\rm p,a}(t-t')$ is the periodic version of the δ-function

$$\delta^{\rm p,a}(t-t')\equiv\sum_{n=-\infty}^{\infty}\delta(t-t'-n\hbar\beta)\left\{\begin{array}{c}1\\(-1)^n\end{array}\right\}, \tag{3.160}$$

and $\Omega(t)$ is assumed to be periodic or antiperiodic in t_b-t_a. This yields again for $\Delta(t,t')$ the homogeneous initial-value problem (3.46), (3.45),

$$[-\partial_t^2-\Omega^2(t)]\Delta(t,t')=0;\quad \Delta(t,t)=0,\ \ \partial_t\Delta(t,t')|_{t'=t}=-1. \tag{3.161}$$

The periodic boundary conditions lead to the system of equations

$$\begin{aligned} a(t)[\xi(t_b)\mp\xi(t_a)]+b(t)[\eta(t_b)\mp\eta(t_a)] &= -\Delta(t_b,t),\\ a(t)[\dot\xi(t_b)\mp\dot\xi(t_a)]+b(t)[\dot\eta(t_b)\mp\dot\eta(t_a)] &= -\partial_t\Delta(t_b,t). \end{aligned} \tag{3.162}$$

Defining now the constant 2×2 -matrices

$$\bar{\Lambda}^{\rm p,a}(t_a,t_b) = \left(\begin{array}{cc} \xi(t_b) \mp \xi(t_a) & \eta(t_b) \mp \eta(t_a) \\ \dot{\xi}(t_b) \mp \dot{\xi}(t_a) & \dot{\eta}(t_b) \mp \dot{\eta}(t_a) \end{array} \right), \tag{3.163}$$

the condition analogous to (3.58),

$$\det \bar{\Lambda}^{\rm p,a}(t_a,t_b) = W\, \bar{\Delta}^{\rm p,a}(t_a,t_b) \neq 0, \tag{3.164}$$

with

$$\bar{\Delta}^{\rm p,a}(t_a,t_b) = 2 \pm \partial_t \Delta(t_a,t_b) \pm \partial_t \Delta(t_b,t_a), \tag{3.165}$$

enables us to obtain the unique solution to Eqs. (3.162). After some algebra using the identities (3.51) and (3.52), the expression (3.159) for Green functions with periodic and antiperiodic boundary conditions can be cast into the form

$$G^{\rm p,a}_{\Omega^2}(t,t') = G_{\Omega^2}(t,t') \mp \frac{[\Delta(t,t_a) \pm \Delta(t_b,t)][\Delta(t',t_a) \pm \Delta(t_b,t')]}{\bar{\Delta}^{\rm p,a}(t_a,t_b)\Delta(t_a,t_b)}, \tag{3.166}$$

where $G_{\Omega^2}(t,t')$ is the Green function (3.59) with Dirichlet boundary conditions. As in (3.59) we may replace the functions on the right-hand side by the solutions $D_a(t)$ and $D_b(t)$ defined in Eqs. (2.228) and (2.229) with the help of (3.60).

The right-hand side of (3.166) is well-defined unless the operator $K(t) = -\partial_t^2 - \Omega^2(t)$ has a zero-mode, say $\eta(t)$, with periodic or antiperiodic boundary conditions $\eta(t_b) = \pm\eta(t_a)$, $\dot{\eta}(t_b) = \pm\dot{\eta}(t_a)$, which would make the determinant of the 2×2 -matrix $\bar{\Lambda}^{\rm p,a}$ vanish.

3.6 Time Evolution Amplitude in Presence of Source Term

Given the Green function $G_{\omega^2}(t,t')$, we can write down an explicit expression for the time evolution amplitude. The quadratic source contribution to the fluctuation factor (3.21) is given explicitly by

$$\begin{aligned} \mathcal{A}_{j,\rm fl} &= -\frac{1}{2M}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\, G_{\omega^2}(t,t')\, j(t)j(t') \qquad (3.167)\\ &= -\frac{1}{M}\frac{1}{\omega \sin\omega(t_b-t_a)}\int_{t_a}^{t_b} dt \int_{t_a}^{t} dt'\, \sin\omega(t_b-t)\sin\omega(t'-t_a)j(t)j(t'). \end{aligned}$$

Altogether, the path integral in the presence of an external source $j(t)$ reads

$$(x_bt_b|x_at_a)^j_\omega = \int \mathcal{D}x\, \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\left[\frac{M}{2}(\dot{x}^2 - \omega^2 x^2) + jx\right]\right\} = e^{(i/\hbar)\mathcal{A}_{j,\rm cl}}F_{\omega,j}(t_b,t_a), \tag{3.168}$$

with a total classical action

$$\begin{aligned} \mathcal{A}_{j,\rm cl} &= \frac{1}{2}\frac{M\omega}{\sin\omega(t_b-t_a)}\left[(x_b^2+x_a^2)\cos\omega(t_b-t_a) - 2x_bx_a\right] \\ &+ \frac{1}{\sin\omega(t_b-t_a)}\int_{t_a}^{t_b} dt[x_a\sin\omega(t_b-t) + x_b\sin\omega(t-t_a)]j(t), \qquad (3.169) \end{aligned}$$

and the fluctuation factor composed of (2.171) and a contribution from the current term $e^{i\mathcal{A}_{j,\rm fl}/\hbar}$:

$$F_{\omega,j}(t_b,t_a) \;=\; F_\omega(t_b,t_a)e^{i\mathcal{A}_{j,\rm fl}/\hbar} = \frac{1}{\sqrt{2\pi i\hbar/M}}\sqrt{\frac{\omega}{\sin\omega(t_b-t_a)}}$$
$$\times\exp\left\{-\frac{i}{\hbar M\omega\sin\omega(t_b-t_a)}\int_{t_a}^{t_b}dt\int_{t_a}^{t}dt'\sin\omega(t_b-t)\sin\omega(t'-t_a)j(t)j(t')\right\}. \quad (3.170)$$

This expression is easily generalized to arbitrary time-dependent frequencies. Using the two independent solutions $D_a(t)$ and $D_b(t)$ of the homogenous differential equations (3.48), which were introduced in Eqs. (2.228) and (2.229), we find for the action (3.169) the general expression, composed of the harmonic action (2.268) and the current term $\int_{t_a}^{t_b} dt x_{\rm cl}(t)j(t)$ with the classical solution (2.248):

$$\mathcal{A}_{j,\rm cl} = \frac{M}{2D_a(t_b)}\left[x_b^2\dot{D}_a(t_b)-x_a^2\dot{D}_b(t_a)-2x_bx_a\right] + \frac{1}{D_a(t_b)}\int_{t_a}^{t_b}dt\,[x_bD_a(t)+x_aD_b(t)]j(t). \quad (3.171)$$

The fluctuation factor is composed of the expression (2.263) for the current-free action, and the generalization of (3.167) with the Green function (3.61):

$$F_{\omega,j}(t_b,t_a) \;=\; F_\omega(t_b,t_a)e^{i\mathcal{A}_{j,\rm fl}/\hbar} = \frac{1}{\sqrt{2\pi i\hbar/M}}\frac{1}{\sqrt{D_a(t_b)}}\exp\left\{-\frac{i}{2\hbar MD_a(t_b)}\right.$$
$$\left.\times\int_{t_a}^{t_b}dt\int_{t_a}^{t}dt'\,j(t)\left[\bar\Theta(t-t')D_b(t)D_a(t')+\bar\Theta(t'-t)D_a(t)D_b(t')\right]j(t')\right\}. \quad (3.172)$$

For applications to statistical mechanics which becomes possible after an analytic continuation to imaginary times, it is useful to write (3.169) and (3.170) in another form. We introduce the Fourier transforms of the current

$$A(\omega) \;\equiv\; \frac{1}{M\omega}\int_{t_a}^{t_b}dte^{-i\omega(t-t_a)}j\,(t)\,, \quad (3.173)$$
$$B(\omega) \;\equiv\; \frac{1}{M\omega}\int_{t_a}^{t_b}dte^{-i\omega(t_b-t)}j(t) = -e^{-i\omega(t_b-t_a)}A(-\omega), \quad (3.174)$$

and see that the classical source term in the exponent of (3.168) can be written as

$$\mathcal{A}_{j,\rm cl} = -i\frac{M\omega}{\sin\omega(t_b-t_a)}\left\{\left[x_b(e^{i\omega(t_b-t_a)}A-B)\right]+x_a(e^{i\omega(t_b-t_a)}B-A)\right\}. \quad (3.175)$$

The source contribution to the quadratic fluctuations in Eq. (3.167), on the other hand, can be rearranged to yield

$$\mathcal{A}_{j,\rm fl} = \frac{i}{4M\omega}\int_{t_a}^{t_b}dt\int_{t_b}^{t_b}dt'e^{-i\omega|t-t'|}j(t)j(t') - \frac{M\omega}{2\sin\omega(t_b-t_a)}\left[e^{i\omega(t_b-t_a)}(A^2+B^2)-2AB\right]. \quad (3.176)$$

This is seen as follows: We write the Green function between $j(t), j(t')$ in (3.168) as

$$
\begin{aligned}
&-\left[\sin\omega(t_b-t)\sin\omega(t'-t_a)\bar{\Theta}(t-t')+\sin\omega(t_b-t')\sin\omega(t-t_a)\bar{\Theta}(t'-t)\right]\\
&=\frac{1}{4}\left[\left(e^{i\omega(t_b-t_a)}e^{-i\omega(t-t')}+\text{c.c.}\right)-\left(e^{i\omega(t_b+t_a)}e^{-i\omega(t+t')}+\text{c.c.}\right)\right]\bar{\Theta}(t-t')\\
&\qquad\qquad\qquad\qquad+\left\{t\leftrightarrow t'\right\}.
\end{aligned}
\tag{3.177}
$$

Using $\bar{\Theta}(t-t')+\bar{\Theta}(t'-t)=1$, this becomes

$$
\begin{aligned}
\frac{1}{4}\Big\{&-\left(e^{i\omega(t_b+t_a)}e^{-i\omega(t'+t)}+\text{c.c.}\right)\\
&+e^{i\omega(t_b-t_a)}\left(e^{-i\omega(t-t')}\bar{\Theta}(t-t')+e^{-i\omega(t'-t)}\bar{\Theta}(t'-t)\right)\\
&+e^{-i\omega(t_b-t_a)}\left[e^{i\omega(t-t')}(1-\bar{\Theta}(t'-t))+e^{i\omega(t'-t)}(1-\bar{\Theta}(t-t'))\right]\Big\}.
\end{aligned}
\tag{3.178}
$$

A multiplication by $j(t), j(t')$ and an integration over the times $t,\ t'$ yield

$$
\begin{aligned}
\frac{1}{4}\Big[&-e^{i\omega(t_b-t_a)}4M^2\omega^2(B^2+A^2)\\
&+\left(e^{i\omega(t_b-t_a)}-e^{-i\omega(t_b-t_a)}\right)\int_{t_a}^{t_b}dt\int_{t_b}^{t_b}dt'e^{-i\omega|t-t'|}j(t)j(t')+4M^2\omega^2 2AB\Big],
\end{aligned}
\tag{3.179}
$$

thus leading to (3.176).

If the source $j(t)$ is time-independent, the integrals in the current terms of the exponential of (3.169) and (3.170) can be done, yielding the j-dependent exponent

$$
\begin{aligned}
\frac{i}{\hbar}\mathcal{A}_j=\frac{i}{\hbar}\left(\mathcal{A}_{j,\text{cl}}+\mathcal{A}_{j,\text{fl}}\right)=\frac{i}{\hbar}\Bigg\{&\frac{1}{\omega\sin\omega(t_b-t_a)}[1-\cos\omega(t_b-t_a)](x_b+x_a)j\\
&+\frac{1}{2M\omega^3}\left[\omega(t_b-t_a)+2\frac{\cos\omega(t_b-t_a)-1}{\sin\omega(t_b-t_a)}\right]j^2\Bigg\}.
\end{aligned}
\tag{3.180}
$$

Substituting $(1-\cos\alpha)$ by $\sin\alpha\tan(\alpha/2)$, this yields the total source action becomes

$$
\mathcal{A}_j=\frac{1}{\omega}\tan\frac{\omega(t_b-t_a)}{2}(x_b+x_a)j+\frac{1}{2M\omega^3}\left[\omega\left(t_b-t_a\right)-2\tan\frac{\omega(t_b-t_a)}{2}\right]j^2. \tag{3.181}
$$

This result could also have been obtained more directly by taking the potential plus a constant-current term in the action

$$
-\int_{t_a}^{t_b}dt\left(\frac{M}{2}\omega^2x^2-xj\right), \tag{3.182}
$$

and by completing it quadratically to the form

$$
-\int_{t_a}^{t_b}dt\frac{M}{2}\omega^2\left(x-\frac{j}{M\omega^2}\right)^2+\frac{t_b-t_a}{2M\omega^2}j^2. \tag{3.183}
$$

This is a harmonic potential shifted in x by $-j/M\omega^2$. The time evolution amplitude can thus immediately be written down as

$$
\begin{aligned}
(x_b t_b|x_a t_a)_\omega^{j=\mathrm{const}} = & \sqrt{\frac{M\omega}{2\pi i\hbar \sin\omega(t_b-t_a)}} \exp\left(\frac{i}{2\hbar}\frac{M\omega}{\sin\omega(t_b-t_a)}\right. \\
& \times\left\{\left[\left(x_b-\frac{j}{M\omega^2}\right)^2+\left(x_a-\frac{j}{M\omega^2}\right)^2\right]\cos\omega(t_b-t_a)\right. \\
& \left.\left. -2\left(x_b-\frac{j}{M\omega^2}\right)\left(x_a-\frac{j}{M\omega^2}\right)\right\}+\frac{i}{\hbar}\frac{t_b-t_a}{2M\omega^2}j^2\right).
\end{aligned}
\tag{3.184}
$$

In the free-particle limit $\omega \to 0$, the result becomes particularly simple:

$$
\begin{aligned}
(x_b t_a|x_a t_a)_0^{j=\mathrm{const}} = & \frac{1}{\sqrt{2\pi i\hbar(t_b-t_a)/M}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x_b-x_a)^2}{t_b-t_a}\right] \\
& \times \exp\left\{\frac{i}{\hbar}\left[\frac{1}{2}(x_b+x_a)(t_b-t_a)j-\frac{1}{24M}(t_b-t_a)^3 j^2\right]\right\}.
\end{aligned}
\tag{3.185}
$$

As a cross check, we verify that the total exponent is equal to $i/\hbar$ times the classical action

$$
\mathcal{A}_{j,\mathrm{cl}} = \int_{t_a}^{t_b} dt\left(\frac{M}{2}\dot{x}_{j,\mathrm{cl}}^2 + j x_{j,\mathrm{cl}}\right), \tag{3.186}
$$

calculated for the classical orbit $x_{j,\mathrm{cl}}(t)$ connecting x_a and x_b in the presence of the constant current j. This satisfies the Euler-Lagrange equation

$$
\ddot{x}_{j,\mathrm{cl}} = j/M, \tag{3.187}
$$

which is solved by

$$
x_{j,\mathrm{cl}}(t) = x_a + \left[x_b - x_a - \frac{j}{2M}(t_b-t_a)^2\right]\frac{t-t_a}{t_b-t_a} + \frac{j}{2M}(t-t_a)^2. \tag{3.188}
$$

Inserting this into the action yields

$$
\mathcal{A}_{j,\mathrm{cl}} = \frac{M}{2}\frac{(x_b-x_a)^2}{t_b-t_a} + \frac{1}{2}(x_b+x_a)(t_b-t_a)j - \frac{(t_b-t_a)^3}{24}\frac{j^2}{M}, \tag{3.189}
$$

just as in the exponent of (3.185).

Let us remark that the calculation of the oscillator amplitude $(x_a t_b|x_a t)_\omega^j$ in (3.168) could have proceeded alternatively by using the orbital separation

$$
x(t) = x_{j,\mathrm{cl}}(t) + \delta x(t), \tag{3.190}
$$

where $x_{j,\mathrm{cl}}(t)$ satisfies the Euler-Lagrange equations with the time-dependent source term

$$
\ddot{x}_{j,\mathrm{cl}}(t) + \omega^2 x_{j,\mathrm{cl}}(t) = j(t)/M, \tag{3.191}
$$

rather than the orbital separation of Eq. (3.7),

$$x(t) = x_{\rm cl}(t) + \delta x(t),$$

where $x_{\rm cl}(t)$ satisfied the Euler-Lagrange equation with no source. For this *inhomogeneous* differential equation we would have found the following solution passing through x_a at $t = t_a$ and x_b at $t = t_b$:

$$x_{j,{\rm cl}}(t) = x_a \frac{\sin\omega(t_b - t)}{\sin\omega(t_b - t_a)} + x_b \frac{\sin\omega(t - t_a)}{\sin\omega(t_b - t_a)} + \frac{1}{M}\int_{t_a}^{t_b} dt' G_{\omega^2}(t,t') j(t'). \qquad (3.192)$$

The Green function $G_{\omega^2}(t,t')$ appears now at the classical level. The separation (3.190) in the total action would have had the advantage over (3.7) that the source causes no linear term in $\delta x(t)$. Thus, there would be no need for a quadratic completion; the classical action would be found from a pure surface term plus one half of the source part of the action

$$\begin{aligned}
\mathcal{A}_{\rm cl} &= \int_{t_a}^{t_b} dt \left[\frac{M}{2}(\dot{x}_{{\rm cl},j}^2 - \omega^2 x_{j,{\rm cl}}^2) + j x_{j,{\rm cl}}\right] = \frac{M}{2} x_{j,{\rm cl}} \dot{x}_{j,{\rm cl}}\Big|_{t_a}^{t_b} \\
&+ \int_{t_a}^{t_b} dt \left[\frac{M}{2} x_{j,{\rm cl}} \left(-\ddot{x}_{j,{\rm cl}} - \omega^2 x_{j,{\rm cl}} + \frac{j}{M}\right)\right] + \frac{1}{2}\int_{t_a}^{t_b} dt x_{j,{\rm cl}} j \\
&= \frac{M}{2}\left(x_b \dot{x}_b - x_a \dot{x}_a\right)\Big|_{x = x_{j,{\rm cl}}} + \frac{1}{2}\int_{t_a}^{t_b} dt x_{j,{\rm cl}}(t) j(t). \qquad (3.193)
\end{aligned}$$

Inserting $x_{j,{\rm cl}}$ from (3.192) and $G_{\omega^2}(t,t')$ from (3.36) leads once more to the exponent in (3.168). The fluctuating action quadratic in $\delta x(t)$ would have given the same fluctuation factor as in the $j = 0$ -case, i.e., the prefactor in (3.168) with no further j^2 (due to the absence of a quadratic completion).

3.7 Time Evolution Amplitude at Fixed Path Average

Another interesting quantity to be needed in Chapter 15 is the Fourier transform of the amplitude (3.184):

$$(x_b t_b | x_a t_a)_\omega^{x_0} = (t_b - t_a)\int_{-\infty}^{\infty} \frac{dj}{2\pi\hbar} e^{-ij(t_b - t_a)x_0/\hbar} (x_b t_b | x_a t_a)_\omega^j. \qquad (3.194)$$

This is the amplitude for a particle to run from x_a to x_b along restricted paths whose temporal average $\bar{x} \equiv (t_b - t_a)^{-1} \int_{t_a}^{t_b} dt\, x(t)$ is held fixed at x_0:

$$(x_b t_b | x_a t_a)_\omega^{x_0} = \int \mathcal{D}x\, \delta(x_0 - \bar{x}) \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \frac{M}{2}(\dot{x}^2 - \omega^2 x^2)\right\}. \qquad (3.195)$$

This property of the paths follows directly from the fact that the integral over the time-independent source j (3.194) produces a δ-function $\delta((t_b - t_a)x_0 - \int_{t_a}^{t_b} dt\, x(t))$. Restricted amplitudes of this type will turn out to have important applications later in Subsection 3.25.1 and in Chapters 5, 10, and 15.

The integral over j in (3.194) is done after a quadratic completion in $\mathcal{A}_j - j(t_b - t_a)x_0$ with $\mathcal{A}_j$ of (3.181):

$$\mathcal{A}_j - j(t_b - t_a)x_0 = \frac{1}{2M\omega^3}\left[\omega\,(t_b - t_a) - 2\tan\frac{\omega(t_b - t_a)}{2}\right](j - j_0)^2 + \mathcal{A}^{x_0}, \quad (3.196)$$

with

$$j_0 = \frac{M\omega^2}{\omega(t_b - t_a) - 2\tan\frac{\omega(t_b - t_a)}{2}}\left[\omega(t_b - t_a)\,x_0 - \tan\frac{\omega(t_b - t_a)}{2}(x_b + x_a)\right], \quad (3.197)$$

and

$$\mathcal{A}^{x_0} = -\frac{M\omega}{2\left[\omega(t_b - t_a) - 2\tan\frac{\omega(t_b - t_a)}{2}\right]}\left[\omega(t_b - t_a)x_0 - \tan\frac{\omega(t_b - t_a)}{2}(x_a + x_b)\right]^2 \quad (3.198)$$

With the completed quadratic exponent (3.196), the Gaussian integral over j in (3.194) can immediately be done, yielding

$$(x_b t_b|x_a t_a)_\omega^{x_0} = (x_b t_b|x_a t_a)\frac{t_b - t_a}{\sqrt{2\pi\hbar}}\sqrt{\frac{iM\omega^3}{\omega(t_b - t_a) - 2\tan\frac{\omega(t_b - t_a)}{2}}}\exp\left(\frac{i}{\hbar}\mathcal{A}^{x_0}\right). \quad (3.199)$$

In the free-particle limit $\omega \to 0$, this reduces to

$$(x_b t_b|x_a t_a)_\omega^{x_0} = \frac{\sqrt{3}M}{\pi\hbar i(t_b - t_a)}\exp\left\{\frac{Mi}{2\hbar(t_b - t_a)}\left[(x_b - x_a)^2 + 12\left(x_0 - \frac{x_b + x_a}{2}\right)^2\right]\right\}. \quad (3.200)$$

If we set $x_b = x_a$ in (3.199) and integrate over $x_b = x_a$, we find the quantum-mechanical version of the partition function at fixed x_0:

$$Z_\omega^{x_0} = \frac{1}{\sqrt{2\pi\hbar(t_b - t_a)/Mi}}\frac{\omega(t_b - t_a)/2}{\sin[\omega(t_b - t_a)/2]}\exp\left[-\frac{i}{2\hbar}(t_b - t_a)M\omega^2 x_0^2\right]. \quad (3.201)$$

As a check we integrate this over x_0 and recover the correct Z_ω of Eq. (2.412).

We may also integrate over both ends independently to obtain the partition function

$$Z_\omega^{\text{open},x_0} = \sqrt{\frac{\omega(t_b - t_a)}{\sin\omega(t_b - t_a)}}\exp\left[-\frac{i}{2\hbar}(t_b - t_a)M\omega^2 x_0^2\right]. \quad (3.202)$$

Integrating this over x_0 and going to imaginary times leads back to the partition function Z_ω^{open} of Eq. (2.413).

3.8 External Source in Quantum-Statistical Path Integral

In the last section we have found the quantum-mechanical time evolution amplitude in the presence of an external source term. Let us now do the same thing for the quantum-statistical case and calculate the path integral

$$(x_b\hbar\beta|x_a 0)_\omega^j = \int \mathcal{D}x(\tau)\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\left[\frac{M}{2}(\dot{x}^2 + \omega^2 x^2) - j(\tau)x(\tau)\right]\right\}. \quad (3.203)$$

This will be done in two ways.

3.8.1 Continuation of Real-Time Result

The desired result is obtained most easily by an analytic continuation of the quantum-mechanical results (3.23), (3.168) in the time difference $t_b - t_a$ to an imaginary time $-i\hbar(\tau_b - \tau_a) = -i\hbar\beta$. This gives immediately

$$(x_b\hbar\beta|x_a 0)^j_\omega = \sqrt{\frac{M}{2\pi\hbar^2\beta}}\sqrt{\frac{\omega\hbar\beta}{\sinh\omega\hbar\beta}}\exp\left\{-\frac{1}{\hbar}\mathcal{A}^{\rm ext}_{\rm e}[j]\right\}, \tag{3.204}$$

with the extended classical Euclidean oscillator action

$$\mathcal{A}^{\rm ext}_{\rm e}[j] = \mathcal{A}_{\rm e} + \mathcal{A}^j_{\rm e} = \mathcal{A}_{\rm e} + \mathcal{A}^j_{1,\rm e} + \mathcal{A}^j_{2,\rm e}, \tag{3.205}$$

where $\mathcal{A}_{\rm e}$ is the Euclidean action

$$\mathcal{A}_{\rm e} = \frac{M\omega}{2\sinh\beta\hbar\omega}\left[(x_b^2 + x_a^2)\cosh\omega\hbar\beta - 2x_b x_a\right], \tag{3.206}$$

while the linear and quadratic Euclidean source terms are

$$\mathcal{A}^j_{1,\rm e} = -\frac{1}{\sinh\omega\hbar\beta}\int_{\tau_a}^{\tau_b} d\tau[x_a\sinh\omega(\hbar\beta - \tau) + x_b\ \sinh\omega\tau]j(\tau), \tag{3.207}$$

and

$$\mathcal{A}^j_{2,\rm e} = -\frac{1}{M}\int_0^{\hbar\beta} d\tau\int_0^\tau d\tau'\ j(\tau)\, G_{\omega^2,\rm e}(\tau,\tau')j(\tau'), \tag{3.208}$$

where $G_{\omega^2,\rm e}(\tau,\tau')$ is the Euclidean version of the Green function (3.36) with Dirichlet boundary conditions:

$$\begin{aligned} G_{\omega^2,\rm e}(\tau,\tau') &= \frac{\sinh\omega(\hbar\beta - \tau_>)\sinh\omega\tau_<}{\omega\sinh\omega\hbar\beta} \\ &= \frac{\cosh\omega(\hbar\beta - |\tau-\tau'|) - \cosh\omega(\hbar\beta - \tau - \tau')}{2\omega\sinh\omega\hbar\beta}, \end{aligned} \tag{3.209}$$

satisfying the differential equation

$$(-\partial_\tau^2 + \omega^2)\, G_{\omega^2,\rm e}(\tau,\tau') = \delta(\tau - \tau'). \tag{3.210}$$

It is related to the real-time Green function (3.36) by

$$G_{\omega^2,\rm e}(\tau,\tau') = i\, G_{\omega^2}(-i\tau, -i\tau'), \tag{3.211}$$

the overall factor i accounting for the replacement $\delta(t-t') \to i\delta(\tau - \tau')$ on the right-hand side of (3.148) in going to (3.210) when going from the real time t to the Euclidean time $-i\tau$. The symbols $\tau_>$ and $\tau_<$ in the first line (3.209) denote the larger and the smaller of the Euclidean times τ and τ', respectively.

The source terms (3.207) and (3.208) can be rewritten as follows:

$$\mathcal{A}^j_{1,\mathrm{e}} = -\frac{M\omega}{\sinh\omega\hbar\beta}\left\{\left[x_b(e^{-\beta\hbar\omega}A_\mathrm{e} - B_\mathrm{e})\right] x_a(e^{-\beta\hbar\omega}B_\mathrm{e} - A_\mathrm{e})\right\}, \tag{3.212}$$

and

$$\mathcal{A}^j_{2,\mathrm{e}} = -\frac{1}{4M\omega}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' e^{-\omega|\tau-\tau'|} j(\tau)j(\tau') + \frac{M\omega}{2\sinh\omega\hbar\beta}\left[e^{\beta\hbar\omega}(A_\mathrm{e}^2 + B_\mathrm{e}^2) - 2A_\mathrm{e}B_\mathrm{e}\right]. \tag{3.213}$$

We have introduced the Euclidean versions of the functions $A(\omega)$ and $B(\omega)$ in Eqs. (3.173) and (3.174) as

$$A_\mathrm{e}(\omega) \equiv iA(\omega)|_{t_b-t_a=-i\hbar\beta} = \frac{1}{M\omega}\int_0^{\hbar\beta} d\tau e^{-\omega\tau} j(\tau), \tag{3.214}$$

$$B_\mathrm{e}(\omega) \equiv iB(\omega)|_{t_b-t_a=-i\hbar\beta} = \frac{1}{M\omega}\int_0^{\hbar\beta} d\tau e^{-\omega(\hbar\beta-\tau)} j(\tau) = -e^{-\beta\hbar\omega}A_\mathrm{e}(-\omega). \tag{3.215}$$

From (3.204) we now calculate the quantum-statistical partition function. Setting $x_b = x_a = x$, the first term in the action (3.205) becomes

$$\mathcal{A}_\mathrm{e} = \frac{M\omega}{\sinh\beta\hbar\omega}\, 2\sinh^2(\omega\hbar\beta/2)x^2. \tag{3.216}$$

If we ignore the second and third action terms in (3.205) and integrate (3.204) over x, we obtain, of course, the free partition function

$$Z_\omega = \frac{1}{2\sinh(\beta\hbar\omega/2)}. \tag{3.217}$$

In the presence of j, we perform a quadratic completion in x and obtain a source-dependent part of the action (3.205):

$$\mathcal{A}^j_\mathrm{e} = \mathcal{A}^j_{\mathrm{fl,e}} + \mathcal{A}^j_{\mathrm{r,e}}, \tag{3.218}$$

where the additional term $\mathcal{A}^j_{\mathrm{r,e}}$ is the remainder left by a quadratic completion. It reads

$$\mathcal{A}^j_{\mathrm{r,e}} = -\frac{M\omega}{2\sinh\omega\beta}e^{\beta\hbar\omega}(A_\mathrm{e} + B_\mathrm{e})^2. \tag{3.219}$$

Combining this with $\mathcal{A}^j_{\mathrm{fl,e}}$ of (3.213) gives

$$\mathcal{A}^j_{\mathrm{fl,e}} + \mathcal{A}^j_{\mathrm{r,e}} = -\frac{1}{4M\omega}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' e^{-\omega|\tau-\tau'|} j(\tau)j(\tau') - \frac{M\omega}{\sinh(\beta\hbar\omega/2)}e^{\beta\hbar\omega/2}A_\mathrm{e}B_\mathrm{e}. \tag{3.220}$$

This can be rearranged to the total source term

$$\mathcal{A}_{\mathrm{e}}^{j} = -\frac{1}{4M\omega}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \frac{\cosh\omega(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\beta\hbar\omega/2)} j(\tau)j(\tau'). \tag{3.221}$$

This is proved by rewriting the latter integrand as

$$\frac{1}{2\sinh(\beta\hbar\omega/2)}\left\{\left[e^{\omega(\tau-\tau')}e^{-\beta\hbar\omega/2} + (\omega\to-\omega)\right]\bar\Theta(\tau-\tau')\right.$$
$$\left. + \left[e^{\omega(\tau'-\tau)}e^{-\beta\hbar\omega/2} + (\omega\to-\omega)\right]\bar\Theta(\tau'-\tau)\right\} j(\tau)j(\tau').$$

In the second and fourth terms we replace $e^{\beta\hbar\omega/2}$ by $e^{-\beta\hbar\omega/2} + 2\sinh(\beta\hbar\omega/2)$ and integrate over τ, τ', with the result (3.220).

The expression between the currents in (3.221) is recognized as the Euclidean version of the periodic Green function $G^{\mathrm{p}}_{\omega^2}(\tau)$ in (3.99):

$$\begin{aligned} G^{\mathrm{p}}_{\omega^2,\mathrm{e}}(\tau) &\equiv iG^{\mathrm{p}}_{\omega^2}(-i\tau)|_{t_b-t_a=-i\hbar\beta} \\ &= \frac{1}{2\omega}\frac{\cosh\omega(\tau-\hbar\beta/2)}{\sinh(\beta\hbar\omega/2)}, \quad \tau\in[0,\hbar\beta]. \end{aligned} \tag{3.222}$$

In terms of (3.221), the partition function of an oscillator in the presence of the source term is

$$Z_\omega[j] = Z_\omega \exp\left(-\frac{1}{\hbar}\mathcal{A}_{\mathrm{e}}^{j}\right). \tag{3.223}$$

For completeness, let us also calculate the partition function of all paths with open ends in the presence of the source $j(t)$, thus generalizing the result (2.413). Integrating (3.204) over initial and final positions x_a and x_b we obtain

$$Z_\omega^{\mathrm{open}}[j] = \sqrt{\frac{2\pi\hbar}{M\omega}}\frac{1}{\sqrt{\sinh[\omega(\tau_b-\tau_a)]}}e^{-(\mathcal{A}^j_{2,\mathrm{e}}+\tilde{\mathcal{A}}^j_{2,\mathrm{e}})/\hbar}, \tag{3.224}$$

where

$$\tilde{\mathcal{A}}^j_{2,\mathrm{e}} = -\frac{1}{M}\int_0^{\hbar\beta} d\tau\int_0^{\tau} d\tau' j(\tau)\tilde G_{\omega^2}(\tau,\tau')j(\tau'), \tag{3.225}$$

with

$$\tilde G_{\omega^2}(\tau,\tau') = \frac{1}{2\omega\sinh^3\omega\hbar\beta}\{\cosh\omega\hbar\beta[\sinh\omega(\hbar\beta-\tau)\sinh\omega(\hbar\beta-\tau')+\sinh\omega\tau\sinh\omega\tau']$$
$$+\sinh\omega(\hbar\beta-\tau)\sinh\omega\tau' + \sinh\omega(\hbar\beta-\tau')\sinh\omega\tau\}. \tag{3.226}$$

By some trigonometric identities, this can be simplified to

$$\tilde G_{\omega^2}(\tau,\tau') = \frac{1}{\omega}\frac{\cosh\omega(\hbar\beta-\tau-\tau')}{\sinh\omega\hbar\beta}. \tag{3.227}$$

The first step is to rewrite the curly brackets in (3.226) as

$$\sinh\omega\tau\Big[\cosh\omega\hbar\beta\sinh\omega\tau' + \sinh\omega(\hbar\beta-\tau')\Big]$$
$$+\sinh\omega(\hbar\beta-\tau')\Big[\cosh\omega\hbar\beta\sinh\omega(\hbar\beta-\tau) + \sinh\omega(\hbar\beta-\,((\hbar\beta-\tau))\Big]. \quad (3.228)$$

The first bracket is equal to $\sinh\beta\hbar\omega\cosh\omega\tau$, the second to $\sinh\beta\hbar\omega\cosh\omega(\hbar\beta-\tau')$, so that we arrive at

$$\sinh\omega\hbar\beta\Big[\sinh\omega\tau\cosh\omega\tau' + \sinh\omega(\hbar\beta-\tau)\cosh\omega(\hbar\beta-\tau')\Big]. \quad (3.229)$$

The bracket is now rewritten as

$$\frac{1}{2}\Big[\sinh\omega(\tau+\tau') + \sinh\omega(\tau-\tau') + \sinh\omega(2\hbar\beta-\tau-\tau') + \sinh\omega(\tau'-\tau)\Big], \quad (3.230)$$

which is equal to

$$\frac{1}{2}\Big[\sinh\omega(\hbar\beta+\tau+\tau'-\hbar\beta) + \sinh\omega(\hbar\beta+\hbar\beta-\tau-\tau')\Big], \quad (3.231)$$

and thus to

$$\frac{1}{2}\Big[2\sinh\omega\hbar\beta\cosh\omega(\hbar\beta-\tau-\tau')\Big], \quad (3.232)$$

such that we arrive indeed at (3.227). The source action in the exponent in (3.224) is therefore:

$$(\mathcal{A}^j_{2,\mathrm{e}} + \tilde{\mathcal{A}}^j_{2,\mathrm{e}}) = -\frac{1}{M}\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\tau'\, j(\tau) G^{\mathrm{open}}_{\omega^2,\mathrm{e}}(\tau,\tau') j(\tau'), \quad (3.233)$$

with (3.208)

$$\begin{aligned} G^{\mathrm{open}}_{\omega^2,\mathrm{e}}(\tau,\tau') &= \frac{\cosh\omega(\hbar\beta-|\tau-\tau'|) + \cosh\omega(\hbar\beta-\tau-\tau')}{2\omega\sinh\omega\hbar\beta} \\ &= \frac{\cosh\omega(\hbar\beta-\tau_>)\cosh\omega\tau_<}{\omega\sinh\omega\hbar\beta}. \end{aligned} \quad (3.234)$$

This Green function coincides precisely with the Euclidean version of Green function $G^{\mathrm{N}}_{\omega^2}(t,t')$ in Eq. (3.151) using the relation (3.211). This coincidence should have been expected after having seen in Section 2.12 that the partition function of all paths with open ends can be calculated, up to a trivial factor $l_{\mathrm{e}}(\hbar\beta)$ of Eq. (2.353), as a sum over all paths satisfying Neumann boundary conditions (2.451), which is calculated using the measure (2.454) for the Fourier components.

In the limit of small-ω, the Green function (3.234) reduces to

$$G^{\mathrm{open}}_{\omega^2,\mathrm{e}}(\tau,\tau') \underset{\omega^2\approx 0}{\approx} \frac{1}{\beta\omega^2} + \frac{\beta}{3} - \frac{1}{2}|\tau-\tau'| - \frac{1}{2}(\tau+\tau') + \frac{1}{2\beta}\left(\tau^2+\tau'^2\right), \quad (3.235)$$

which is the imaginary-time version of (3.157).

3.8.2 Calculation at Imaginary Time

Let us now see how the partition function with a source term is calculated directly in the imaginary-time formulation, where the periodic boundary condition is used from the outset. Thus we consider

$$Z_\omega[j] = \int \mathcal{D}x(\tau)\, e^{-\mathcal{A}_{\rm e}[j]/\hbar}, \tag{3.236}$$

with the Euclidean action

$$\mathcal{A}_{\rm e}[j] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}(\dot{x}^2 + \omega^2 x^2) - j(\tau)x(\tau)\right]. \tag{3.237}$$

Since $x(\tau)$ satisfies the periodic boundary condition, we can perform a partial integration of the kinetic term without picking up a boundary term $x\dot{x}|_{t_a}^{t_b}$. The action becomes

$$\mathcal{A}_{\rm e}[j] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}x(\tau)(-\partial_\tau^2 + \omega^2)x(\tau) - j(\tau)x(\tau)\right]. \tag{3.238}$$

Let $D_e(\tau,\tau')$ be the functional matrix

$$D_{\omega^2,{\rm e}}(\tau,\tau') \equiv (-\partial_\tau^2 + \omega^2)\delta(\tau-\tau'), \quad \tau-\tau' \in [0,\hbar\beta]. \tag{3.239}$$

Its functional inverse is the Euclidean Green function,

$$G^{\rm p}_{\omega^2,{\rm e}}(\tau,\tau') = G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau') = D^{-1}_{\omega^2,{\rm e}}(\tau,\tau') = (-\partial_\tau^2+\omega^2)^{-1}\delta(\tau-\tau'), \tag{3.240}$$

with the periodic boundary condition.

Next we perform a quadratic completion by shifting the path:

$$x \to x' = x - \frac{1}{M}G^P_{\omega^2,{\rm e}}\,j. \tag{3.241}$$

This brings the Euclidean action to the form

$$\mathcal{A}_{\rm e}[j] = \int_0^{\hbar\beta} d\tau \frac{M}{2}x'(-\partial_\tau^2+\omega^2)x' - \frac{1}{2M}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' j(\tau)G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau')j(\tau'). \tag{3.242}$$

The fluctuations over the periodic paths $x'(\tau)$ can now be integrated out and yield for $j(\tau)\equiv 0$

$$Z_\omega = {\rm Det}\, D^{-1/2}_{\omega^2,{\rm e}}. \tag{3.243}$$

As in Subsection 2.15.2, we find the functional determinant by rewriting the product of eigenvalues as

$${\rm Det}\, D_{\omega^2,{\rm e}} = \prod_{m=-\infty}^{\infty}(\omega_m^2+\omega^2) = \exp\left[\sum_{m=-\infty}^{\infty}\log(\omega_m^2+\omega^2)\right], \tag{3.244}$$

and evaluating the sum in the exponent according to the rules of analytic regularization. This leads directly to the partition function of the harmonic oscillator as in Eq. (2.409):

$$Z_\omega = \frac{1}{2\sinh(\beta\hbar\omega/2)}. \tag{3.245}$$

The generating functional for $j(\tau) \neq 0$ is therefore

$$Z[j] = Z_\omega \exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\rm e}^j[j]\right\}, \tag{3.246}$$

with the source term:

$$\mathcal{A}_{\rm e}^j[j] = -\frac{1}{2M}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' j(\tau) G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau') j(\tau'). \tag{3.247}$$

The Green function of imaginary time is calculated as follows. The eigenfunctions of the differential operator $-\partial_\tau^2$ are $e^{-i\omega_m\tau}$ with eigenvalues ω_m^2, and the periodic boundary condition forces ω_m to be equal to the thermal Matsubara frequencies $\omega_m = 2\pi m/\hbar\beta$ with $m = 0, \pm1, \pm2, \dots$. Hence we have the Fourier expansion

$$G^{\rm p}_{\omega^2,{\rm e}}(\tau) \;=\; \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\frac{1}{\omega_m^2+\omega^2}e^{-i\omega_m\tau}. \tag{3.248}$$

In the zero-temperature limit, the Matsubara sum becomes an integral, yielding

$$G^{\rm p}_{\omega^2,{\rm e}}(\tau) \underset{T=0}{=} \int\frac{d\omega_m}{2\pi}\frac{1}{\omega_m^2+\omega^2}e^{-i\omega_m\tau} = \frac{1}{2\omega}e^{-\omega|\tau|}. \tag{3.249}$$

The frequency sum in (3.248) may be written as such an integral over ω_m, provided the integrand contains an additional Poisson sum (3.81):

$$\sum_{\bar m=-\infty}^{\infty}\delta(m-\bar m) = \sum_{n=-\infty}^{\infty}e^{i2\pi nm} = \sum_{n=-\infty}^{\infty}e^{in\omega_m\hbar\beta}. \tag{3.250}$$

This implies that the finite-temperature Green function (3.248) is obtained from (3.249) by a periodic repetition:

$$\begin{aligned} G^{\rm p}_{\omega^2,{\rm e}}(\tau) &= \sum_{n=-\infty}^{\infty}\frac{1}{2\omega}e^{-\omega|\tau+n\hbar\beta|} \\ &= \frac{1}{2\omega}\frac{\cosh\omega(\tau-\hbar\beta/2)}{\sinh(\beta\hbar\omega/2)}, \qquad \tau\in[0,\hbar\beta]. \end{aligned} \tag{3.251}$$

A comparison with (3.97), (3.99) shows that $G^{\rm p}_{\omega^2,{\rm e}}(\tau)$ coincides with $G^{\rm p}_{\omega^2}(t)$ at imaginary times, as it should.

Note that for small ω, the Green function has the expansion

$$G^{\rm p}_{\omega^2,{\rm e}}(\tau) = \frac{1}{\hbar\beta\omega^2} + \frac{\tau^2}{2\hbar\beta} - \frac{\tau}{2} + \frac{\hbar\beta}{12} + \dots\;. \tag{3.252}$$

The first term diverges in the limit $\omega \to 0$. Comparison with the spectral representation (3.248) shows that it stems from the zero Matsubara frequency contribution to the sum. If this term is omitted, the subtracted Green function

$$G^{\mathrm{p}\prime}_{\omega^2,\mathrm{e}}(\tau) \equiv G^{\mathrm{p}}_{\omega^2,\mathrm{e}}(\tau) - \frac{1}{\hbar\beta\omega^2} \tag{3.253}$$

has a well-defined $\omega \to 0$ limit

$$G^{\mathrm{p}\prime}_{0,\mathrm{e}}(\tau) = \frac{1}{\hbar\beta} \sum_{m=\pm1,\pm2,\dots} \frac{1}{\omega_m^2} e^{-i\omega_m\tau} = \frac{\tau^2}{2\hbar\beta} - \frac{\tau}{2} + \frac{\hbar\beta}{12}, \tag{3.254}$$

the right-hand side being correct only for $\tau \in [0, \hbar\beta]$. Outside this interval it must be continued periodically. The subtracted Green function $G^{\mathrm{p}\prime}_{\omega^2,\mathrm{e}}(\tau)$ is plotted for different frequencies ω in Fig. 3.4.

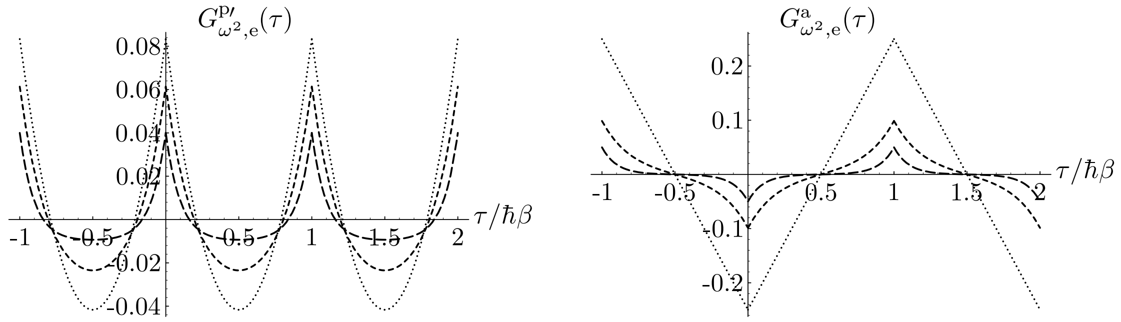

Figure 3.4 Subtracted periodic Green function $G^{\mathrm{p}\prime}_{\omega^2,\mathrm{e}}(\tau) \equiv G^{\mathrm{p}}_{\omega^2,\mathrm{e}}(\tau) - 1/\hbar\beta\omega^2$ and antiperiodic Green function $G^{\mathrm{a}}_{\omega^2,\mathrm{e}}(\tau)$ for frequencies $\omega = (0,\, 5,\, 10)/\hbar\beta$ (with increasing dash length). Compare Fig. 3.2.

The limiting expression (3.254) can, incidentally, be derived using the methods developed in Subsection 2.15.6. We rewrite the sum as

$$\frac{1}{\hbar\beta} \sum_{m=\pm1,\pm2,\dots} \frac{(-1)^m}{\omega_m^2} e^{-i\omega_m(\tau-\hbar\beta/2)} \tag{3.255}$$

and expand

$$-\frac{2}{\hbar\beta}\left(\frac{\hbar\beta}{2\pi}\right)^2 \sum_{n=0,2,4,\dots} \frac{1}{n!}\left[-i\frac{2\pi}{\hbar\beta}(\tau-\hbar\beta/2)\right]^n \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m^{2-n}}. \tag{3.256}$$

The sum over m on the right-hand side is Riemann's eta function[1]

$$\eta(z) \equiv \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m^z}, \tag{3.257}$$

[1] M. Abramowitz and I. Stegun, op. cit., Formula 23.2.19.

which is related to the zeta function (2.521) by

$$\eta(z) = (1 - 2^{1-z})\zeta(z). \tag{3.258}$$

Since the zeta functions of negative integers are all zero [recall (2.587)], only the terms with $n = 0$ and 2 contribute in (3.256). Inserting

$$\eta(0) = -\zeta(0) = 1/2, \quad \eta(2) = \zeta(2)/2 = \pi^2/12, \tag{3.259}$$

we obtain

$$-\frac{2}{\hbar\beta}\left(\frac{\hbar\beta}{2\pi}\right)^2 \left[\frac{\pi^2}{12} - \frac{1}{4}\left(\frac{2\pi}{\hbar\beta}\right)^2 (\tau - \hbar\beta/2)^2\right] = \frac{\tau^2}{2\hbar\beta} - \frac{\tau}{2} + \frac{\hbar\beta}{12}, \tag{3.260}$$

in agreement with (3.254).

It is worth remarking that the Green function (3.254) is directly proportional to the Bernoulli polynomial $B_2(z)$:

$$G^{\mathrm{p}\prime}_{0,\mathrm{e}}(\tau) = \frac{\hbar\beta}{2} B_2(\tau/\hbar\beta). \tag{3.261}$$

These polynomials are defined in terms of the Bernoulli numbers B_k as[2]

$$B_n(x) = \sum_{k=0}^{n} \binom{n}{k} B_k z^{n-k}. \tag{3.262}$$

They appear in the expansion of the generating function[3]

$$\frac{e^{zt}}{e^t - 1} = \sum_{n=0}^{\infty} B_n(z) \frac{t^{n-1}}{n!}, \tag{3.263}$$

and have the expansion

$$B_{2n}(z) = (-1)^{n-1} \frac{2(2n)!}{(2\pi)^{2n}} \sum_{k=0}^{\infty} \frac{\cos(2\pi k z)}{k^{2n}}, \tag{3.264}$$

with the special cases

$$B_1(z) = z - 1/2, \quad B_2(z) = z^2 - z + 1/6, \dots . \tag{3.265}$$

By analogy with (3.251), the antiperiodic Green function can be obtained from an antiperiodic repetition

$$\begin{aligned} G^{\mathrm{a}}_{\omega^2,\mathrm{e}}(\tau) &= \sum_{n=-\infty}^{\infty} \frac{(-1)^n}{2\omega} e^{-\omega|\tau + n\hbar\beta|} \\ &= \frac{1}{2\omega} \frac{\sinh \omega(\tau - \hbar\beta/2)}{\cosh(\beta\hbar\omega/2)}, \quad \tau \in [0, \hbar\beta], \end{aligned} \tag{3.266}$$

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[2] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formula 9.620.

[3] ibid. Formula 9.621.

which is an analytic continuation of (3.113) to imaginary times. In contrast to (3.252), this has a finite $\omega \to 0$ limit

$$G^{\rm a}_{\omega^2,{\rm e}}(\tau) \;=\; \frac{\tau}{2} - \frac{\hbar\beta}{4}, \quad \tau \in [0, \hbar\beta]. \tag{3.267}$$

For a plot of the antiperiodic Green function for different frequencies ω see again Fig. 3.4.

The limiting expression (3.267) can again be derived using an expansion of the type (3.256). The spectral representation in terms of odd Matsubara frequencies (3.104)

$$G^{\rm a}_{\omega^2,{\rm e}}(\tau) \;\equiv\; \frac{1}{\hbar\beta} \sum_{m=-\infty}^{\infty} \frac{1}{\omega^{{\rm f}\,2}_m} e^{-i\omega^{\rm f}_m \tau} \tag{3.268}$$

is rewritten as

$$\frac{1}{\hbar\beta} \sum_{m=-\infty}^{\infty} \frac{1}{\omega^{{\rm f}\,2}_m} \cos(\omega^{\rm f}_m \tau) = \frac{1}{\hbar\beta} \sum_{m=-\infty}^{\infty} \frac{(-1)^m}{\omega^{{\rm f}\,2}_m} \sin[\omega^{\rm f}_m(\tau - \hbar\beta/2)]. \tag{3.269}$$

Expanding the sin function yields

$$\frac{2}{\hbar\beta}\left(\frac{\hbar\beta}{2\pi}\right)^2 \sum_{n=1,3,5,\dots} \frac{(-1)^{(n-1)/2}}{n!} \left[\frac{2\pi}{\hbar\beta}(\tau - \hbar\beta/2)\right]^n \sum_{m=0}^{\infty} \frac{(-1)^m}{\left(m+\frac{1}{2}\right)^{2-n}}. \tag{3.270}$$

The sum over m at the end is 2^{2-n} times Riemann's beta function[4] $\beta(2-n)$, which is defined as

$$\beta(z) \equiv \frac{1}{2^z} \sum_{m=0}^{\infty} \frac{(-1)^m}{\left(m+\frac{1}{2}\right)^z}, \tag{3.271}$$

and is related to Riemann's zeta function

$$\zeta(z,q) \equiv \sum_{m=0}^{\infty} \frac{1}{(m+q)^z}. \tag{3.272}$$

Indeed, we see immediately that

$$\sum_{m=0}^{\infty} \frac{(-1)^m}{(m+q)^z} = \zeta(z,q) - 2^{2-z}\zeta(z,(q+1)/2), \tag{3.273}$$

so that

$$\beta(z) \equiv \frac{1}{2^z}\left[\zeta(z,1/2) - 2^{2-z}\zeta(z,3/4)\right]. \tag{3.274}$$

Near $z = 1$, the function $\zeta(z,q)$ behaves like[5]

$$\zeta(z,q) = \frac{1}{z-1} - \psi(q) + \mathcal{O}(z-1), \tag{3.275}$$

[4] M. Abramowitz and I. Stegun, op. cit., Formula 23.2.21.
[5] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formula 9.533.2.

where $\psi(z)$ is the Digamma function (2.573). Thus we obtain in the limit $z \to 1$:

$$\beta(1) = \lim_{z\to 1} \frac{1}{2}\left[\zeta(z,1/2) - 2^{1-z}\zeta(z,3/4)\right] = \frac{1}{2}\left[-\psi(1/2) + \psi(3/4) + \log 2\right] = \frac{\pi}{4}. \tag{3.276}$$

The last result follows from the specific values [compare (2.575)]:

$$\psi(1/2) = -\gamma - 2\log 2, \quad \psi(3/4) = -\gamma - 3\log 2 + \frac{\pi}{2}. \tag{3.277}$$

For negative odd arguments, the beta function (3.271) vanishes, so that there are no further contributions. Inserting this into (3.270) the only surviving e $n = 1$ -term yields once more (3.267).

Note that the relation (3.276) could also have been found directly from the expansion (2.574) of the Digamma function, which yields

$$\beta(1) = \frac{1}{4}\left[\psi(3/2) - \psi(1/4)\right], \tag{3.278}$$

and is equal to (3.276) due to $\psi(1/4) = -\gamma - 3\log 2 - \pi/2$.

For currents $j(\tau)$, which are periodic in $\hbar\beta$, the source term (3.247) can also be written more simply:

$$\mathcal{A}_{\rm e}^{j}[j] = -\frac{1}{4M\omega}\int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\tau' e^{-\omega|\tau-\tau'|} j(\tau)j(\tau'). \tag{3.279}$$

This follows directly by rewriting (3.279), by analogy with (3.149), as a sum over all periodic repetitions of the zero-temperature Green function (3.249):

$$G^{\rm p}_{\omega^2,{\rm e}}(\tau) = \frac{1}{2\omega}\sum_{n=-\infty}^{\infty} e^{-\omega|\tau+n\hbar\beta|}. \tag{3.280}$$

When inserted into (3.247), the factors $e^{-n\beta\hbar\omega}$ can be removed by an irrelevant periodic temporal shift in the current $j(\tau') \to j(\tau' - n\hbar\beta)$ leading to (3.279).

For a time-dependent periodic or antiperiodic potential $\Omega(\tau)$, the Green function $G^{\rm p,a}_{\omega^2,{\rm e}}(\tau)$ solving the differential equation

$$[\partial_\tau^2 - \Omega^2(\tau)]G^{\rm p,a}_{\omega^2,{\rm e}}(\tau,\tau') = \delta^{\rm p,a}(\tau-\tau'), \tag{3.281}$$

with the periodic or antiperiodic δ-function

$$\delta^{\rm p,a}(\tau-\tau') = \sum_{n=-\infty}^{\infty}\delta(\tau-\tau'-n\hbar\beta)\left\{\begin{array}{c}1\\(-1)^n\end{array}\right\}, \tag{3.282}$$

can be expressed[6] in terms of two arbitrary solutions $\xi(\tau)$ and $\eta(\tau)$ of the homogenous differential equation in the same way as the real-time Green functions in Section 3.5:

$$G^{\rm p,a}_{\omega^2,{\rm e}}(\tau,\tau') = G_{\omega^2,{\rm e}}(\tau,\tau') \mp \frac{[\Delta(\tau,\tau_a) \pm \Delta(\tau_b,\tau)][\Delta(\tau',\tau_a) \pm \Delta(\tau_b,\tau')]}{\bar{\Delta}^{\rm p,a}(\tau_a,\tau_b)\Delta(\tau_a,\tau_b)}, \tag{3.283}$$

[6]See H. Kleinert and A. Chervyakov, Phys. Lett. A *245*, 345 (1998) (quant-ph/9803016); J. Math. Phys. B *40*, 6044 (1999) (physics/9712048).

where $G_{\omega^2,\mathrm{e}}(\tau,\tau')$ is the imaginary-time Green function with Dirichlet boundary conditions corresponding to (3.209):

$$G_{\omega^2,\mathrm{e}}(\tau,\tau') = \frac{\bar\Theta(\tau-\tau')\Delta(\tau_b,\tau)\Delta(\tau',\tau_a)+\bar\Theta(\tau-\tau')\Delta(\tau_b,\tau')\Delta(\tau,\tau_a)}{\Delta(\tau_a,\tau_b)}, \qquad (3.284)$$

with

$$\Delta(\tau,\tau') = \frac{1}{W}\left[\xi(\tau)\eta(\tau')-\xi(\tau')\eta(\tau)\right], \qquad W=\xi(\tau)\dot\eta(\tau)-\dot\xi(\tau)\eta(\tau), \qquad (3.285)$$

and

$$\bar\Delta^{\mathrm{p,a}}(\tau_a,\tau_b) = 2\pm\partial_\tau\Delta(\tau_a,\tau_b)\pm\partial_\tau\Delta(\tau_b,\tau_a). \qquad (3.286)$$

Let also write down the imaginary-time versions of the periodic or antiperiodic Green functions for time-dependent frequencies. Recall the expressions for constant frequency $G^{\mathrm{p}}_\omega(t)$ and $G^{\mathrm{a}}_\omega(t)$ of Eqs. (3.94) and (3.112) for $\tau\in(0,\hbar\beta)$:

$$\begin{aligned} G^{\mathrm{p}}_{\omega,\mathrm{e}}(\tau) &= \frac{1}{\hbar\beta}\sum_m e^{-i\omega_m\tau}\frac{-1}{i\omega_m-\omega} = e^{-\omega(\tau-\hbar\beta/2)}\frac{1}{2\sinh(\beta\hbar\omega/2)} \\ &= (1+n^{\mathrm{b}}_\omega)e^{-\omega\tau}, \end{aligned} \qquad (3.287)$$

and

$$\begin{aligned} G^{\mathrm{a}}_{\omega,\mathrm{e}}(\tau) &= \frac{1}{\hbar\beta}\sum_m e^{-i\omega^{\mathrm{f}}_m\tau}\frac{-1}{i\omega^{\mathrm{f}}_m-\omega} = e^{-\omega(\tau-\hbar\beta/2)}\frac{1}{2\cosh(\beta\hbar\omega/2)} \\ &= (1-n^{\mathrm{f}}_\omega)e^{-\omega\tau}, \end{aligned} \qquad (3.288)$$

the first sum extending over the even Matsubara frequencies, the second over the odd ones. The Bose and Fermi distribution functions $n^{\mathrm{b,f}}_\omega$ were defined in Eqs. (3.93) and (3.111).

For $\tau<0$, periodicity or antiperiodicity determine

$$G^{\mathrm{p,a}}_{\omega,\mathrm{e}}(\tau) = \pm G^{\mathrm{p,a}}_{\omega,\mathrm{e}}(\tau+\hbar\beta). \qquad (3.289)$$

The generalization of these expressions to time-dependent periodic and antiperiodic frequencies $\Omega(\tau)$ satisfying the differential equations

$$[-\partial_\tau-\Omega(\tau)]G^{\mathrm{p,a}}_{\Omega,\mathrm{e}}(\tau,\tau') = \delta^{\mathrm{p,a}}(\tau-\tau') \qquad (3.290)$$

has for $\beta\to\infty$ the form

$$G^{\mathrm{p,a}}_{\Omega,\mathrm{e}}(\tau,\tau') = \bar\Theta(\tau-\tau')e^{-\int_0^\tau d\tau'\,\Omega(\tau')}. \qquad (3.291)$$

Its periodic superposition yields for finite β a sum analogous to (3.280):

$$G^{\mathrm{p,a}}_{\Omega,\mathrm{e}}(\tau,\tau') = \sum_{n=0}^{\infty} e^{-\int_0^{\tau+n\hbar\beta} d\tau'\,\Omega(\tau')}\left\{\begin{array}{c}1\\(-1)^n\end{array}\right\}, \qquad \hbar\beta>\tau>\tau'>0, \qquad (3.292)$$

which reduces to (3.287), (3.288) for a constant frequency $\Omega(\tau)\equiv\omega$.

3.9 Lattice Green Function

As in Chapter 2, it is easy to calculate the above results also on a sliced time axis. This is useful when it comes to comparing analytic results with Monte Carlo lattice simulations. We consider here only the Euclidean versions; the quantum-mechanical ones can be obtained by analytic continuation to real times.

The Green function $G_{\omega^2}(\tau,\tau')$ on an imaginary-time lattice with infinitely many lattice points of spacing ϵ reads [instead of the Euclidean version of (3.147)]:

$$G_{\omega^2}(\tau,\tau') = \frac{\epsilon}{2\sinh \epsilon\tilde{\omega}_{\rm e}} e^{-\tilde{\omega}_{\rm e}|\tau-\tau'|} = \frac{1}{2\omega}\frac{1}{\cosh(\epsilon\tilde{\omega}_{\rm e}/2)} e^{-\tilde{\omega}_{\rm e}|\tau-\tau'|}, \tag{3.293}$$

where $\tilde{\omega}_{\rm e}$ is given, as in (2.406), by

$$\tilde{\omega}_{\rm e} = \frac{2}{\epsilon}\text{arsinh}\frac{\epsilon\omega}{2}. \tag{3.294}$$

This is derived from the spectral representation

$$G_{\omega^2}(\tau,\tau') = G_{\omega^2}(\tau-\tau') = \int \frac{d\omega'}{2\pi} e^{-i\omega'(\tau-\tau')} \frac{\epsilon^2}{2(1-\cos\epsilon\omega')+\epsilon^2\omega^2} \tag{3.295}$$

by rewriting it as

$$G_{\omega^2}(\tau,\tau') = \int_0^\infty ds \int \frac{d\omega'}{2\pi} e^{-i\omega'\epsilon n} e^{-s[2(1-\cos\epsilon\omega')+\epsilon^2\omega^2]/\epsilon^2}, \tag{3.296}$$

with $n \equiv (\tau'-\tau)/\epsilon$, performing the ω'-integral which produces a Bessel function $I_{(\tau-\tau')/\epsilon}(2s/\epsilon^2)$, and subsequently the integral over s with the help of formula (2.475). The Green function (3.293) is defined only at discrete $\tau_n = n\hbar\beta/(N+1)$. If it is summed over all periodic repetitions $n \to n + k(N+1)$ with $k = 0, \pm 1, \pm 2, \ldots$, one obtains the lattice analog of the periodic Green function (3.251):

$$\begin{aligned} G_{\rm e}^{\rm p}(\tau) &= \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty} \frac{\epsilon^2}{2(1-\cos\epsilon\omega_m)+\epsilon^2\omega^2} e^{-i\omega_m\tau} \\ &= \frac{1}{2\omega}\frac{1}{\cosh(\epsilon\tilde{\omega}/2)}\frac{\cosh\tilde{\omega}(\tau-\hbar\beta/2)}{\sinh(\hbar\tilde{\omega}\beta/2)}, \quad \tau\in[0,\hbar\beta]. \end{aligned} \tag{3.297}$$

3.10 Correlation Functions, Generating Functional, and Wick Expansion

Equipped with the path integral of the harmonic oscillator in the presence of an external source it is easy to calculate the correlation functions of any number of position variables $x(\tau)$. We consider here only a system in thermal equilibrium and study the behavior at imaginary times. The real-time correlation functions can be discussed similarly. The precise relation between them will be worked out in Chapter 18.

In general, i.e., also for nonharmonic actions, the thermal correlation functions of n-variables $x(\tau)$ are defined as the functional averages

$$\begin{aligned} G_{\omega^2}^{(n)}(\tau_1,\ldots,\tau_n) &\equiv \langle x(\tau_1)x(\tau_2)\cdots x(\tau_n)\rangle \\ &\equiv Z^{-1}\int \mathcal{D}x\, x(\tau_1)x(\tau_2)\cdots x(\tau_n)\exp\left(-\frac{1}{\hbar}\mathcal{A}_{\rm e}\right). \end{aligned} \tag{3.298}$$

They are also referred to as *n-point functions*. In operator quantum mechanics, the same quantities are obtained from the thermal expectation values of time-ordered products of Heisenberg position operators $\hat{x}_H(\tau)$:

$$G^{(n)}_{\omega^2}(\tau_1,\dots,\tau_n) = Z^{-1}\mathrm{Tr}\left\{\hat{T}_\tau\left[\hat{x}_H(\tau_1)\hat{x}_H(\tau_2)\cdots\hat{x}_H(\tau_n)e^{-\hat{H}/k_BT}\right]\right\}, \tag{3.299}$$

where Z is the partition function

$$Z = e^{-F/k_BT} = \mathrm{Tr}(e^{-\hat{H}/k_BT}) \tag{3.300}$$

and $\hat{T}_\tau$ is the time-ordering operator. Indeed, by slicing the imaginary-time evolution operator $e^{-\hat{H}\tau/\hbar}$ at discrete times in such a way that the times τ_i of the n position operators $x(\tau_i)$ are among them, we find that $G^{(n)}_{\omega^2}(\tau_1,\dots,\tau_n)$ has precisely the path integral representation (3.298).

By definition, the path integral with the product of $x(\tau_i)$ in the integrand is calculated as follows. First we sort the times τ_i according to their time order, denoting the reordered times by $\tau_{t(i)}$. We also set $\tau_b \equiv \tau_{t(n+1)}$ and $\tau_a \equiv \tau_{t(0)}$. Assuming that the times $\tau_{t(i)}$ are different from one another, we slice the time axis $\tau \in [\tau_a, \tau_b]$ into the intervals $[\tau_b, \tau_{t(n)}]$, $[\tau_{t(n)}, \tau_{t(n-1)}]$, $[\tau_{t(n-2)}, \tau_{t(n-3)}]$,. . ., $[\tau_{t(4)}, \tau_{t(3)}]$, $[\tau_{t(2)}, \tau_{t(1)}]$, $[\tau_{t(1)}, \tau_a]$. For each of these intervals we calculate the time evolution amplitude $(x_{t(i+1)}\tau_{t(i+1)}|x_{t(i)}\tau_{t(i)})$ as usual. Finally, we recombine the amplitudes by performing the intermediate $x(\tau_{t(i)})$-integrations, with an extra factor $x(\tau_i)$ at each τ_i, i.e.,

$$\begin{aligned}G^{(n)}_{\omega^2}(\tau_1,\dots,\tau_n) = &\prod_{i=1}^{n+1}\left[\int_{-\infty}^{\infty} dx_{\tau_{t(i)}}\right](x_{t(n+1)}\tau_b|x_{t(n)}\tau_{t(n)})\cdot x(\tau_{t(n)})\cdot\ldots\\ &\cdot(x_{t(i+1)}\tau_{t(i+1)}|x_{t(i)}\tau_{t(i)})\cdot x(\tau_{t(i)})\cdot(x_{t(i)}\tau_{t(i)}|x_{t(i-1)}\tau_{t(i-1)})\cdot x(\tau_{t(i-1)})\\ &\cdot\ldots\cdot(x_{t(2)}\tau_{t(2)}|x_{t(1)}\tau_{t(1)})\cdot x(\tau_{t(1)})\cdot(x_{t(1)}\tau_{t(1)}|x_{t(0)}\tau_a).\end{aligned} \tag{3.301}$$

We have set $x_{t(n+1)} \equiv x_b = x_a \equiv x_{t(0)}$, in accordance with the periodic boundary condition. If two or more of the times τ_i are equal, the intermediate integrals are accompanied by the corresponding power of $x(\tau_i)$.

Fortunately, this rather complicated-looking expression can be replaced by a much simpler one involving functional derivatives of the thermal partition function $Z[j]$ in the presence of an external current j. From the definition of $Z[j]$ in (3.236) it is easy to see that all correlation functions of the system are obtained by the functional formula

$$G^{(n)}_{\omega^2}(\tau_1,\dots,\tau_n) = \left[Z[j]^{-1}\hbar\frac{\delta}{\delta j(\tau_1)}\cdots\hbar\frac{\delta}{\delta j(\tau_n)}Z[j]\right]_{j=0}. \tag{3.302}$$

This is why $Z[j]$ is called the *generating functional* of the theory.

In the present case of a harmonic action, $Z[j]$ has the simple form (3.246), (3.247), and we can write

$$G^{(n)}_{\omega^2}(\tau_1,\dots,\tau_n) \;\;=\;\; \left[\hbar\frac{\delta}{\delta j(\tau_1)}\cdots\hbar\frac{\delta}{\delta j(\tau_n)}\right. \tag{3.303}$$

$$\times \quad \exp\left\{\frac{1}{2\hbar M}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' j(\tau) G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau') j(\tau')\right\}\Bigg]_{j=0},$$

where $G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau')$ is the Euclidean Green function (3.251). Expanding the exponential into a Taylor series, the differentiations are easy to perform. Obviously, any odd number of derivatives vanishes. Differentiating (3.246) twice yields the two-point function [recall (3.251)]

$$G^{(2)}_{\omega^2}(\tau,\tau') = \langle x(\tau)x(\tau')\rangle = \frac{\hbar}{M} G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau'). \qquad (3.304)$$

Thus, up to the constant prefactor, the two-point function coincides with the Euclidean Green function (3.251). Inserting (3.304) into (3.303), all n-point functions are expressed in terms of the two-point function $G^{(2)}_{\omega^2}(\tau,\tau')$: Expanding the exponential into a power series, the expansion term of order $n/2$ carries the numeric prefactors $1/(n/2)! \cdot 1/2^{n/2}$ and consists of a product of $n/2$ factors $\int_0^{\hbar\beta} d\tau' j(\tau) G^{(2)}_{\omega^2}(\tau,\tau') j(\tau')/\hbar^2$. The n-point function is obtained by functionally differentiating this term n times. The result is a sum over products of $n/2$ factors $G^{(2)}_{\omega^2}(\tau,\tau')$ with $n!$ permutations of the n time arguments. Most of these products coincide, for symmetry reasons. First, $G^{(2)}_{\omega^2}(\tau,\tau')$ is symmetric in its arguments. Hence $2^{n/2}$ of the permutations correspond to identical terms, their number canceling one of the prefactors. Second, the $n/2$ Green functions $G^{(2)}_{\omega^2}(\tau,\tau')$ in the product are identical. Of the $n!$ permutations, subsets of $(n/2)!$ permutations produce identical terms, their number canceling the other prefactor. Only $n!/[(n/2)!2^{n/2}] = (n-1)\cdot(n-3)\cdots 1 = (n-1)!!$ terms are different. They all carry a unit prefactor and their sum is given by the so-called *Wick rule* or *Wick expansion*:

$$G^{(n)}_{\omega^2}(\tau_1,\dots,\tau_n) = \sum_{\rm pairs} G^{(2)}_{\omega^2}(\tau_{p(1)},\tau_{p(2)})\cdots G^{(2)}_{\omega^2}(\tau_{p(n-1)},\tau_{p(n)}). \qquad (3.305)$$

Each term is characterized by a different pair configurations of the time arguments in the Green functions. These pair configurations are found most simply by the following rule: Write down all time arguments in the n-point function $\tau_1\tau_2\tau_3\tau_4\dots\tau_n$. Indicate a pair by a common symbol, say $\dot\tau_{p(i)}\dot\tau_{p(i+1)}$, and call it a *pair contraction* to symbolize a Green function $G^{(2)}_{\omega^2}(\tau_{p(i)},\tau_{p(i+1)})$. The desired $(n-1)!!$ pair configurations in the Wick expansion (3.305) are then found iteratively by forming $n-1$ single contractions

$$\dot\tau_1\dot\tau_2\tau_3\tau_4\dots\tau_n + \dot\tau_1\tau_2\dot\tau_3\tau_4\dots\tau_n + \dot\tau_1\tau_2\tau_3\dot\tau_4\dots\tau_n + \dots + \dot\tau_1\tau_2\tau_3\tau_4\dots\dot\tau_n, \qquad (3.306)$$

and by treating the remaining $n-2$ uncontracted variables in each of these terms likewise, using a different contraction symbol. The procedure is continued until all variables are contracted.

In the literature, one sometimes another shorter formula under the name of Wick's rule, stating that a single harmonically fluctuating variable satisfies the equality of expectations:

$$\left\langle e^{Kx}\right\rangle = e^{K^2\left\langle x^2\right\rangle/2}. \tag{3.307}$$

This follows from the observation that the generating functional (3.236) may also be viewed as Z_ω times the expectation value of the source exponential

$$Z_\omega[j] = Z_\omega \times \left\langle e^{\int d\tau j(\tau)x(\tau)/\hbar}\right\rangle. \tag{3.308}$$

Thus we can express the result (3.246) also as

$$\left\langle e^{\int d\tau j(\tau)x(\tau)/\hbar}\right\rangle = e^{(1/2M\hbar)\int d\tau\int d\tau' j(\tau)G^{\rm p}_{\omega^2,{\rm e}}(\tau,\tau')j(\tau')}. \tag{3.309}$$

Since $(\hbar/M)G^{\rm p}_{\omega^2,{\rm e}}(\tau,\tau')$ in the exponent is equal to the correlation function $G^{(2)}_{\omega^2}(\tau,\tau') = \langle x(\tau)x(\tau')\rangle$ by Eq. (3.304), we may also write

$$\left\langle e^{\int d\tau j(\tau)x(\tau)/\hbar}\right\rangle = e^{\int d\tau\int d\tau' j(\tau)\langle x(\tau)x(\tau')\rangle j(\tau')/2\hbar^2}. \tag{3.310}$$

Considering now a discrete time axis sliced at $t = t_n$, and inserting the special source current $j(\tau_n) = K\delta_{n,0}$, for instance, we find directly (3.307).

The Wick theorem in this form has an important physical application. The intensity of the sharp diffraction peaks observed in *Bragg scattering* of X-rays on crystal planes is reduced by thermal fluctuations of the atoms in the periodic lattice. The reduction factor is usually written as e^{-2W} and called the *Debye-Waller factor*. In the Gaussian approximation it is given by

$$e^{-W} \equiv \langle e^{-\boldsymbol{\nabla}\cdot\mathbf{u}(\mathbf{x})}\rangle = e^{-\Sigma_{\mathbf{k}}\langle\,|\mathbf{k}\cdot\mathbf{u}(\mathbf{k})]^2\rangle/2}, \tag{3.311}$$

where $\mathbf{u}(\mathbf{x})$ is the atomic displacement field.

If the fluctuations take place around $\langle x(\tau)\rangle \neq 0$, then (3.307) goes obviously over into

$$\langle e^{Px}\rangle = e^{P\langle x(\tau)\rangle + P^2\langle x-\langle x(\tau)\rangle\rangle^2/2}. \tag{3.312}$$

3.10.1 Real-Time Correlation Functions

The translation of these results to real times is simple. Consider, for example, the harmonic fluctuations $\delta x(t)$ with Dirichlet boundary conditions, which vanish at t_b and t_a. Their correlation functions can be found by using the amplitude (3.23) as a generating functional, if we replace $x(t) \to \delta x(t)$ and $x_b = x_a \to 0$. Differentiating twice with respect to the external currents $j(t)$ we obtain

$$G^{(2)}_{\omega^2}(t,t') = \langle x(t)x(t')\rangle = i\frac{\hbar}{M}G_{\omega^2}(t-t'), \tag{3.313}$$

with the Green function $G_{\omega^2}(t-t')$ of Eq. (3.36), which vanishes if $t=t_b$ or $t=t_a$. The correlation function of $\dot{x}(t)$ is

$$\langle \dot{x}(t)\dot{x}(t')\rangle = i\frac{\hbar}{M}\frac{\cos\omega(t_b-t_>)\,\cos\omega(t_<-t_a)}{\omega\sin\omega(t_b-t_a)}, \tag{3.314}$$

and has the value

$$\langle \dot{x}(t_b)\dot{x}(t_b)\rangle = i\frac{\hbar}{M}\cot\omega(t_b-t_a). \tag{3.315}$$

As an application, we use this result to calculate once more the time evolution amplitude $(\mathbf{x}_bt_b|\mathbf{x}_at_a)$ in a way closely related to the operator method in Section 2.23. We observe that the time derivative of this amplitude has the path integral representation [compare (2.763)]

$$i\hbar\partial_{t_b}(\mathbf{x}_bt_b|\mathbf{x}_at_a) = -\int\mathcal{D}^Dx\,L(\mathbf{x}_b,\dot{\mathbf{x}}_b)e^{i\int_{t_a}^{t_b}dt\,L(\mathbf{x},\dot{\mathbf{x}})/\hbar} = -\langle L(\mathbf{x}_b,\dot{\mathbf{x}}_b)\rangle\,(\mathbf{x}_bt_b|\mathbf{x}_at_a), \tag{3.316}$$

and calculate the expectation value $\langle L(\mathbf{x}_b,\dot{\mathbf{x}}_b)\rangle$ as a sum of the classical Lagrangian $L(\mathbf{x}_{\rm cl}(t_b),\dot{\mathbf{x}}_{\rm cl}(t_b))$ and the expectation value of the fluctuating part of the Lagrangian $\langle L_{\rm fl}(\mathbf{x}_b,\dot{\mathbf{x}}_b)\rangle \equiv \langle\,[L(\mathbf{x}_b,\dot{\mathbf{x}}_b)-L(\mathbf{x}_{\rm cl}(t_b),\dot{\mathbf{x}}_{\rm cl}(t_b))]\,\rangle$. If the Lagrangian has the standard form $L=M\dot{\mathbf{x}}^2/2-V(\mathbf{x})$, then only the kinetic term contributes to $\langle L_{\rm fl}(\mathbf{x}_b,\dot{\mathbf{x}}_b)\rangle$, so that

$$\langle L_{\rm fl}(\mathbf{x}_b,\dot{\mathbf{x}}_b)\rangle = \frac{M}{2}\langle\delta\dot{\mathbf{x}}_b^2\rangle. \tag{3.317}$$

There is no contribution from $\langle V(\mathbf{x}_b)-V(\mathbf{x}_{\rm cl}(t_b))\rangle$, due to the Dirichlet boundary conditions.

The temporal integral over $-[L(\mathbf{x}_{\rm cl}(t_b),\dot{\mathbf{x}}_{\rm cl}(t_b))-\langle L_{\rm fl}(\mathbf{x}_b,\dot{\mathbf{x}}_b)\rangle]$ agrees with the operator result (2.790), and we obtain the time evolution amplitude from the formula

$$(\mathbf{x}_bt_b|\mathbf{x}_at_a) = C(\mathbf{x}_b,\mathbf{x}_a)e^{iA(\mathbf{x}_b,\mathbf{x}_a;t_b-t_a)/\hbar}\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}dt_{b'}\frac{M}{2}\langle\delta\dot{\mathbf{x}}_{b'}^2\rangle\right), \tag{3.318}$$

where $A(\mathbf{x}_b,\mathbf{x}_a;t_b-t_a)$ is the classical action $\mathcal{A}[\mathbf{x}_{\rm cl}]$ expressed as a function of the endpoints [recall (4.87)]. The constant of integration $C(\mathbf{x}_b,\mathbf{x}_a)$ is fixed as in (2.776) by solving the differential equation

$$-i\hbar\nabla_b(\mathbf{x}_bt_b|\mathbf{x}_at_a) = \langle\mathbf{p}_b\rangle(\mathbf{x}_bt_b|\mathbf{x}_at_a) = \mathbf{p}_{\rm cl}(t_b)(\mathbf{x}_bt_b|\mathbf{x}_at_a), \tag{3.319}$$

and a similar equation for $\mathbf{x}_a$ [compare (2.777)]. Since the prefactor $\mathbf{p}_{\rm cl}(t_b)$ on the right-hand side is obtained from the derivative of the exponential $e^{iA(\mathbf{x}_b,\mathbf{x}_a;t_b-t_a)/\hbar}$ in (3.318), due to the general relation (4.88), the constant of integration $C(\mathbf{x}_b,\mathbf{x}_a)$ is actually independent of $\mathbf{x}_b$ and $\mathbf{x}_a$. Thus we obtain from (3.318) once more the known result (3.318).

As an example, take the harmonic oscillator. The terms linear in $\delta\mathbf{x}(t)=\mathbf{x}(t)-\mathbf{x}_{\rm cl}(t)$ vanish since they are they are odd in $\delta\mathbf{x}(t)$ while the exponent in (3.316) is even. Inserting on the right-hand side of (3.317) the correlation function (3.314), we obtain in D dimensions

$$\langle L_{\mathrm{fl}}(\mathbf{x}_b, \dot{\mathbf{x}}_b)\rangle = \frac{M}{2}\langle \delta\dot{\mathbf{x}}_b^2\rangle = i\frac{\hbar\omega}{2} D\cot\omega(t_b - t_a), \tag{3.320}$$

which is precisely the second term in Eq. (2.789), with the appropriate opposite sign.

3.11 Correlation Functions of Charged Particle in Magnetic Field and Harmonic Potential

It is straightforward to find the correlation functions of a charged particle in a magnetic and an extra harmonic potential discussed in Section 2.19. They are obtained by inverting the functional matrix (2.693):

$$\mathbf{G}^{(2)}_{\omega^2,B}(\tau,\tau') = \frac{\hbar}{M}\mathbf{D}^{-1}_{\omega^2,B}(\tau,\tau'). \tag{3.321}$$

By an ordinary matrix inversion of (2.696), we obtain the Fourier expansion

$$\mathbf{G}^{(2)}_{B}(\tau,\tau') = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\tilde{\mathbf{G}}_{\omega^2,B}(\omega_m)e^{-i\omega_m(\tau-\tau')}, \tag{3.322}$$

with

$$\tilde{\mathbf{G}}^{(2)}_{\omega^2,B}(\omega_m) = \frac{\hbar}{M}\frac{1}{(\omega_m^2+\omega_+^2)(\omega_m^2+\omega_-^2)}\begin{pmatrix}\omega_m^2+\omega^2-\omega_B^2 & 2\omega_B\omega_m\\ -2\omega_B\omega_m & \omega_m^2+\omega^2-\omega_B^2,\end{pmatrix}. \tag{3.323}$$

Since $\omega_+^2+\omega_-^2 = 2(\omega^2+\omega_B^2)$ and $\omega_+^2-\omega_-^2 = 4\omega\omega_B$, the diagonal elements can be written as

$$\begin{aligned}\frac{1}{2(\omega_m^2+\omega_+^2)(\omega_m^2+\omega_-^2)}&\left[(\omega_m^2+\omega_+^2)+(\omega_m^2+\omega_-^2)-4\omega_B^2\right]\\ &= \frac{1}{2}\left\{\left[\frac{1}{\omega_m^2+\omega_+^2}+\frac{1}{\omega_m^2+\omega_-^2}\right]+\frac{\omega_B}{\omega}\left[\frac{1}{\omega_m^2+\omega_+^2}-\frac{1}{\omega_m^2+\omega_-^2}\right]\right\}.\end{aligned} \tag{3.324}$$

Recalling the Fourier expansion (3.248), we obtain directly the diagonal periodic correlation function

$$G^{(2)}_{\omega^2,B,xx} = \frac{\hbar}{4M\omega}\left[\frac{\cosh\omega_+(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\omega_+\hbar\beta/2)}+\frac{\cosh\omega_-(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\omega_-\hbar\beta/2)}\right], \tag{3.325}$$

which is equal to $G^{(2)}_{\omega^2,B,yy}$. The off-diagonal correlation functions have the Fourier components

$$\frac{2\omega_B\omega_m}{(\omega_m^2+\omega_+^2)(\omega_m^2+\omega_-^2)} = \frac{\omega_m}{2\omega}\left[\frac{1}{\omega_m^2+\omega_+^2}-\frac{1}{\omega_m^2+\omega_-^2}\right]. \tag{3.326}$$

Since ω_m are the Fourier components of the derivative $i\partial_\tau$, we can write

$$G^{(2)}_{\omega^2,B,xy}(\tau,\tau')=-G^{(2)}_{\omega^2,B,yx}(\tau,\tau')=\frac{\hbar}{2M}\,i\partial_\tau\left[\frac{1}{2\omega_+}\frac{\cosh\omega_+(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\omega_+\hbar\beta/2)}\right.$$
$$\left.-\frac{1}{2\omega_-}\frac{\cosh\omega_-(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\omega_-\hbar\beta/2)}\right].\quad(3.327)$$

Performing the derivatives yields

$$G^{(2)}_{\omega^2,B,xy}(\tau,\tau')=G^{(2)}_{\omega^2,B,yx}(\tau,\tau')=\frac{\hbar\epsilon(\tau-\tau')}{2Mi}\left[\frac{1}{2\omega_+}\frac{\sinh\omega_+(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\omega_+\hbar\beta/2)}\right.$$
$$\left.-\frac{1}{2\omega_-}\frac{\sinh\omega_-(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\omega_-\hbar\beta/2)}\right],\quad(3.328)$$

where $\epsilon(\tau-\tau')$ is the step function (1.315).

For a charged particle in a magnetic field without an extra harmonic oscillator we have to take the limit $\omega\to\omega_B$ in these equations. Due to translational invariance of the limiting system, this exists only after removing the zero-mode in the Matsubara sum. This is done most simply in the final expressions by subtracting the high-temperature limits at $\tau=\tau'$. In the diagonal correlation functions (3.325) this yields

$$G^{(2)\,\prime}_{\omega^2,B,xx}(\tau,\tau')=G^{(2)\,\prime}_{\omega^2,B,yy}(\tau,\tau')=G^{(2)}_{\omega^2,B,xx}-\frac{1}{\beta M\omega_+\omega_-},\quad(3.329)$$

where the prime indicates the subtraction. Now one can easily go to the limit $\omega\to\omega_B$ with the result

$$G^{(2)\,\prime}_{\omega^2,B,xx}(\tau,\tau')=G^{(2)\,\prime}_{\omega^2,B,yy}(\tau,\tau')=\frac{\hbar}{4M\omega}\left[\frac{\cosh 2\omega(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\beta\hbar\omega)}-\frac{1}{\omega\hbar\beta}\right].\quad(3.330)$$

For the subtracted off-diagonal correlation functions (3.328) we find

$$G^{(2)\,\prime}_{\omega^2,B,xy}(\tau,\tau')=-G^{(2)\,\prime}_{\omega^2,B,yx}(\tau,\tau')=G^{(2)}_{\omega^2,B,xy}+\frac{\hbar\omega_B}{2Mi\omega_+\omega_-}\epsilon(\tau-\tau').\quad(3.331)$$

For more details see the literature.[7]

3.12 Correlation Functions in Canonical Path Integral

Sometimes it is desirable to know the correlation functions of position and momentum variables

$$G^{(m,n)}_{\omega^2}(\tau_1,\dots,\tau_m;\tau_1,\dots,\tau_n)\equiv\langle x(\tau_1)x(\tau_2)\cdots x(\tau_m)p(\tau_1)p(\tau_2)\cdots p(\tau_n)\rangle\quad(3.332)$$
$$\equiv Z^{-1}\int\mathcal{D}x(\tau)\int\frac{\mathcal{D}p(\tau)}{2\pi}x(\tau_1)x(\tau_2)\cdots x(\tau_m)p(\tau)\,p(\tau_1)p(\tau_2)\cdots p(\tau_n)\exp\left(-\frac{1}{\hbar}\mathcal{A}_{\rm e}\right).$$

These can be obtained from a direct extension of the generating functional (3.236) by another source $k(\tau)$ coupled linearly to the momentum variable $p(\tau)$:

$$Z[j,k]=\int\mathcal{D}x(\tau)\,e^{-\mathcal{A}_{\rm e}[j,k]/\hbar}.\quad(3.333)$$

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[7]M. Bachmann, H. Kleinert, and A. Pelster, Phys. Rev. A *62*, 52509 (2000) (quant-ph/0005074); Phys. Lett. A *279*, 23 (2001) (quant-ph/0005100).

3.12.1 Harmonic Correlation Functions

For the harmonic oscillator, the generating functional (3.333) is denoted by $Z_\omega[j,k]$ and its Euclidean action reads

$$\mathcal{A}_{\rm e}[j,k]=\int_0^{\hbar\beta}d\tau\left[-ip(\tau)\dot{x}(\tau)+\frac{1}{2M}p^2+\frac{M}{2}\omega^2x^2-j(\tau)x(\tau)-k(\tau)p(\tau)\right], \tag{3.334}$$

the partition function is denoted by $Z_\omega[j,k]$. Introducing the vectors in phase space $\mathbf{V}(\tau)=(p(\tau),x(\tau))$ and $\mathbf{J}(\tau)=(j(\tau),k(\tau))$, this can be written in matrix form as

$$\mathcal{A}_{\rm e}[\mathbf{J}]=\int_0^{\hbar\beta}d\tau\left(\frac{1}{2}\mathbf{V}^T\,\mathbf{D}_{\omega^2,{\rm e}}\,\mathbf{V}\;-\;\mathbf{V}^T\mathbf{J}\right), \tag{3.335}$$

where $\mathbf{D}_{\omega^2,{\rm e}}(\tau,\tau')$ is the functional matrix

$$\mathbf{D}_{\omega^2,{\rm e}}(\tau,\tau')\equiv\begin{pmatrix} M\omega^2 & i\partial_\tau\\ -i\partial_\tau & M^{-1}\end{pmatrix}\delta(\tau-\tau'),\quad \tau-\tau'\in[0,\hbar\beta]. \tag{3.336}$$

Its functional inverse is the Euclidean Green function,

$$\begin{aligned}\mathbf{G}^{\rm p}_{\omega^2,{\rm e}}(\tau,\tau') &= \mathbf{G}^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau')=\mathbf{D}^{-1}_{\omega^2,{\rm e}}(\tau,\tau')\\ &= \begin{pmatrix} M^{-1} & -i\partial_\tau\\ i\partial_\tau & M\omega^2\end{pmatrix}(-\partial_\tau^2+\omega^2)^{-1}\delta(\tau-\tau'),\end{aligned} \tag{3.337}$$

with the periodic boundary condition. After performing a quadratic completion as in (3.241) by shifting the path:

$$\mathbf{V}\to\mathbf{V}'=\mathbf{V}+\mathbf{G}^{\rm p}_{\omega^2,{\rm e}}\mathbf{J}, \tag{3.338}$$

the Euclidean action takes the form

$$\mathcal{A}_{\rm e}[\mathbf{J}]=\int_0^{\hbar\beta}d\tau\frac{1}{2}\mathbf{V}'^T\,\mathbf{D}_{\omega^2,{\rm e}}\mathbf{V}'-\frac{1}{2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\mathbf{J}^T(\tau')\mathbf{G}^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau')\mathbf{J}(\tau'). \tag{3.339}$$

The fluctuations over the periodic paths $\mathbf{V}'(\tau)$ can now be integrated out and yield for $\mathbf{J}(\tau)\equiv 0$ the oscillator partition function

$$Z_\omega=\mathrm{Det}\,\mathbf{D}^{-1/2}_{\omega^2,{\rm e}}. \tag{3.340}$$

A Fourier decomposition into Matsubara frequencies

$$\mathbf{D}_{\omega^2,{\rm e}}(\tau,\tau') = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\mathbf{D}^{\rm p}_{\omega^2,{\rm e}}(\omega_m)e^{-i\omega_m(\tau-\tau')}, \tag{3.341}$$

has the components

$$\mathbf{D}^{\rm p}_{\omega^2,{\rm e}}(\omega_m)=\begin{pmatrix} M^{-1} & \omega_m\\ -\omega_m & M\omega^2\end{pmatrix}, \tag{3.342}$$

with the determinants

$$\det\mathbf{D}^{\rm p}_{\omega^2,{\rm e}}(\omega_m)=\omega_m^2+\omega^2, \tag{3.343}$$

and the inverses

$$\mathbf{G}^{\rm p}_{\rm e}(\omega_m)=[\mathbf{D}^{\rm p}_{\omega^2,{\rm e}}(\omega_m)]^{-1}=\begin{pmatrix} M\omega^2 & -\omega_m\\ \omega_m & M^{-1}\end{pmatrix}\frac{1}{\omega_m^2+\omega^2}. \tag{3.344}$$

The product of determinants (3.343) for all ω_m required in the functional determinant of Eq. (3.340) is calculated with the rules of analytic regularization in Section 2.15, and yields the same partition function as in (3.244), and thus the same partition function (3.245):

$$Z_\omega = \frac{1}{\prod_{m=1}^{\infty}\sqrt{\omega_m^2+\omega^2}} = \frac{1}{2\sinh(\beta\hbar\omega/2)}. \tag{3.345}$$

We therefore obtain for arbitrary sources $\mathbf{J}(\tau) = (j(\tau), k(\tau)) \neq 0$ the generating functional

$$Z[\mathbf{J}] = Z_\omega \exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\rm e}^{\mathbf{J}}[\mathbf{J}]\right\}, \tag{3.346}$$

with the source term

$$\mathcal{A}_{\rm e}^{\mathbf{J}}[\mathbf{J}] = -\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, \mathbf{J}^T(\tau)\mathbf{G}^{\rm p}_{\omega^2,{\rm e}}(\tau,\tau')\mathbf{J}(\tau'). \tag{3.347}$$

The Green function $\mathbf{G}^{\rm p}_{\omega^2,{\rm e}}(\tau,\tau')$ follows immediately from Eq. (3.337) and (3.240):

$$\mathbf{G}^{\rm p}_{\omega^2,{\rm e}}(\tau,\tau') = \mathbf{G}^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau') = \mathbf{D}^{-1}_{\omega^2,{\rm e}}(\tau,\tau') = \begin{pmatrix} M^{-1} & -i\partial_\tau \\ i\partial_\tau & M\omega^2 \end{pmatrix} G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau'), \tag{3.348}$$

where $G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau')$ is the simple periodic Green function (3.251). From the functional derivatives of (3.346) with respect to $j(\tau)/\hbar$ and $k(\tau)/\hbar$ as in (3.302), we now find the correlation functions

$$G^{(2)}_{\omega^2,{\rm e},xx}(\tau,\tau') \equiv \langle x(\tau)x(\tau')\rangle = \frac{\hbar}{M}G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau'), \tag{3.349}$$

$$G^{(2)}_{\omega^2,{\rm e},xp}(\tau,\tau') \equiv \langle x(\tau)p(\tau')\rangle = -i\hbar\dot{G}^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau'), \tag{3.350}$$

$$G^{(2)}_{\omega^2,{\rm e},px}(\tau,\tau') \equiv \langle p(\tau)x(\tau')\rangle = i\hbar\dot{G}^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau'), \tag{3.351}$$

$$G^{(2)}_{\omega^2,{\rm e},pp}(\tau,\tau') \equiv \langle p(\tau)p(\tau')\rangle = \hbar M\omega^2 G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau'). \tag{3.352}$$

The correlation function $\langle x(\tau)x(\tau')\rangle$ is the same as in the pure configuration space formulation (3.304). The mixed correlation function $\langle p(\tau)x(\tau')\rangle$ is understood immediately by rewriting the current-free part of the action (3.334) as

$$\mathcal{A}_{\rm e}[0,0] = \int_0^{\hbar\beta} d\tau \left[\frac{1}{2M}(p-iM\dot{x})^2 + \frac{M}{2}\left(\dot{x}^2+\omega^2x^2\right)\right], \tag{3.353}$$

which shows that $p(\tau)$ fluctuates harmonically around the classical momentum for imaginary time $iM\dot{x}(\tau)$. It is therefore not surprising that the correlation function $\langle p(\tau)x(\tau')\rangle$ comes out to be the same as that of $iM\langle\dot{x}(\tau)x(\tau')\rangle$. Such an analogy is no longer true for the correlation function $\langle p(\tau)p(\tau')\rangle$. In fact, the correlation function $\langle\dot{x}(\tau)\dot{x}(\tau')\rangle$ is equal to

$$\langle\dot{x}(\tau)\dot{x}(\tau')\rangle = -\hbar M\partial_\tau^2 G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau'). \tag{3.354}$$

Comparison with (3.352) reveals the relation

$$\begin{aligned}\langle p(\tau)p(\tau')\rangle &= \langle\dot{x}(\tau)\dot{x}(\tau')\rangle + \frac{\hbar}{M}\left(-\partial_\tau^2+\omega^2\right)G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau') \\ &= \langle\dot{x}(\tau)\dot{x}(\tau')\rangle + \frac{\hbar}{M}\delta(\tau-\tau').\end{aligned} \tag{3.355}$$

The additional δ-function on the right-hand side is the consequence of the fact that $p(\tau)$ is not equal to $iM\dot{x}$, but fluctuates around it harmonically.

For the canonical path integral of a particle in a uniform magnetic field solved in Section 2.18, there are analogous relations. Here we write the canonical action (2.643) with a vector potential (2.640) in the Euclidean form as

$$\mathcal{A}_{\rm e}[\mathbf{p},\mathbf{x}]=\int_0^{\hbar\beta}d\tau\left\{\frac{1}{2M}\left[\mathbf{p}-\frac{e}{c}\mathbf{B}\times\mathbf{x}-iM\dot{\mathbf{x}}\right]^2+\frac{M}{2}\omega^2\mathbf{x}^2\right\},\tag{3.356}$$

showing that $\mathbf{p}(\tau)$ fluctuates harmonically around the classical momentum $\mathbf{p}_{\rm cl}(\tau)=(e/c)\mathbf{B}\times\mathbf{x}-iM\dot{\mathbf{x}}$. For a magnetic field pointing in the z-direction we obtain, with the frequency $\omega_B=\omega_L/2$ of Eq. (2.648), the following relations between the correlation functions involving momenta and those involving only coordinates given in (3.325), (3.327), (3.327):

$$G^{(2)}_{\omega^2,B,xp_x}(\tau,\tau')\equiv\langle x(\tau)p_x(\tau')\rangle=iM\partial_{\tau'}G^{(2)}_{\omega^2,B,xx}(\tau,\tau')-M\omega_BG^{(2)}_{\omega^2,B,xy}(\tau,\tau'),\tag{3.357}$$

$$G^{(2)}_{\omega^2,B,xp_y}(\tau,\tau')\equiv\langle x(\tau)p_y(\tau')\rangle=iM\partial_{\tau'}G^{(2)}_{\omega^2,B,xy}(\tau,\tau')+M\omega_BG^{(2)}_{\omega^2,B,xx}(\tau,\tau'),\tag{3.358}$$

$$G^{(2)}_{\omega^2,B,zp_z}(\tau,\tau')\equiv\langle z(\tau)p_z(\tau')\rangle=iM\partial_{\tau'}G^{(2)}_{\omega^2,B,zz}(\tau,\tau'),\tag{3.359}$$

$$\begin{aligned}G^{(2)}_{\omega^2,B,p_xp_x}(\tau,\tau')\equiv\langle p_x(\tau)p_x(\tau')\rangle=&-M^2\partial_\tau\partial_{\tau'}G^{(2)}_{\omega^2,B,xx}(\tau,\tau')-2iM^2\omega_B\partial_\tau G^{(2)}_{\omega^2,B,xy}(\tau,\tau')\\&+M^2\omega_B^2\,G^{(2)}_{\omega^2,B,xx}(\tau,\tau')+\hbar M\delta(\tau-\tau'),\end{aligned}\tag{3.360}$$

$$\begin{aligned}G^{(2)}_{\omega^2,B,p_xp_y}(\tau,\tau')\equiv\langle p_x(\tau)p_y(\tau')\rangle=&-M^2\partial_\tau\partial_{\tau'}G^{(2)}_{\omega^2,B,xy}(\tau,\tau')+iM^2\partial_\tau G^{(2)}_{\omega^2,B,xx}(\tau,\tau')\\&+M^2\omega_B^2G^{(2)}_{\omega^2,B,xy}(\tau,\tau'),\end{aligned}\tag{3.361}$$

$$G^{(2)}_{\omega^2,B,p_zp_z}(\tau,\tau')\equiv\langle p_z(\tau)p_z(\tau')\rangle=-M^2\partial_\tau\partial_{\tau'}G^{(2)}_{\omega^2,B,zz}(\tau,\tau')+\hbar M\delta(\tau-\tau').\tag{3.362}$$

Only diagonal correlations between momenta contain the extra δ-function on the right-hand side according to the rule (3.355). Note that $\partial_\tau\partial_{\tau'}G^{(2)}_{\omega^2,B,ab}(\tau,\tau')=-\partial_\tau^2G^{(2)}_{\omega^2,B,ab}(\tau,\tau')$. Each correlation function is, of course, invariant under time translations, depending only on the time difference $\tau-\tau'$.

The correlation functions $\langle x(\tau)x(\tau')\rangle$ and $\langle x(\tau)y(\tau')\rangle$ are the same as before in Eqs. (3.327) and (3.328).

3.12.2 Relations between Various Amplitudes

A slight generalization of the generating functional (3.333) contains paths with fixed endpoints rather than all periodic paths. If the endpoints are held fixed in configuration space, one defines

$$(x_b\,\hbar\beta|x_a\,0)[j,k]=\int_{x(0)=x_a}^{x(\hbar\beta)=x_b}Dx\frac{Dp}{2\pi\hbar}\exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\rm e}[j,k]\right\}.\tag{3.363}$$

If the endpoints are held fixed in momentum space, one defines

$$(p_b\,\hbar\beta|p_a\,0)[j,k]=\int_{p(0)=p_a}^{p(\hbar\beta)=p_b}Dx\frac{Dp}{2\pi\hbar}\exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\rm e}[j,k]\right\}.\tag{3.364}$$

The two are related by a Fourier transformation

$$(p_b\,\hbar\beta|p_a\,0)[j,k]=\int_{-\infty}^{+\infty}dx_a\int_{-\infty}^{+\infty}dx_be^{-i(p_bx_b-p_ax_a)/\hbar}(x_b\,\hbar\beta|x_a\,0)[j,k]\,.\tag{3.365}$$

We now observe that in the canonical path integral, the amplitudes (3.363) and (3.364) with fixed endpoints can be reduced to those with vanishing endpoints with modified sources. The modification consists in shifting the current $k(\tau)$ in the action by the source term $ix_b\delta(\tau_b-\tau)-$

$ix_a\delta(\tau-\tau_a)$ and observe that this produces in (3.364) an overall phase factor in the limit $\tau_b\uparrow\hbar\beta$ and $\tau_a\downarrow 0$:

$$\lim_{\tau_b\uparrow\hbar\beta}\lim_{\tau_a\downarrow 0}(p_b\,\hbar\beta|p_a\,0)[j(\tau),k(\tau)+ix_b\delta(\tau_b-\tau)-ix_a\delta(\tau-\tau_a)]$$
$$=\exp\left\{\frac{i}{\hbar}(p_bx_b-p_ax_a)\right\}(p_b\,\hbar\beta|p_a\,0)[j(\tau),k(\tau)]\,. \tag{3.366}$$

By inserting (3.366) into the inverse of the Fourier transformation (3.365),

$$(x_b\,\hbar\beta|x_a\,0)[j,k]=\int_{-\infty}^{+\infty}\frac{dp_a}{2\pi\hbar}\int_{-\infty}^{+\infty}\frac{dp_b}{2\pi\hbar}e^{i(p_bx_b-p_ax_a)/\hbar}(p_b\,\hbar\beta|p_a\,0)[j,k], \tag{3.367}$$

we obtain

$$(x_b\,\hbar\beta|x_a\,0)[j,k]=\lim_{\tau_b\uparrow\hbar\beta}\lim_{\tau_a\downarrow 0}(0\,\hbar\beta|0\,0)[j(\tau),k(\tau)+ix_b\delta(\tau_b-\tau)-ix_a\delta(\tau-\tau_a)]\,. \tag{3.368}$$

In this way, the fixed-endpoint path integral (3.363) can be reduced to a path integral with vanishing endpoints but additional δ-terms in the current $k(\tau)$ coupled to the momentum $p(\tau)$.

There is also a simple relation between path integrals with fixed equal endpoints and periodic path integrals. The measures of integration are related by

$$\int_{x(0)=x}^{x(\hbar\beta)=x}\frac{\mathcal{D}x\mathcal{D}p}{2\pi\hbar}=\oint\frac{\mathcal{D}x\mathcal{D}p}{2\pi\hbar}\,\delta(x(0)-x)\,. \tag{3.369}$$

Using the Fourier decomposition of the delta function, we rewrite (3.369) as

$$\int_{x(0)=x}^{x(\hbar\beta)=x}\frac{\mathcal{D}x\mathcal{D}p}{2\pi\hbar}=\lim_{\tau_a'\downarrow 0}\int_{-\infty}^{+\infty}\frac{dp_a}{2\pi\hbar}e^{ip_ax/\hbar}\oint\frac{\mathcal{D}x\mathcal{D}p}{2\pi\hbar}e^{-i\int_0^{\hbar\beta}d\tau\,p_a\delta(\tau-\tau_a')x(\tau)/\hbar}. \tag{3.370}$$

Inserting now (3.370) into (3.368) leads to the announced desired relation

$$\begin{aligned}(x_b\,\hbar\beta|x_a0)[k,j] \;=\;& \lim_{\tau_b\uparrow\hbar\beta}\lim_{\tau_a\downarrow 0}\lim_{\tau_a'\downarrow 0}\int_{-\infty}^{+\infty}\frac{dp_a}{2\pi\hbar}\\ &\times Z\left[j(\tau)-ip_a\delta(\tau-\tau_a'),k(\tau)+ix_b\delta(\tau_b-\tau)-ix_a\delta(\tau-\tau_a)\right],\end{aligned} \tag{3.371}$$

where $Z[j,k]$ is the thermodynamic partition function (3.333) summing all periodic paths. When using (3.371) we must be careful in evaluating the three limits. The limit $\tau_a'\downarrow 0$ has to be evaluated prior to the other limits $\tau_b\uparrow\hbar\beta$ and $\tau_a\downarrow 0$.

3.12.3 Harmonic Generating Functionals

Here we write down explicitly the harmonic generating functionals with the above shifted source terms:

$$\tilde{k}(\tau)=k(\tau)+ix_b\delta(\tau_b-\tau)-ix_a\delta(\tau-\tau_a)\,,\quad \tilde{j}(\tau)=j(\tau)-ip\delta(\tau-\tau_a'), \tag{3.372}$$

leading to the factorized generating functional

$$Z_\omega[\tilde{k},\tilde{j}]=Z_\omega^{(0)}[0,0]Z_\omega^{(1)}[k,j]Z_\omega^{\rm p}[k,j]\,. \tag{3.373}$$

The respective terms on the right-hand side of (3.373) read in detail

$$Z_\omega^{(0)}[0,0] \;=\; Z_\omega\exp\left(\frac{1}{2\hbar^2}\left\{-p^2G^{\rm p}_{xx}(\tau_a',\tau_a')-2p\left[x_aG^{\rm p}_{xp}(\tau_a',\tau_a)+x_bG^{\rm p}_{xp}(\tau_a',\tau_b)\right]\right.\right.$$

$$-x_a^2 G_{pp}^{\rm p}(\tau_a,\tau_a) - x_b^2 G_{pp}^{\rm p}(\tau_b,\tau_b) + 2x_a x_b G_{pp}^{\rm p}(\tau_a,\tau_b)\}\big), \tag{3.374}$$

$$Z_\omega^{(1)}[k,j] = \exp\left(\frac{1}{\hbar^2}\int_0^{\hbar\beta} d\tau\,\{j(\tau)[-ipG_{xx}^{\rm p}(\tau,\tau_a') + ix_b G_{xp}^{\rm p}(\tau,\tau_b) - ix_a G_{xp}^{\rm p}(\tau,\tau_a)] \right.$$
$$\left. +k(\tau)[-ipG_{xp}^{\rm p}(\tau,\tau_a') + ix_b G_{pp}^{\rm p}(\tau,\tau_b) - ix_a G_{pp}^{\rm p}(\tau,\tau_a)]\}\right), \tag{3.375}$$

$$Z_\omega^{\rm p}[k,j] = \exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\,[(j(\tau_1),k(\tau_2)) \right.$$
$$\left. \times \begin{pmatrix} G_{xx}^{\rm p}(\tau_1,\tau_1) & G_{xp}^{\rm p}(\tau_1,\tau_2) \\ G_{px}^{\rm p}(\tau_1,\tau_2) & G_{pp}^{\rm p}(\tau_1,\tau_2)\end{pmatrix}\begin{pmatrix} j(\tau_2) \\ k(\tau_2)\end{pmatrix}\Big]\right\}, \tag{3.376}$$

where Z_ω is given by (3.345) and $G_{xp}^{\rm p}(\tau_1,\tau_2)$ etc. are the periodic Euclidean Green functions $G_{\omega^2,{\rm e},ab}^{(2)}(\tau_1,\tau_2)$ defined in Eqs. (3.349)–(3.352) in an abbreviated notation. Inserting (3.373) into (3.371) and performing the Gaussian momentum integration, over the exponentials in $Z_\omega^{(0)}[0,0]$ and $Z_\omega^{(1)}[k,j]$, the result is

$$(x_b\,\hbar\beta|x_a\,0)[k,j] = (x_b\,\hbar\beta|x_a\,0)[0,0]\times\exp\left\{\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\,[x_{\rm cl}(\tau)j(\tau)+p_{\rm cl}(\tau)k(\tau)]\right\}$$
$$\times\exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau_1\int_0^{\hbar\beta} d\tau_2\,[(j(\tau_1),k(\tau_2))\begin{pmatrix} G_{xx}^{\rm (D)}(\tau_1,\tau_2) & G_{xp}^{\rm (D)}(\tau_1,\tau_2) \\ G_{px}^{\rm (D)}(\tau_1,\tau_2) & G_{pp}^{\rm (D)}(\tau_1,\tau_2)\end{pmatrix}\begin{pmatrix} j(\tau_2) \\ k(\tau_2)\end{pmatrix}\Big]\right\}, \tag{3.377}$$

where the Green functions $G_{ab}^{\rm (D)}(\tau_1,\tau_2)$ have now Dirichlet boundary conditions. In particular, the Green function $G_{ab}^{\rm (D)}(\tau_1,\tau_2)$ is equal to (3.36) continued to imaginary time. The Green functions $G_{xp}^{\rm (D)}(\tau_1,\tau_2)$ and $G_{pp}^{\rm (D)}(\tau_1,\tau_2)$ are Dirichlet versions of Eqs. (3.349)–(3.352) which arise from the above Gaussian momentum integrals.

After performing the integrals, the first factor without currents is

$$(x_b\,\hbar\beta|x_a 0)[0,0] = \lim_{\tau_b\uparrow\hbar\beta}\lim_{\tau_a\downarrow 0}\lim_{\tau_a'\downarrow 0}\frac{Z_\omega}{2\pi\hbar}\sqrt{\frac{2\pi\hbar^2}{G_{xx}^{\rm p}(\tau_a',\tau_a')}}$$
$$\times\exp\left[\frac{1}{2\hbar^2}\left(x_a^2\left\{\frac{{G_{xp}^{\rm p}}^2(\tau_a',\tau_a)}{G_{xx}^{\rm p}(\tau_a',\tau_a')} - G_{pp}^{\rm p}(\tau_a,\tau_a)\right\} + x_b^2\left\{\frac{{G_{xp}^{\rm p}}^2(\tau_a',\tau_b)}{G_{xx}^{\rm p}(\tau_a',\tau_a')} - G_{pp}^{\rm p}(\tau_b,\tau_b)\right\}\right.\right.$$
$$\left.\left. -2x_a x_b\left\{\frac{G_{xp}^{\rm p}(\tau_a',\tau_a)G_{xp}^{\rm p}(\tau_a',\tau_b)}{G_{xx}^{\rm p}(\tau_a',\tau_a')} - G_{pp}^{\rm p}(\tau_a,\tau_b)\right\}\right)\right]. \tag{3.378}$$

Performing the limits using

$$\lim_{\tau_a\downarrow 0}\lim_{\tau_a'\downarrow 0} G_{xp}^{\rm p}(\tau_a',\tau_a) = -i\frac{\hbar}{2}, \tag{3.379}$$

where the order of the respective limits turns out to be important, we obtain the amplitude (2.411):

$$(x_b\,\hbar\beta|x_a 0)[0,0] = \sqrt{\frac{M\omega}{2\pi\hbar\sinh\hbar\beta\omega}}$$
$$\times\ \exp\left\{-\frac{M\omega}{2\hbar\sinh\hbar\beta\omega}\left[(x_a^2+x_b^2)\cosh\hbar\beta\omega - 2x_a x_b\right]\right\}. \tag{3.380}$$

The first exponential in (3.377) contains a complicated representation of the classical path

$$x_{\rm cl}(\tau) = \lim_{\tau_b\uparrow\hbar\beta}\lim_{\tau_a\downarrow 0}\lim_{\tau_a'\downarrow 0}\frac{i}{\hbar}\left\{\ x_a\left[\frac{G_{xp}^{\rm p}(\tau_a',\tau_a)G_{xx}^{\rm p}(\tau,\tau_a')}{G_{xx}^{\rm p}(\tau_a',\tau_a')} + G_{xp}^{\rm p}(\tau_a,\tau)\right]\right.$$

$$-x_b \left[\frac{G^{\rm p}_{xp}(\tau'_a,\tau_b)G^{\rm p}_{xx}(\tau,\tau'_a)}{G^{\rm p}_{xx}(\tau'_a,\tau'_a)} + G^{\rm p}_{xp}(\tau_b,\tau)\right]\Bigg\}\,, \tag{3.381}$$

and of the classical momentum

$$\begin{aligned} p_{\rm cl}(\tau) \;\;=\;\; \lim_{\tau_b\uparrow\hbar\beta}\lim_{\tau_a\downarrow 0}\lim_{\tau'_a\downarrow 0}\frac{i}{\hbar}\Bigg\{ & x_a\left[\frac{G^{\rm p}_{xp}(\tau'_a,\tau_a)G^{\rm p}_{xp}(\tau'_a,\tau)}{G^{\rm p}_{xx}(\tau'_a,\tau'_a)} - G^{\rm p}_{pp}(\tau_a,\tau)\right] \\ & -x_b\left[\frac{G^{\rm p}_{xp}(\tau'_a,\tau_b)G^{\rm p}_{xp}(\tau'_a,\tau)}{G^{\rm p}_{xx}(\tau'_a,\tau'_a)} - G^{\rm p}_{pp}(\tau_b,\tau)\right]\Bigg\}\,. \end{aligned} \tag{3.382}$$

Indeed, inserting the explicit periodic Green functions (3.349)–(3.352) and going to the limits we obtain

$$x_{\rm cl}(\tau) \;\;=\;\; \frac{x_a\sinh\omega(\hbar\beta-\tau)+x_b\sinh\omega\tau}{\sinh\hbar\beta\omega} \tag{3.383}$$

and

$$p_{\rm cl}(\tau) \;\;=\;\; iM\omega\frac{-x_a\cosh\omega(\hbar\beta-\tau)+x_b\cosh\omega\tau}{\sinh\hbar\beta\omega}\,, \tag{3.384}$$

the first being the imaginary-time version of the classical path (3.6), the second being related to it by the classical relation $p_{\rm cl}(\tau) = iM dx_{\rm cl}(\tau)/d\tau$.

The second exponential in (3.377) quadratic in the currents contains the Green functions with Dirichlet boundary conditions

$$G^{\rm (D)}_{xx}(\tau_1,\tau_2) \;\; = G^{\rm p}_{xx}(\tau_1,\tau_2) - \frac{G^{\rm p}_{xx}(\tau_1,0)G^{\rm p}_{xx}(\tau_2,0)}{G^{\rm p}_{xx}(\tau_1,\tau_1)}, \tag{3.385}$$

$$G^{\rm (D)}_{xp}(\tau_1,\tau_2) \;\; = G^{\rm p}_{xp}(\tau_1,\tau_2) + \frac{G^{\rm p}_{xx}(\tau_1,0)G^{\rm p}_{xp}(\tau_2,0)}{G^{\rm p}_{xx}(\tau_1,\tau_1)}, \tag{3.386}$$

$$G^{\rm (D)}_{px}(\tau_1,\tau_2) \;\; = G^{\rm p}_{px}(\tau_1,\tau_2) + \frac{G^{\rm p}_{xp}(\tau_1,0)G^{\rm p}_{xx}(\tau_2,0)}{G^{\rm p}_{xx}(\tau_1,\tau_1)}, \tag{3.387}$$

$$G^{\rm (D)}_{pp}(\tau_1,\tau_2) \;\; = G^{\rm p}_{pp}(\tau_1,\tau_2) - \frac{G^{\rm p}_{xp}(\tau_1,0)G^{\rm p}_{xp}(\tau_2,0)}{G^{\rm p}_{xx}(\tau_1,\tau_1)}. \tag{3.388}$$

After applying some trigonometric identities, these take the form

$$G^{\rm (D)}_{xx}(\tau_1,\tau_2) \;\;=\;\; \frac{\hbar}{2M\omega\sinh\hbar\beta\omega}\left[\cosh\omega(\hbar\beta-|\tau_1-\tau_2|)-\cosh\omega(\hbar\beta-\tau_1-\tau_2)\right], \tag{3.389}$$

$$\begin{aligned} G^{\rm (D)}_{xp}(\tau_1,\tau_2) \;\;=\;\; & \frac{i\hbar}{2\sinh\hbar\beta\omega}\left\{\theta(\tau_1-\tau_2)\sinh\omega(\hbar\beta-|\tau_1-\tau_2|)\right. \\ & \left.-\theta(\tau_2-\tau_1)\sinh\omega(\hbar\beta-|\tau_2-\tau_1|)+\sinh\omega(\hbar\beta-\tau_1-\tau_2)\right\}, \end{aligned} \tag{3.390}$$

$$\begin{aligned} G^{\rm (D)}_{px}(\tau_1,\tau_2) \;\;=\;\; & -\frac{i\hbar}{2\sinh\hbar\beta\omega}\left\{\theta(\tau_1-\tau_2)\sinh\omega(\hbar\beta-|\tau_1-\tau_2|)\right. \\ & \left.-\theta(\tau_2-\tau_1)\sinh\omega(\hbar\beta-|\tau_2-\tau_1|)-\sinh\omega(\hbar\beta-\tau_1-\tau_2)\right\}, \end{aligned} \tag{3.391}$$

$$G^{\rm (D)}_{pp}(\tau_1,\tau_2) \;\;=\;\; \frac{M\hbar\omega}{2\sinh\hbar\beta\omega}\left[\cosh\omega(\hbar\beta-|\tau_1-\tau_2|)+\cosh\omega(\hbar\beta-\tau_1-\tau_2)\right]. \tag{3.392}$$

The first correlation function is, of course, the imaginary-time version of the Green function (3.209). Observe the symmetry properties under interchange of the time arguments:

$$G^{\rm (D)}_{xx}(\tau_1,\tau_2) = G^{\rm (D)}_{xx}(\tau_2,\tau_1)\,, \qquad G^{\rm (D)}_{xp}(\tau_1,\tau_2) = -G^{\rm (D)}_{xp}(\tau_2,\tau_1)\,, \tag{3.393}$$

$$G^{\rm (D)}_{px}(\tau_1,\tau_2) = -G^{\rm (D)}_{px}(\tau_2,\tau_1)\,, \quad G^{\rm (D)}_{pp}(\tau_1,\tau_2) = G^{\rm (D)}_{pp}(\tau_2,\tau_1)\,, \tag{3.394}$$

and the identity

$$G_{xp}^{(\mathrm{D})}(\tau_1,\tau_2) = G_{px}^{(\mathrm{D})}(\tau_2,\tau_1). \tag{3.395}$$

In addition, there are the following derivative relations between the Green functions with Dirichlet boundary conditions:

$$G_{xp}^{(\mathrm{D})}(\tau_1,\tau_2) = -iM\frac{\partial}{\partial\tau_1}G_{xx}^{(\mathrm{D})}(\tau_1,\tau_2) = iM\frac{\partial}{\partial\tau_2}G_{xx}^{(\mathrm{D})}(\tau_1,\tau_2), \tag{3.396}$$

$$G_{px}^{(\mathrm{D})}(\tau_1,\tau_2) = iM\frac{\partial}{\partial\tau_1}G_{xx}^{(\mathrm{D})}(\tau_1,\tau_2) = -iM\frac{\partial}{\partial\tau_2}G_{xx}^{(\mathrm{D})}(\tau_1,\tau_2), \tag{3.397}$$

$$G_{pp}^{(\mathrm{D})}(\tau_1,\tau_2) = \hbar M\delta(\tau_1-\tau_2) - M^2\frac{\partial^2}{\partial\tau_1\partial\tau_2}G_{xx}^{(\mathrm{D})}(\tau_1-\tau_2). \tag{3.398}$$

Note that Eq. (3.385) is a nonlinear alternative to the additive decomposition (3.142) of a Green function with Dirichlet boundary conditions: into Green functions with periodic boundary conditions.

3.13 Particle in Heat Bath

The results of Section 3.8 are the key to understanding the behavior of a quantum-mechanical particle moving through a dissipative medium at a fixed temperature T. We imagine the coordinate $x(t)$ a particle of mass M to be coupled linearly to a *heat bath* consisting of a great number of harmonic oscillators $X_i(\tau)$ $(i = 1, 2, 3, \ldots)$ with various masses M_i and frequencies Ω_i. The imaginary-time path integral in this heat bath is given by

$$\begin{aligned}
(x_b\hbar\beta|x_a0) &= \prod_i \oint \mathcal{D}X_i(\tau) \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}x(\tau)\\
&\times \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \sum_i \left[\frac{M_i}{2}(\dot{X}_i^{\,2} + \Omega_i^2 X_i^2)\right]\right\}\\
&\times \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}^2 + V(x(\tau)) - \sum_i c_i X_i(\tau)x(\tau)\right]\right\} \times \frac{1}{\prod_i Z_i},
\end{aligned} \tag{3.399}$$

where we have allowed for an arbitrary potential $V(x)$. The partition functions of the individual bath oscillators

$$\begin{aligned}
Z_i &\equiv \oint \mathcal{D}X_i(\tau) \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M_i}{2}(\dot{X}_i^{\,2} + \Omega_i^2 X_i^2)\right]\right\}\\
&= \frac{1}{2\sinh(\hbar\beta\Omega_i/2)}
\end{aligned} \tag{3.400}$$

have been divided out, since their thermal behavior is trivial and will be of no interest in the sequel. The path integrals over $X_i(\tau)$ can be performed as in Section 3.1 leading for each oscillator label i to a source expression like (3.246), in which $c_i x(\tau)$ plays the role of a current $j(\tau)$. The result can be written as

$$(x_b\hbar\beta|x_a0) = \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}x(\tau) \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}^2 + V(x(\tau))\right] - \frac{1}{\hbar}\mathcal{A}_{\mathrm{bath}}[x]\right\}, \tag{3.401}$$

where $\mathcal{A}_{\rm bath}[x]$ is a *nonlocal* action for the particle motion generated by the bath

$$\mathcal{A}_{\rm bath}[x] = -\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' x(\tau)\alpha(\tau-\tau')x(\tau'). \tag{3.402}$$

The function $\alpha(\tau-\tau')$ is the weighted periodic correlation function (3.251):

$$\begin{aligned}\alpha(\tau-\tau') &= \sum_i c_i^2 \frac{1}{M_i} G^{\rm p}_{\Omega_i^2,{\rm e}}(\tau-\tau') \\ &= \sum_i \frac{c_i^2}{2M_i\Omega_i}\frac{\cosh\Omega_i(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\Omega_i\hbar\beta/2)}.\end{aligned} \tag{3.403}$$

Its Fourier expansion has the Matsubara frequencies $\omega_m = 2\pi k_BT/\hbar$

$$\alpha(\tau-\tau') = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\alpha_m e^{-i\omega_m(\tau-\tau')}, \tag{3.404}$$

with the coefficients

$$\alpha_m = \sum_i \frac{c_i^2}{M_i}\frac{1}{\omega_m^2+\omega_i^2}. \tag{3.405}$$

Alternatively, we can write the bath action in the form corresponding to (3.279) as

$$\mathcal{A}_{\rm bath}[x] = -\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\tau' x(\tau)\alpha_0(\tau-\tau')x(\tau'), \tag{3.406}$$

with the weighted nonperiodic correlation function [recall (3.280)]

$$\alpha_0(\tau-\tau') = \sum_i \frac{c_i^2}{2M_i\Omega_i} e^{-\Omega_i|\tau-\tau'|}. \tag{3.407}$$

The bath properties are conveniently summarized by the *spectral density of the bath*

$$\rho_{\rm b}(\omega') \equiv 2\pi\sum_i \frac{c_i^2}{2M_i\Omega_i}\delta(\omega'-\Omega_i). \tag{3.408}$$

The frequencies Ω_i are by definition positive numbers. The spectral density allows us to express $\alpha_0(\tau-\tau')$ as the spectral integral

$$\alpha_0(\tau-\tau') = \int_0^\infty \frac{d\omega'}{2\pi}\rho_{\rm b}(\omega')e^{-\omega'|\tau-\tau'|}, \tag{3.409}$$

and similarly

$$\alpha(\tau-\tau') = \int_0^\infty \frac{d\omega'}{2\pi}\,\rho_{\rm b}(\omega')\frac{\cosh\omega'(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\omega'\hbar\beta/2)}. \tag{3.410}$$

For the Fourier coefficients (3.405), the spectral integral reads

$$\alpha_m = \int_0^\infty \frac{d\omega'}{2\pi} \rho_{\rm b}(\omega') \frac{2\omega'}{\omega_m^2 + \omega'^2}. \tag{3.411}$$

It is useful to subtract from these coefficients the first term α_0, and to invert the sign of the remainder making it positive definite. Thus we split

$$\alpha_m = 2\int_0^\infty \frac{d\omega'}{2\pi} \frac{\rho_{\rm b}(\omega')}{\omega'} \left(1 - \frac{\omega_m^2}{\omega_m^2 + \omega'^2}\right) = \alpha_0 - g_m. \tag{3.412}$$

Then the Fourier expansion (3.404) separates as

$$\alpha(\tau - \tau') = \alpha_0 \delta^{\rm p}(\tau - \tau') - g(\tau - \tau'), \tag{3.413}$$

where $\delta^{\rm p}(\tau - \tau')$ is the periodic δ-function (3.282):

$$\delta^{\rm p}(\tau - \tau') = \frac{1}{\hbar\beta} \sum_{m=-\infty}^{\infty} e^{-i\omega_m(\tau-\tau')} = \sum_{n=-\infty}^{\infty} \delta(\tau - \tau' - n\hbar\beta), \tag{3.414}$$

the right-hand sum following from Poisson's summation formula (1.197). The subtracted correlation function

$$g(\tau - \tau') = \frac{1}{\hbar\beta} \sum_{m=-\infty}^{\infty} g(\omega_m) e^{-i\omega_m(\tau-\tau')}, \tag{3.415}$$

has the coefficients

$$g_m = \sum_i \frac{c_i^2}{M_i} \frac{\omega_m^2}{\omega_m^2 + \Omega_i^2} = \int_0^\infty \frac{d\omega'}{2\pi} \frac{\rho_{\rm b}(\omega')}{\omega'} \frac{2\omega_m^2}{\omega_m^2 + \omega'^2}. \tag{3.416}$$

The corresponding decomposition of the bath action (3.402) is

$$\mathcal{A}_{\rm bath}[x] = \mathcal{A}_{\rm loc} + \mathcal{A}'_{\rm bath}[x], \tag{3.417}$$

where

$$\mathcal{A}'_{\rm bath}[x] = \frac{1}{2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' x(\tau) g(\tau - \tau') x(\tau'), \tag{3.418}$$

and

$$\mathcal{A}_{\rm loc} = -\frac{\alpha_0}{2} \int_0^{\hbar\beta} d\tau\, x^2(\tau), \tag{3.419}$$

is a local action which can be added to the original action in Eq. (3.401), changing merely the curvature of the potential $V(x)$. Because of this effect, it is useful to introduce a *frequency shift* $\Delta\omega^2$ via the equation

$$M\Delta\omega^2 \equiv -\alpha_0 = -2\int_0^\infty \frac{d\omega'}{2\pi} \frac{\rho_{\rm b}(\omega')}{\omega'} = -\sum_i \frac{c_i^2}{M_i \Omega_i^2}. \tag{3.420}$$

Then the local action (3.419) becomes

$$\mathcal{A}_{\rm loc} = \frac{M}{2}\Delta\omega^2 \int_0^{\hbar\beta} d\tau\, x^2(\tau). \tag{3.421}$$

This can be absorbed into the potential of the path integral (3.401), yielding a *renormalized potential*

$$V_{\rm ren}(x) = V(x) + \frac{M}{2}\Delta\omega^2\, x^2. \tag{3.422}$$

With the decomposition (3.417), the path integral (3.401) acquires the form

$$(x_b\hbar\beta|x_a0) = \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}x(\tau)\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}^2 + V_{\rm ren}(x(\tau))\right] - \frac{1}{\hbar}\mathcal{A}'_{\rm bath}[x]\right\}. \tag{3.423}$$

The subtracted correlation function (3.415) has the property

$$\int_0^{\hbar\beta} d\tau\, g(\tau-\tau') = 0. \tag{3.424}$$

Thus, if we rewrite in (3.418)

$$x(\tau)x(\tau') = \frac{1}{2}\{x^2(\tau) + x^2(\tau') - [x(\tau)-x(\tau')]^2\}, \tag{3.425}$$

the first two terms do not contribute, and we remain with

$$\mathcal{A}'_{\rm bath}[x] = -\frac{1}{4}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' g(\tau-\tau')[x(\tau)-x(\tau')]^2. \tag{3.426}$$

If the oscillator frequencies Ω_i are densely distributed, the function $\rho_{\rm b}(\omega')$ is continuous. As will be shown later in Eqs. (18.208) and (18.317), an oscillator bath introduces in general a *friction force* into classical equations of motion. If this is to have the usual form $-M\gamma\dot{x}(t)$, the spectral density of the bath must have the approximation

$$\rho_{\rm b}(\omega') \approx 2M\gamma\omega' \tag{3.427}$$

[see Eqs. (18.208), (18.317)]. This approximation is characteristic for *Ohmic dissipation*. In general, a typical friction force increases with ω only for small frequencies; for larger ω, it decreases again. An often applicable phenomenological approximation is the so-called *Drude form*

$$\rho_{\rm b}(\omega') \approx 2M\gamma\omega' \frac{\omega_D^2}{\omega_D^2 + \omega'^2}, \tag{3.428}$$

where $1/\omega_D \equiv \tau_D$ is *Drude's relaxation time*. For times much shorter than the Drude time τ_D, there is no dissipation. In the limit of large ω_D, the Drude form describes again Ohmic dissipation.

Inserting (3.428) into (3.416), we obtain the Fourier coefficients for Drude dissipation

$$g_m = 2M\gamma\omega_D^2 \int_0^\infty \frac{d\omega}{2\pi} \frac{1}{\omega_D^2+\omega^2} \frac{2\omega_m^2}{\omega_m^2+\omega^2} = M|\omega_m|\gamma \frac{\omega_D}{|\omega_m|+\omega_D}. \tag{3.429}$$

It is customary, to factorize

$$g_m \equiv M|\omega_m|\gamma_m, \tag{3.430}$$

so that Drude dissipation corresponds to

$$\gamma_m = \gamma \, \frac{\omega_D}{|\omega_m|+\omega_D}, \tag{3.431}$$

and Ohmic dissipation to $\gamma_m \equiv \gamma$.

The Drude form of the spectral density gives rise to a frequency shift (3.420)

$$\Delta\omega^2 = -\gamma\omega_D, \tag{3.432}$$

which goes to infinity in the Ohmic limit $\omega_D \to \infty$.

3.14 Heat Bath of Photons

The heat bath in the last section was a convenient phenomenological tool to reproduce the Ohmic friction observed in many physical systems. In nature, there can be various different sources of dissipation. The most elementary of these is the deexcitation of atoms by radiation, which at zero temperature gives rise to the natural line width of atoms. The photons may form a thermally equilibrated gas, the most famous example being the cosmic black-body radiation which is a gas of the photons of 3 K left over from the big bang 15 billion years ago (and which create a sizable fraction of the blips on our television screens).

The theoretical description is quite simple. We decompose the vector potential $\mathbf{A}(\mathbf{x},t)$ of electromagnetism into Fourier components of wave vector $\mathbf{k}$

$$\mathbf{A}(\mathbf{x},t) = \sum_{\mathbf{k}} c_{\mathbf{k}}(\mathbf{x})\mathbf{X}_{\mathbf{k}}(t), \qquad c_{\mathbf{k}} = \frac{e^{i\mathbf{k}\mathbf{x}}}{\sqrt{2\Omega_{\mathbf{k}}V}}, \qquad \sum_{\mathbf{k}} = \int \frac{d^3kV}{(2\pi)^3}. \tag{3.433}$$

The Fourier components $\mathbf{X}_{\mathbf{k}}(t)$ can be considered as a sum of harmonic oscillators of frequency $\Omega_{\mathbf{k}} = c|\mathbf{k}|$, where c is the light velocity. A photon of wave vector $\mathbf{k}$ is a quantum of $\mathbf{X}_{\mathbf{k}}(t)$. A certain number N of photons with the same wave vector can be described as the Nth excited state of the oscillator $\mathbf{X}_{\mathbf{k}}(t)$. The statistical sum of these harmonic oscillators led Planck to his famous formula for the energy of black-body radiation for photons in an otherwise empty cavity whose walls have a temperature T. These will form the bath, and we shall now study its effect on the quantum mechanics of a charged point particle. Its coupling to the vector potential is given by the interaction (2.634). Comparison with the coupling to the heat bath in Eq. (3.399) shows that we simply have to replace $-\sum_i c_i X_i(\tau)x(\tau)$ by $-\sum_{\mathbf{k}} c_{\mathbf{k}} \mathbf{X}_{\mathbf{k}}(\tau)\dot{\mathbf{x}}(\tau)$. The bath action (3.402) takes then the form

$$\mathcal{A}_{\rm bath}[x] = -\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \dot{x}^i(\tau)\alpha^{ij}(\mathbf{x}(\tau),\tau;\mathbf{x}(\tau'),\tau')\dot{x}^j(\tau'), \tag{3.434}$$

where $\alpha^{ij}(\mathbf{x},\tau;\mathbf{x}',\tau')$ is a 3×3 matrix generalization of the correlation function (3.403):

$$\alpha^{ij}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{e^2}{\hbar c^2}\sum_{\mathbf{k}} c_{-\mathbf{k}}(\mathbf{x})c_{\mathbf{k}}(\mathbf{x}')\langle X^i_{-\mathbf{k}}(\tau)X^j_{\mathbf{k}}(\tau')\rangle. \tag{3.435}$$

We now have to account for the fact that there are two polarization states for each photon, which are transverse to the momentum direction. We therefore introduce a transverse Kronecker symbol

$$^T\delta^{ij}_{\mathbf{k}} \equiv (\delta^{ij} - k^i k^j/\mathbf{k}^2) \tag{3.436}$$

and write the correlation function of a single oscillator $X^i_{-\mathbf{k}}(\tau)$ as

$$G^{ij}_{-\mathbf{k}'\mathbf{k}}(\tau-\tau') = \langle \hat{X}^i_{-\mathbf{k}'}(\tau)\hat{X}^j_{\mathbf{k}'}(\tau')\rangle = \hbar\, ^T\delta^{ij}_{\mathbf{k}}\,\delta_{\mathbf{k}\mathbf{k}'}\, G^{\rm p}_{\omega^2,{\rm e}\,\mathbf{k}}(\tau-\tau'), \tag{3.437}$$

with

$$G^{\rm p}_{\omega^2,{\rm e}\,\mathbf{k}}(\tau-\tau') \equiv \frac{1}{2\Omega_{\mathbf{k}}}\frac{\cosh\Omega_{\mathbf{k}}(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\Omega_{\mathbf{k}}\hbar\beta/2)}. \tag{3.438}$$

Thus we find

$$\alpha^{ij}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{e^2}{c^2}\int\frac{d^3k}{(2\pi)^3}\, ^T\delta^{ij}_{\mathbf{k}}\,\frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}}{2\Omega_{\mathbf{k}}}\frac{\cosh\Omega_{\mathbf{k}}(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\Omega_{\mathbf{k}}\hbar\beta/2)}. \tag{3.439}$$

At zero temperature, and expressing $\Omega_{\mathbf{k}} = c|\mathbf{k}|$, this simplifies to

$$\alpha^{ij}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{e^2}{c^3}\int\frac{d^3k}{(2\pi)^3}\, ^T\delta^{ij}_{\mathbf{k}}\,\frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')-c|\mathbf{k}||\tau-\tau'|}}{2|\mathbf{k}|}. \tag{3.440}$$

Forgetting for a moment the transverse Kronecker symbol and the prefactor e^2/c^2, the integral yields

$$G^R_{\rm e}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{1}{4\pi^2c^2}\frac{1}{(\tau-\tau')^2+(\mathbf{x}-\mathbf{x}')^2/c^2}, \tag{3.441}$$

which is the imaginary-time version of the well-known retarded Green function used in electromagnetism. If the system is small compared to the average wavelengths in the bath we can neglect the retardation and omit the term $(\mathbf{x}-\mathbf{x}')^2/c^2$. In the finite-temperature expression (3.440) this amounts to neglecting the $\mathbf{x}$-dependence.

The transverse Kronecker symbol can then be averaged over all directions of the wave vector and yields simply $2\delta^{ij}/3$, and we obtain the approximate function

$$\alpha^{ij}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{2e^2}{3c^2}\,\delta^{ij}\,\frac{1}{2\pi c^2}\int\frac{d\omega}{2\pi}\,\omega\,\frac{\cosh\omega(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\omega\hbar\beta/2)}. \tag{3.442}$$

This has the generic form (3.410) with the spectral function of the photon bath

$$\rho_{\rm pb}(\omega') = \frac{e^2}{3c^2\pi}\omega'. \tag{3.443}$$

This has precisely the Ohmic form (3.427), but there is now an important difference: the bath action (3.434) contains now the time derivatives of the paths $\mathbf{x}(\tau)$. This gives rise to an extra factor ω'^2 in (3.427), so that we may define a spectral density for the photon bath:

$$\rho_{\rm pb}(\omega') \approx 2M\gamma\omega'^3, \qquad \gamma = \frac{e^2}{6c^2\pi M}. \tag{3.444}$$

In contrast to the usual friction constant γ in the previous section, this has the dimension 1/frequency.

3.15 Harmonic Oscillator in Ohmic Heat Bath

For a harmonic oscillator in an Ohmic heat bath, the partition function can be calculated as follows. Setting

$$V_{\rm ren}(x) = \frac{M}{2}\omega^2 x^2, \tag{3.445}$$

the Fourier decomposition of the action (3.423) reads

$$\mathcal{A}_{\rm e} = \frac{M\hbar}{k_BT}\left\{\frac{\omega^2}{2}x_0^2 + \sum_{m=1}^{\infty}\left[\omega_m^2+\omega^2+\omega_m\gamma_m\right]|x_m|^2\right\}. \tag{3.446}$$

The harmonic potential is the full renormalized potential (3.422). Performing the Gaussian integrals using the measure (2.447), we obtain the partition function for the damped harmonic oscillator of frequency ω [compare (2.408)]

$$Z_\omega^{\rm damp} = \frac{k_BT}{\hbar\omega}\left\{\prod_{m=1}^{\infty}\left[\frac{\omega_m^2+\omega^2+\omega_m\gamma_m}{\omega_m^2}\right]\right\}^{-1}. \tag{3.447}$$

For the Drude dissipation (3.429), this can be written as

$$Z_\omega^{\rm damp} = \frac{k_BT}{\hbar\omega}\prod_{m=1}^{\infty}\frac{\omega_m^2(\omega_m+\omega_D)}{\omega_m^3+\omega_m^2\omega_D+\omega_m(\omega^2+\gamma\omega_D)+\omega_D\omega^2}. \tag{3.448}$$

Let w_1, w_2, w_3 be the roots of the cubic equation

$$w^3 - w^2\omega_D + w(\omega^2+\gamma\omega_D) - \omega^2\omega_D = 0. \tag{3.449}$$

Then we can rewrite (3.448) as

$$Z_\omega^{\rm damp} = \frac{k_BT}{\hbar\omega}\prod_{m=1}^{\infty}\frac{\omega_m}{\omega_m+w_1}\frac{\omega_m}{\omega_m+w_2}\frac{\omega_m}{\omega_m+w_3}\frac{\omega_m+\omega_D}{\omega_m}. \tag{3.450}$$

Using the product representation of the Gamma function[8]

$$\Gamma(z) = \lim_{n\to\infty}\frac{n^z}{z}\prod_{m=1}^{n}\frac{m}{m+z} \tag{3.451}$$

and the fact that

$$w_1+w_2+w_3-\omega_D = 0, \qquad w_1w_2w_3 = \omega^2\omega_D, \tag{3.452}$$

the partition function (3.450) becomes

$$Z_\omega^{\rm damp} = \frac{1}{2\pi}\frac{\omega}{\omega_1}\frac{\Gamma(w_1/\omega_1)\Gamma(w_2/\omega_1)\Gamma(w_3/\omega_1)}{\Gamma(\omega_D/\omega_1)}, \tag{3.453}$$

where $\omega_1 = 2\pi k_BT/\hbar$ is the first Matsubara frequency, such that $w_i/\omega_1 = w_i\beta/2\pi$.

In the Ohmic limit $\omega_D\to\infty$, the roots w_1, w_2, w_3 reduce to

$$w_1 = \gamma/2+i\delta, \qquad w_1 = \gamma/2-i\delta, \qquad w_3 = \omega_D-\gamma, \tag{3.454}$$

with

$$\delta \equiv \sqrt{\omega^2-\gamma^2/4}, \tag{3.455}$$

and (3.453) simplifies further to

$$Z_\omega^{\rm damp} = \frac{1}{2\pi}\frac{\omega}{\omega_1}\Gamma(w_1/\omega_1)\Gamma(w_2/\omega_1). \tag{3.456}$$

For vanishing friction, the roots w_1 and w_2 become simply $w_1 = i\omega,\ \ w_2 = -i\omega$, and the formula[9]

$$\Gamma(1-z)\Gamma(z) = \frac{\pi}{\sin\pi z} \tag{3.457}$$

can be used to calculate

$$\Gamma(i\omega/\omega_1)\Gamma(-i\omega/\omega_1) = \frac{\omega_1}{\omega}\frac{\pi}{\sinh(\pi\omega/\omega_1)} = \frac{\omega_1}{\omega}\frac{\pi}{\sinh(\omega\hbar/2k_BT)}, \tag{3.458}$$

showing that (3.453) goes properly over into the partition function (3.217) of the undamped harmonic oscillator.

The free energy of the system is

$$\begin{aligned} F(T) \;\; = \;\; & -k_BT\left[\log(\omega/2\pi\omega_1) - \log\Gamma(\omega_D/\omega_1)\right. \\ & \left. + \log\Gamma(w_1/\omega_1) + \log\Gamma(w_2/\omega_1) + \log\Gamma(w_3/\omega_1)\right]. \end{aligned} \tag{3.459}$$

[8] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formula 8.322.

[9] *ibid.*, Formula 8.334.3.

Using the large-z behavior of $\log\Gamma(z)$[10]

$$\log\Gamma(z) = \left(z-\frac{1}{2}\right)\log z - z + \frac{1}{2}\log 2\pi + \frac{1}{12z} - \frac{1}{360z^3} - \mathcal{O}(1/z^5), \tag{3.460}$$

we find the free energy at low temperature

$$F(T) \sim E_0 - \left(\frac{1}{w_1}+\frac{1}{w_2}+\frac{1}{w_1}-\frac{\omega^2}{w_1w_2w_3}\right)\frac{\pi}{6\hbar}(k_BT)^2 = E_0 - \frac{\gamma\pi}{6\omega^2\hbar}(k_BT)^2, \tag{3.461}$$

where

$$E_0 = -\frac{\hbar}{2\pi}\left[w_1\log(w_1/\omega_D) + w_2\log(w_2/\omega_D) + w_3\log(w_3/\omega_D)\right] \tag{3.462}$$

is the ground state energy.

For small friction, this reduces to

$$E_0 = \frac{\hbar\omega}{2} + \frac{\gamma}{2\pi}\log\frac{\omega_D}{\omega} - \frac{\gamma^2}{16\omega}\left(1+\frac{4\omega}{\pi\omega_D}\right) + \mathcal{O}(\gamma^3). \tag{3.463}$$

The T^2-behavior of $F(T)$ in Eq. (3.461) is typical for Ohmic dissipation.

At zero temperature, the Matsubara frequencies $\omega_m = 2\pi m k_BT/\hbar$ move arbitrarily close together, so that Matsubara sums become integrals according to the rule

$$\frac{1}{\hbar\beta}\sum_m \xrightarrow[T\to 0]{} \int_0^\infty \frac{d\omega_m}{2\pi}. \tag{3.464}$$

Applying this limiting procedure to the logarithm of the product formula (3.448), the ground state energy can also be written as an integral

$$E_0 = \frac{\hbar}{2\pi}\int_0^\infty d\omega_m \log\left[\frac{\omega_m^3+\omega_m^2\omega_D+\omega_m(\omega^2+\gamma\omega_D)+\omega_D\omega^2}{\omega_m^2(\omega_m+\omega_D)}\right], \tag{3.465}$$

which shows that the energy E_0 increases with the friction coefficient γ.

It is instructive to calculate the density of states defined in (1.583). Inverting the Laplace transform (1.582), we have to evaluate

$$\rho(\varepsilon) = \frac{1}{2\pi i}\int_{\eta-i\infty}^{\eta+i\infty} d\beta\, e^{i\varepsilon\beta}\, Z_\omega^{\rm damp}(\beta), \tag{3.466}$$

where η is an infinitesimally small positive number. In the absence of friction, the integral over $Z_\omega(\beta) = \sum_{n=0}^\infty e^{-\beta\hbar\omega(n+1/2)}$ yields

$$\rho(\varepsilon) = \sum_{n=0}^\infty \delta(\varepsilon-(n+1/2)\hbar\omega). \tag{3.467}$$

In the presence of friction, we expect the sharp δ-function spikes to be broadened. The calculation is done as follows: The vertical line of integration in the complex β-plane in (3.466) is moved all the way to the left, thereby picking up the poles

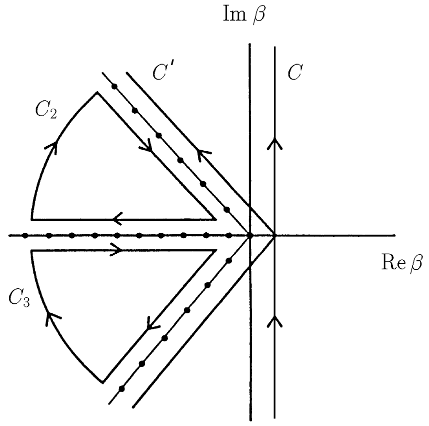


Figure 3.5 Poles in complex β-plane of Fourier integral (3.466) coming from the Gamma functions of (3.453)

of the Gamma functions which lie at negative integer values of $w_i\beta/2\pi$. From the representation of the Gamma function[11]

$$\Gamma(z) = \int_1^\infty dt\, t^{z-1}e^{-t} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(z+n)} \tag{3.468}$$

we see the size of the residues. Thus we obtain the sum

$$\rho(\varepsilon) = \frac{1}{\omega} \sum_{n=1}^{\infty} \sum_{i=1}^{3} R_{n,i} e^{-2\pi n\varepsilon/w_i}, \tag{3.469}$$

$$R_{n,1} = \frac{\omega}{w_1^2} \frac{(-1)^{n-1}}{(n-1)!} \frac{\Gamma(-nw_2/w_1)\Gamma(-nw_3/w_1)}{\Gamma(-n\omega_D/w_1)}, \tag{3.470}$$

with analogous expressions for $R_{n,2}$ and $R_{n,3}$. The sum can be done numerically and yields the curves shown in Fig. 3.6 for typical underdamped and overdamped situations. There is an isolated δ-function at the ground state energy E_0 of (3.462) which is not widened by the friction. Right above E_0, the curve continues from a finite value $\rho(E_0+0) = \gamma\pi/6\omega^2$ determined by the first expansion term in (3.461).

3.16 Harmonic Oscillator in Photon Heat Bath

It is straightforward to extend this result to a photon bath where the spectral density is given by (3.444) and (3.471) becomes

$$Z_\omega^{\text{damp}} = \frac{k_B T}{\hbar\omega} \left\{ \prod_{m=1}^{\infty} \left[\frac{\omega_m^2 + \omega^2 + \omega_m^3 \gamma}{\omega_m^2} \right] \right\}^{-1}, \tag{3.471}$$

[10] *ibid.*, Formula 8.327.
[11] *ibid.*, Formula 8.314.

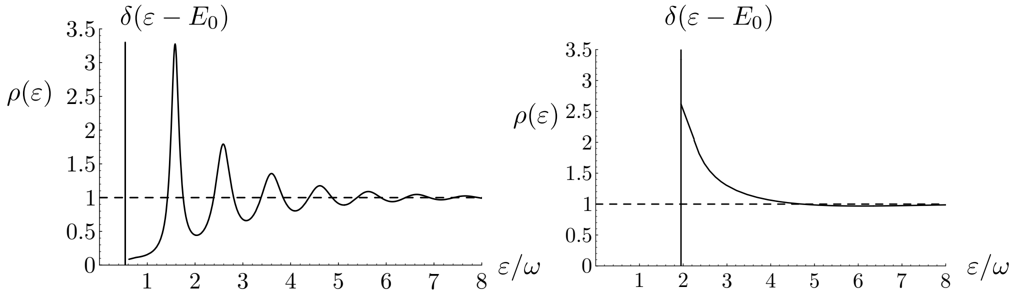


Figure 3.6 Density of states for weak and strong damping in natural units. On the left, the parameters are $\gamma/\omega = 0.2$, $\omega_D/\omega = 10$, on the right $\gamma/\omega = 5$, $\omega_D/\omega = 10$. For more details see Hanke and Zwerger in Notes and References.

with $\gamma = e^2/6c^2\pi M$. The power of ω_m accompanying the friction constant is increased by two units. Adding a Drude correction for the high-frequency behavior we replace γ by $\omega_m/(\omega_m + \omega_D)$ and obtain instead of (3.448)

$$Z_\omega^{\rm damp} = \frac{k_BT}{\hbar\omega} \prod_{m=1}^{\infty} \frac{\omega_m^2(\omega_m + \omega_D)(1 + \gamma\omega_D)}{\omega_m^3(1 + \gamma\omega_D) + \omega_m^2\omega_D + \omega_m\omega^2 + \omega_D\omega^2}. \tag{3.472}$$

The resulting partition function has again the form (3.453), except that w_{123} are the solutions of the cubic equation

$$w^3(1 + \gamma\omega_D) - w^2\omega_D + w\omega^2 - \omega^2\omega_D = 0. \tag{3.473}$$

Since the electromagnetic coupling is small, we can solve this equation to lowest order in γ. If we also assume ω_D to be large compared to ω, we find the roots

$$w_1 \approx \gamma_{\rm pb}^{\rm eff}/2 + i\omega, \qquad w_1 \approx \gamma_{\rm pb}^{\rm eff}/2 - i\omega, \qquad w_3 \approx \omega_D/(1 + \gamma_{\rm pb}^{\rm eff}\omega_D/\omega^2), \tag{3.474}$$

where we have introduced an effective friction constant of the photon bath

$$\gamma_{\rm pb}^{\rm eff} = \frac{e^2}{6c^2\pi M}\omega^2, \tag{3.475}$$

which has the dimension of a frequency, just as the usual friction constant γ in the previous heat bath equations (3.454).

3.17 Perturbation Expansion of Anharmonic Systems

If a harmonic system is disturbed by an additional anharmonic potential $V(x)$, to be called *interaction*, the path integral can be solved exactly only in exceptional cases. These will be treated in Chapters 8, 13, and 14. For sufficiently smooth and small potentials $V(x)$, it is always possible to expand the full partition in powers of the interaction strength. The result is the so-called *perturbation series*. Unfortunately, it only renders reliable numerical results for very small $V(x)$ since, as we shall prove in Chapter 17, the expansion coefficients grow for large orders k like $k!$, making the series strongly divergent. The can only be used for extremely small perturbations. Such expansions are called *asymptotic* (more in Subsection 17.10.1). For this reason we are forced to develop a more powerful technique of studying anharmonic systems in Chapter 5. It combines the perturbation series with a variational approach and will yield very accurate energy levels up to arbitrarily large interaction strengths. It is therefore worthwhile to find the formal expansion in spite of its divergence.

Consider the quantum-mechanical amplitude

$$(x_bt_b|x_at_a)=\int_{x(t_a)=x_a}^{x(t_b)=x_b}\mathcal{D}x\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left[\frac{M}{2}\dot{x}^2-M\frac{\omega^2}{2}x^2-V(x)\right]\right\}\ , \tag{3.476}$$

and expand the integrand in powers of $V(x)$, which leads to the series

$$\begin{aligned}(x_bt_b|x_at_a) \;=\; & \int_{x(t_a)=x_a}^{x(t_b)=x_b}\mathcal{D}x\Big[1-\frac{i}{\hbar}\int_{t_a}^{t_b}dtV(x(t))\\ & -\frac{1}{2!\hbar^2}\int_{t_a}^{t_b}dt_2V(x(t_2))\int_{t_a}^{t_b}dt_1V(x(t_1))\\ & +\frac{i}{3!\hbar^3}\int_{t_a}^{t_b}dt_3V(x(t_3))\int_{t_a}^{t_b}dt_2V(x(t_2))\int_{t_a}^{t_b}dt_1V(x(t_1))+\ldots\Big]\\ & \times\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}dt\frac{M}{2}\left(\dot{x}^2-\omega^2x^2\right)\right].\end{aligned} \tag{3.477}$$

If we decompose the path integral in the nth term into a product (2.4), the expansion can be rewritten as

$$\begin{aligned}(x_bt_b|x_at_a) = (x_bt_b|x_at_a) - \frac{i}{\hbar}\int_{t_a}^{t_b}dt_1\int dx_1(x_bt_b|x_1t_1)V(x_1)(x_bt_b|x_at_a)\\ -\frac{1}{2!\hbar^2}\int_{t_a}^{t_b}dt_2\int_{t_a}^{t_b}dt_1\int dx_1dx_2(x_bt_b|x_2t_2)V(x_2)(x_2t_2|x_1t_1)V(x_1)(x_1t_1|x_at_a)+\ldots.\end{aligned} \tag{3.478}$$

A similar expansion can be given for the Euclidean path integral of a partition function

$$Z=\oint\mathcal{D}x\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\left[\frac{M}{2}(\dot{x}^2+\omega^2x^2)+V(x)\right]\right\}, \tag{3.479}$$

where we obtain

$$\begin{aligned}Z \;=\; & \int\mathcal{D}x\Big[1-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau V(x(\tau))+\frac{1}{2!\hbar^2}\int_0^{\hbar\beta}d\tau_2V(x(\tau_2))\int_0^{\hbar\beta}d\tau_1V(x(\tau_1))\\ & -\frac{1}{3!\hbar^3}\int_0^{\hbar\beta}d\tau_3V(x(\tau_3))\int_0^{\hbar\beta}d\tau_2V(x(\tau_2))\int_0^{\hbar\beta}d\tau_1V(x(\tau_1))+\ldots\Big]\\ & \times\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}dt\left[\frac{M}{2}\dot{x}^2+M\frac{\omega^2}{2}x^2\right]\right\}.\end{aligned} \tag{3.480}$$

The individual terms are obviously expectation values of powers of the Euclidean interaction

$$\mathcal{A}_{\rm int,e}\equiv\int_0^{\hbar\beta}d\tau V(x(\tau)), \tag{3.481}$$

calculated within the harmonic-oscillator partition function Z_ω. The expectation values are defined by

$$\langle \dots \rangle_\omega \equiv Z_\omega^{-1} \int \mathcal{D}x \, \dots \, \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}(\dot{x}^2 + \omega^2 x^2) \right] \right\}. \tag{3.482}$$

With these, the perturbation series can be written in the form

$$Z = \left(1 - \frac{1}{\hbar} \langle \mathcal{A}_{\rm int,e} \rangle_\omega + \frac{1}{2!\hbar^2} \langle \mathcal{A}_{\rm int,e}^2 \rangle_\omega - \frac{1}{3!\hbar^3} \langle \mathcal{A}_{\rm int,e}^3 \rangle_\omega + \dots \right) Z_\omega. \tag{3.483}$$

As we shall see immediately, it is preferable to resum the prefactor into an exponential of a series

$$\begin{aligned} & 1 - \frac{1}{\hbar} \langle \mathcal{A}_{\rm int,e} \rangle_\omega + \frac{1}{2!\hbar^2} \langle \mathcal{A}_{\rm int,e}^2 \rangle_\omega - \frac{1}{3!\hbar^3} \langle \mathcal{A}_{\rm int,e}^3 \rangle_\omega + \dots \\ & = \exp\left\{ -\frac{1}{\hbar} \langle \mathcal{A}_{\rm int,e} \rangle_\omega + \frac{1}{2!\hbar^2} \langle \mathcal{A}_{\rm int,e}^2 \rangle_{\omega,c} - \frac{1}{3!\hbar^3} \langle \mathcal{A}_{\rm int,e}^3 \rangle_{\omega,c} + \dots \right\}. \end{aligned} \tag{3.484}$$

The expectation values $\langle \rangle_{\omega,\rm c}$ are called *cumulants*. They are related to the original expectation values by the *cumulant expansion*:[12]

$$\begin{aligned} \langle \mathcal{A}_{\rm int,e}^2 \rangle_{\omega,c} & \equiv \langle \mathcal{A}_{\rm int,e}^2 \rangle_\omega - \langle \mathcal{A}_{\rm int,e} \rangle_\omega^2 & (3.485) \\ & = \langle [\mathcal{A}_{\rm int,e} - \langle \mathcal{A}_{\rm int,e} \rangle_\omega]^2 \rangle_\omega, & \\ \langle \mathcal{A}_{\rm int,e}^3 \rangle_{\omega,\rm c} & \equiv \langle \mathcal{A}_{\rm int,e}^3 \rangle_\omega - 3 \langle \mathcal{A}_{\rm int,e}^2 \rangle_\omega \langle \mathcal{A}_{\rm int,e} \rangle_\omega + 2 \langle \mathcal{A}_{\rm int,e} \rangle_\omega^3 & (3.486) \\ & = \langle [\mathcal{A}_{\rm int,e} - \langle \mathcal{A}_{\rm int,e} \rangle_\omega]^3 \rangle_\omega, & \\ & \vdots \quad . & \end{aligned}$$

The cumulants contribute directly to the free energy $F = -(1/\beta) \log Z$. From (3.484) and (3.483) we conclude that the anharmonic potential $V(x)$ shifts the free energy of the harmonic oscillator $F_\omega = (1/\beta) \log[2 \sinh(\hbar\beta\omega/2)]$ by

$$\Delta F = \frac{1}{\beta} \left(\frac{1}{\hbar} \langle \mathcal{A}_{\rm int,e} \rangle_\omega - \frac{1}{2!\hbar^2} \langle \mathcal{A}_{\rm int,e}^2 \rangle_{\omega,\rm c} + \frac{1}{3!\hbar^3} \langle \mathcal{A}_{\rm int,e}^3 \rangle_{\omega,\rm c} + \dots \right). \tag{3.487}$$

Whereas the original expectation values $\left\langle \mathcal{A}_{\rm int,e}^n \right\rangle_\omega$ grow for large β with the nth power of β, due to contributions of n disconnected diagrams of first order in g which are integrated independently over τ from 0 to $\hbar\beta$, the cumulants $\left\langle \mathcal{A}_{\rm int,,e}^n \right\rangle_\omega$ are proportional to β, thus ensuring that the free energy F has a finite limit, the ground state energy E_0. In comparison with the ground state energy of the unperturbed harmonic system, the energy E_0 is shifted by

$$\Delta E_0 = \lim_{\beta\to\infty} \frac{1}{\beta} \left(\frac{1}{\hbar} \langle \mathcal{A}_{\rm int,e} \rangle_\omega - \frac{1}{2!\hbar^2} \langle \mathcal{A}_{\rm int,e}^2 \rangle_{\omega,\rm c} + \frac{1}{3!\hbar^3} \langle \mathcal{A}_{\rm int,e}^3 \rangle_{\omega,\rm c} + \dots \right). \tag{3.488}$$

[12]Note that the subtracted expressions in the second lines of these equations are particularly simple only for the lowest two cumulants given here.

There exists a simple functional formula for the perturbation expansion of the partition function in terms of the generating functional $Z_\omega[j]$ of the unperturbed harmonic system. Adding a source term into the action of the path integral (3.479), we define the generating functional of the interacting theory:

$$Z[j] = \oint \mathcal{D}x \, \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\left(\dot{x}^2+\omega^2x^2\right)+V(x)-jx\right]\right\}. \tag{3.489}$$

The interaction can be brought outside the path integral in the form

$$Z[j] = e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau V(\delta/\delta j(\tau))}\, Z_\omega[j] \ . \tag{3.490}$$

The interacting partition function is obviously

$$Z = Z[0]. \tag{3.491}$$

Indeed, after inserting on the right-hand side the explicit path integral expression for $Z[j]$ from (3.236):

$$Z_\omega[j] = \int \mathcal{D}x \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}(\dot{x}^2+\omega^2x^2)-jx\right]\right\}, \tag{3.492}$$

and expanding the exponential in the prefactor

$$\begin{aligned} e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau V(\delta/\delta j(\tau))} &= 1-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau V(\delta/\delta j(\tau)) \\ &+\frac{1}{2!\hbar^2}\int_0^{\hbar\beta} d\tau_2 V(\delta/\delta j(\tau_2))\int_0^{\hbar\beta} d\tau_1 V(\delta/\delta j(\tau_1)) \\ &-\frac{1}{3!\hbar^3}\int_0^{\hbar\beta} d\tau_3 V(\delta/\delta j(\tau_3))\int_0^{\hbar\beta} d\tau_2 V(\delta/\delta(\tau_2))\int_0^{\hbar\beta} d\tau_1 V(\delta/\delta(\tau_1))+\dots\ , \end{aligned} \tag{3.493}$$

the functional derivatives of $Z[j]$ with respect to the source $j(\tau)$ generate inside the path integral precisely the expansion (3.483), whose cumulants lead to formula (3.487) for the shift in the free energy.

Before continuing, let us mention that the partition function (3.479) can, of course, be viewed as a generating functional for the calculation of the expectation values of the action and its powers. We simply have to form the derivatives with respect to $\hbar^{-1}$:

$$\langle \mathcal{A}^n\rangle = Z^{-1}\frac{\partial^n}{\partial\hbar^{-1n}}Z_\omega[j]\bigg|_{\hbar^{-1}=0}. \tag{3.494}$$

For a harmonic oscillator where Z is given by (3.245), this yields

$$\langle \mathcal{A}\rangle = \lim_{\hbar\to\infty} Z_\omega^{-1}\,\hbar^2\frac{\partial}{\partial\hbar}Z_\omega = \lim_{\hbar\to\infty}\hbar\frac{\hbar\omega\beta}{2\sinh\hbar\omega\beta/2} = 0. \tag{3.495}$$

The same result is, incidentally, obtained by calculating the expectation value of the action with analytic regularization:

$$\left\langle \dot{x}^2(\tau)\right\rangle_\omega + \omega^2\left\langle x^2(\tau)\right\rangle_\omega = \int \frac{d\omega'}{2\pi}\frac{\omega'^2}{\omega'^2+\omega^2} + \int\frac{d\omega'}{2\pi}\frac{\omega^2}{\omega'^2+\omega^2} = \int\frac{d\omega'}{2\pi} = 0. \tag{3.496}$$

The integral vanishes by Veltman's rule (2.508).

3.18 Rayleigh-Schrödinger and Brillouin-Wigner Perturbation Expansion

The expectation values in formula (3.487) can be evaluated by means of the so-called *Rayleigh-Schrödinger perturbation expansion*, also referred to as *old-fashioned perturbation expansion*. This expansion is particularly useful if the potential $V(x)$ is not a polynomial in x. Examples are $V(x) = \delta(x)$ and $V(x) = 1/x$. In these two cases the perturbation expansions can be summed to all orders, as will be shown for the first example in Section 9.5. For the second example the reader is referred to the literature.[13] We shall explicitly demonstrate the procedure for the ground state and the excited energies of an anharmonic oscillator. Later we shall also give expansions for scattering amplitudes.

To calculate the free-energy shift ΔF in Eq. (3.487) to first order in $V(x)$, we need the expectation

$$\langle \mathcal{A}_{\rm int,e} \rangle_\omega \equiv Z_\omega^{-1} \int_0^{\hbar\beta} d\tau_1 \int dx dx_1 (x\,\hbar\beta|x_1\,\tau_1)_\omega V(x_1)(x_1\tau_1|x\,0)_\omega. \tag{3.497}$$

The time evolution amplitude on the right describes the temporal development of the harmonic oscillator located initially at the point x, from the imaginary time 0 up to τ_1. At the time τ_1, the state is subject to the interaction depending on its position $x_1 = x(\tau_1)$ with the amplitude $V(x_1)$. After that, the state is carried to the final state at the point x by the other time evolution amplitude.

To second order we have to calculate the expectation in $V(x)$:

$$\begin{aligned}\frac{1}{2}\langle \mathcal{A}_{\rm int,e}^2 \rangle_\omega \equiv\ & Z_\omega^{-1} \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_1 \int dx dx_2 dx_1 (x\,\hbar\beta|x_2\tau_2)_\omega V(x_2) \\ & \times (x_2\tau_2|x_1\tau_1)_\omega V(x_1)(x_1\tau_1|x\,0)_\omega. \end{aligned} \tag{3.498}$$

The integration over τ_1 is taken only up to τ_2 since the contribution with $\tau_1 > \tau_2$ would merely render a factor 2.

The explicit evaluation of the integrals is facilitated by the spectral expansion (2.300). The time evolution amplitude at imaginary times is given in terms of the eigenstates $\psi_n(x)$ of the harmonic oscillator with the energy $E_n = \hbar\omega(n + 1/2)$:

$$(x_b\tau_b|x_a\tau_a)_\omega = \sum_{n=0}^{\infty} \psi_n(x_b)\psi_n^*(x_a)e^{-E_n(\tau_b-\tau_a)/\hbar}. \tag{3.499}$$

The same type of expansion exists also for the real-time evolution amplitude. This leads to the Rayleigh-Schrödinger perturbation expansion for the energy shifts of all excited states, as we now show.

The amplitude can be projected onto the eigenstates of the harmonic oscillator. For this, the two sides are multiplied by the harmonic wave functions $\psi_n^*(x_b)$ and

[13] M.J. Goovaerts and J.T. Devreese, J. Math. Phys. *13*, 1070 (1972).

$\psi_n(x_a)$ of quantum number n and integrated over x_b and x_a, respectively, resulting in the expansion

$$\int dx_b dx_a \psi_n^*(x_b)(x_b t_b|x_a t_a)\psi_n(x_a) = \int dx_b dx_a \psi_n^*(x_b)(x_b t_b|x_a t_a)_\omega \psi_n(x_a) \\ \times\left(1+\frac{i}{\hbar}\langle n|\mathcal{A}_{\rm int}|n\rangle_\omega - \frac{1}{2!\hbar^2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_\omega - \frac{i}{3!\hbar^3}\langle n|\mathcal{A}_{\rm int}^3|n\rangle_\omega + \dots\right), \tag{3.500}$$

with the interaction

$$\mathcal{A}_{\rm int} \equiv -\int_{t_a}^{t_b} dt\, V(x(t)). \tag{3.501}$$

The expectation values are defined by

$$\langle n|\dots|n\rangle_\omega \equiv Z_{{\rm QM},\omega,n}^{-1}\int dx_b dx_a \psi_n^*(x_b)\left(\int_{x(t_a)=x_a}^{x(t_b)=x_b}\mathcal{D}x \dots e^{i\mathcal{A}_\omega/\hbar}\right)\psi_n(x_a), \tag{3.502}$$

where

$$Z_{{\rm QM},\omega,n} \equiv e^{-i\omega(n+1/2)(t_b-t_a)} \tag{3.503}$$

is the projection of the quantum-mechanical partition function of the harmonic oscillator

$$Z_{{\rm QM},\omega} = \sum_{n=0}^{\infty} e^{-i\omega(n+1/2)(t_b-t_a)}$$

[see (2.42)] onto the nth excited state.

The expectation values are calculated as in (3.497), (3.498). To first order in $V(x)$, one has

$$\langle n|\mathcal{A}_{\rm int}|n\rangle_\omega \equiv -Z_{{\rm QM},\omega,n}^{-1}\int_{t_a}^{t_b} dt_1 \int dx_b dx_a dx_1 \psi_n^*(x_b)(x_b t_b|x_1 t_1)_\omega \\ \times V(x_1)(x_1 t_1|x_a t_a)_\omega \psi_n(x_a). \tag{3.504}$$

The time evolution amplitude on the right-hand side describes the temporal development of the initial state $\psi_n(x_a)$ from the time t_a to the time t_1, where the interaction takes place with an amplitude $-V(x_1)$. After that, the time evolution amplitude on the left-hand side carries the state to $\psi_n^*(x_b)$.

To second order in $V(x)$, the expectation value is given by the double integral

$$\frac{1}{2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_\omega \equiv Z_{{\rm QM},\omega,n}^{-1}\int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_2} dt_1 \int dx_b dx_a dx_2 dx_1 \\ \times \psi_n^*(x_b)(x_b t_b|x_2 t_2)_\omega V(x_2)(x_2 t_2|x_1 t_1)_\omega V(x_1)(x_1 t_1|x_a t_a)_\omega \psi_n(x_a). \tag{3.505}$$

As in (3.498), the integral over t_1 ends at t_2.

By analogy with (3.484), we resum the corrections in (3.500) to bring them into the exponent:

$$1+\frac{i}{\hbar}\langle n|\mathcal{A}_{\rm int}|n\rangle_\omega - \frac{1}{2!\hbar^2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_\omega - \frac{i}{3!\hbar^3}\langle n|\mathcal{A}_{\rm int}^3|n\rangle_\omega + \dots \\ = \exp\left\{\frac{i}{\hbar}\langle n|\mathcal{A}_{\rm int}|n\rangle_\omega - \frac{1}{2!\hbar^2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_{\omega,\rm c} - \frac{i}{3!\hbar^3}\langle n|\mathcal{A}_{\rm int}^3|n\rangle_{\omega,\rm c} + \dots\right\}. \tag{3.506}$$

The cumulants in the exponent are

$$\begin{aligned}
\langle n|\mathcal{A}_{\rm int}^2|n\rangle_{\omega,{\rm c}} &\equiv \langle n|\mathcal{A}_{\rm int}^2|n\rangle_\omega - \langle n|\mathcal{A}_{\rm int}|n\rangle_\omega^2 \\
&= \langle n|[\mathcal{A}_{\rm int} - \langle n|\mathcal{A}_{\rm int}|n\rangle_\omega]^2|n\rangle_\omega, \qquad (3.507)\\
\langle n|\mathcal{A}_{\rm int}^3|n\rangle_{\omega,{\rm c}} &\equiv \langle n|\mathcal{A}_{\rm int}^3|n\rangle_\omega - 3\langle n|\mathcal{A}_{\rm int}^2|n\rangle_\omega\langle n|\mathcal{A}_{\rm int}|n\rangle_\omega + 2\langle n|\mathcal{A}_{\rm int}|n\rangle_\omega^3 \\
&= \langle n|[\mathcal{A}_{\rm int} - \langle n|\mathcal{A}_{\rm int}|n\rangle_\omega]^3|n\rangle_\omega, \qquad (3.508)\\
&\;\vdots \\
&\;.
\end{aligned}$$

From (3.506), we obtain the energy shift of the nth oscillator energy

$$\begin{aligned}
\Delta E_n = \lim_{t_b-t_a\to\infty} \frac{i\hbar}{t_b-t_a}\bigg\{ \frac{i}{\hbar}\langle n|\mathcal{A}_{\rm int}|n\rangle_\omega - \frac{1}{2!\hbar^2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_{\omega,{\rm c}} \\
- \frac{i}{3!\hbar^3}\langle n|\mathcal{A}_{\rm int}^3|n\rangle_{\omega,{\rm c}} + \dots\bigg\}, \qquad (3.509)
\end{aligned}$$

which is a generalization of formula (3.488) which was valid only for the ground state energy. At $n=0$, the new formula goes over into (3.488), after the usual analytic continuation of the time variable.

The cumulants can be evaluated further with the help of the real-time version of the spectral expansion (3.499):

$$(x_bt_b|x_at_a)_\omega = \sum_{n=0}^{\infty}\psi_n(x_b)\psi_n^*(x_a)e^{-iE_n(t_b-t_a)/\hbar}. \qquad (3.510)$$

To first order in $V(x)$, it leads to

$$\langle n|\mathcal{A}_{\rm int}|n\rangle_\omega \equiv -\int_{t_a}^{t_b}dt\int dx\psi_n^*(x)V(x)\psi_n(x) \equiv -(t_b-t_a)V_{nn}. \qquad (3.511)$$

To second order in $V(x)$, it yields

$$\begin{aligned}
\frac{1}{2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_\omega \equiv Z_{{\rm QM},\omega,n}^{-1}\int_{t_a}^{t_b}dt_2\int_{t_a}^{t_2}dt_1 \qquad (3.512)\\
\times\sum_k e^{-iE_n(t_b-t_2)/\hbar-iE_k(t_2-t_1)/\hbar-iE_n(t_1-t_a)/\hbar}V_{nk}V_{kn}.
\end{aligned}$$

The right-hand side can also be written as

$$\int_{t_a}^{t_b}dt_2\int_{t_a}^{t_2}dt_1\sum_k e^{i(E_n-E_k)t_2/\hbar+i(E_k-E_n)t_1/\hbar}V_{nk}V_{kn} \qquad (3.513)$$

and becomes, after the time integrations,

$$-\sum_k\frac{V_{nk}V_{kn}}{E_k-E_n}\left\{i\hbar(t_b-t_a)-\frac{\hbar^2}{E_n-E_k}\left[e^{i(E_n-E_k)(t_b-t_a)/\hbar}-1\right]\right\}. \qquad (3.514)$$

As it stands, the sum makes sense only for the $E_k \neq E_n$ -terms. In these, the second term in the curly brackets can be neglected in the limit of large time differences $t_b - t_a$. The term with $E_k = E_n$ must be treated separately by doing the integral directly in (3.513). This yields

$$V_{nn}V_{nn}\frac{(t_b - t_a)^2}{2}, \tag{3.515}$$

so that

$$\frac{1}{2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_\omega = -\sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_m - E_n}i\hbar(t_b - t_a) + V_{nn}V_{nn}\frac{(t_b - t_a)^2}{2}. \tag{3.516}$$

The same result could have been obtained without the special treatment of the $E_k = E_n$ -term by introducing artificially an infinitesimal energy difference $E_k - E_n = \epsilon$ in (3.514), and by expanding the curly brackets in powers of $t_b - t_a$.

When going over to the cumulants $\frac{1}{2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_{\omega,{\rm c}}$ according to (3.507), the $k = n$ -term is eliminated and we obtain

$$\frac{1}{2}\langle n|\mathcal{A}_{\rm int}^2|n\rangle_{\omega,{\rm c}} = -\sum_{k\neq n}\frac{V_{nk}V_{kn}}{E_k - E_n}i\hbar(t_b - t_a). \tag{3.517}$$

For the energy shifts up to second order in $V(x)$, we thus arrive at the simple formula

$$\Delta_1 E_n + \Delta_2 E_n = V_{nn} - \sum_{k\neq n}\frac{V_{nk}V_{kn}}{E_k - E_n}. \tag{3.518}$$

The higher expansion coefficients become rapidly complicated. The correction of third order in $V(x)$, for example, is

$$\Delta_3 E_n = \sum_{k\neq n}\sum_{l\neq n}\frac{V_{nk}V_{kl}V_{ln}}{(E_k - E_n)(E_l - E_n)} - V_{nn}\sum_{k\neq n}\frac{V_{nk}V_{kn}}{(E_k - E_n)^2}. \tag{3.519}$$

For comparison, we recall the well-known formula of *Brillouin-Wigner equation*[14]

$$\Delta E_n = \bar{R}_{nn}(E_n + \Delta E_n), \tag{3.520}$$

where $\bar{R}_{nn}(E)$ are the diagonal matrix elements $\langle n|\hat{\bar{R}}(E)|n\rangle$ of the *level shift operator* $\hat{\bar{R}}(E)$ which solves the integral equation

$$\hat{\bar{R}}(E) = \hat{V} + \hat{V}\frac{1 - \hat{P}_n}{E - \hat{H}_\omega}\hat{\bar{R}}(E). \tag{3.521}$$

The operator $\hat{P}_n \equiv |n\rangle\langle n|$ is the projection operator onto the state $|n\rangle$. The factors $1 - \hat{P}_n$ ensure that the sums over the intermediate states exclude the quantum

[14] L. Brillouin and E.P. Wigner, J. Phys. Radium **4**, 1 (1933); M.L. Goldberger and K.M. Watson, *Collision Theory*, John Wiley & Sons, New York, 1964, pp. 425–430.

number n of the state under consideration. The integral equation is solved by the series expansion in powers of $\hat{V}$:

$$\hat{\hat{R}}(E) = \hat{V} + \hat{V}\frac{1-\hat{P}_n}{E-\hat{H}_\omega}\hat{V} + \hat{V}\frac{1-\hat{P}_n}{E-\hat{H}_\omega}\hat{V}\frac{1-\hat{P}_n}{E-\hat{H}_\omega}\hat{V} + \dots \,. \tag{3.522}$$

Up to the third order in $\hat{V}$, Eq. (3.520) leads to the *Brillouin-Wigner perturbation expansion*

$$E - E_n \,=\, R_{nn}(E) = V_{nn} + \sum_{k\neq n}\frac{V_{nk}V_{kn}}{E-E_k} + \sum_{k\neq n}\sum_{l\neq n}\frac{V_{nk}V_{kl}V_{ln}}{(E-E_k)(E-E_l)} + \dots \,, \tag{3.523}$$

which is an implicit equation for $\Delta E_n = E - E_n$. The Brillouin-Wigner equation (3.520) may be converted into an explicit equation for the level shift ΔE_n:

$$\begin{aligned}\Delta E_n &= R_{nn}(E_n) + R_{nn}(E_n)R'_{nn}(E_n) + [R_{nn}(E_n)R'_{nn}(E_n)^2 + \tfrac{1}{2}R^2_{nn}(E_n)R''_{nn}(E_n)]\\ &+[R_{nn}(E_n)R'_{nn}(E_n)^3 + \tfrac{3}{2}R^2_{nn}(E_n)R'_{nn}(E_n)R''_{nn}(E_n) + \tfrac{1}{6}R^3_{nn}(E_n)R'''_{nn}(E_n)] + \dots\,.\end{aligned} \tag{3.524}$$

Inserting (3.523) on the right-hand side, we recover the standard *Rayleigh-Schrödinger perturbation expansion* of quantum mechanics,which coincides precisely with the above perturbation expansion of the path integral whose first three terms were given in (3.518) and (3.519). Note that starting from the third order, the explicit solution (3.524) for the level shift introduces more and more extra disconnected terms with respect to the simple systematics in the Brillouin-Wigner expansion (3.523).

For arbitrary potentials, the calculation of the matrix elements V_{nk} can become quite tedious. A simple technique to find them is presented in Appendix 3A.

The calculation of the energy shifts for the particular interaction $V(x) = gx^4/4$ is described in Appendix 3B. Up to order g^3, the result is

$$\begin{aligned}\Delta E_n \;&=\; \frac{\hbar\omega}{2}(2n+1) + \frac{g}{4}3(2n^2+2n+1)a^4\\ &-\; \left(\frac{g}{4}\right)^2 2(34n^3+51n^2+59n+21)a^8\frac{1}{\hbar\omega}\\ &+\; \left(\frac{g}{4}\right)^3 4\cdot 3(125n^4+250n^3+472n^2+347n+111)a^{12}\frac{1}{\hbar^2\omega^2}.\end{aligned} \tag{3.525}$$

The perturbation series for this as well as arbitrary polynomial potentials can be carried out to high orders via recursion relations for the expansion coefficients. This is done in Appendix 3C.

3.19 Level-Shifts and Perturbed Wave Functions from Schrödinger Equation

It is instructive to rederive the perturbation expansion from ordinary operator Schrödinger theory. This derivation provides us also with the perturbed eigenstates to any desired order.

The Hamiltonian operator $\hat{H}$ is split into a free and an interacting part

$$\hat{H} = \hat{H}_0 + \hat{V}. \tag{3.526}$$

Let $|n\rangle$ be the eigenstates of $\hat{H}_0$ and $|\psi^{(n)}\rangle$ those of $\hat{H}$:

$$\hat{H}_0|n\rangle = E_0^{(n)}|n\rangle, \qquad \hat{H}|\psi^{(n)}\rangle = E^{(n)}|\psi^{(n)}\rangle. \tag{3.527}$$

We shall assume that the two sets of states $|n\rangle$ and $|\psi^{(n)}\rangle$ are orthogonal sets, the first with unit norm, the latter normalized by scalar products

$$a_n^{(n)} \equiv \langle n|\psi^{(n)}\rangle = 1. \tag{3.528}$$

Due to the completeness of the states $|n\rangle$, the states $|\psi^{(n)}\rangle$ can be expanded as

$$|\psi^{(n)}\rangle = |n\rangle + \sum_{m\neq n} a_m^{(n)}|m\rangle, \tag{3.529}$$

where

$$a_m^{(n)} \equiv \langle m|\psi^{(n)}\rangle \tag{3.530}$$

are the components of the interacting states in the free basis. Projecting the right-hand Schrödinger equation in (3.527) onto $\langle m|$ and using (3.530), we obtain

$$E_0^{(m)} a_m^{(n)} + \langle m|\hat{V}|\psi^{(n)}\rangle = E^{(n)} a_m^{(n)}. \tag{3.531}$$

Inserting here (3.529), this becomes

$$E_0^{(m)} a_m^{(n)} + \langle m|\hat{V}|n\rangle + \sum_{k\neq n} a_k^{(n)} \langle m|\hat{V}|k\rangle = E^{(n)} a_m^{(n)}, \tag{3.532}$$

and for $m = n$, due to the special normalization (3.528),

$$E_0^{(n)} + \langle n|\hat{V}|n\rangle + \sum_{k\neq n} a_k^{(n)} \langle n|\hat{V}|k\rangle = E^{(n)}. \tag{3.533}$$

Multiplying this equation with $a_m^{(n)}$ and subtracting it from (3.532), we eliminate the unknown exact energy $E^{(n)}$, and obtain a set of coupled algebraic equations for $a_m^{(n)}$:

$$a_m^{(n)} = \frac{1}{E_0^{(n)} - E_0^{(m)}} \left[\langle m - a_m^{(n)} n|\hat{V}|n\rangle + \sum_{k\neq n} a_k^{(n)} \langle m - a_m^{(n)} n|\hat{V}|k\rangle \right], \tag{3.534}$$

where we have introduced the notation $\langle m - a_m^{(n)} n|$ for the combination of states $\langle m| - a_m^{(n)}\langle n|$, for brevity.

This equation can now easily be solved perturbatively order by order in powers of the interaction strength. To count these, we replace $\hat{V}$ by $g\hat{V}$ and expand $a_m^{(n)}$ as well as the energies $E^{(n)}$ in powers of g as:

$$a_m^{(n)}(g) = \sum_{l=1}^{\infty} a_{m,l}^{(n)} (-g)^l \qquad (m \neq n), \tag{3.535}$$

and

$$E^{(n)} = E_0^{(n)} - \sum_{l=1}^{\infty} (-g)^l E_l^{(n)}. \tag{3.536}$$

Inserting these expansions into (3.533), and equating the coefficients of g, we immediately find the perturbation expansion of the energy of the nth level

$$E_1^{(n)} = \langle n|\hat{V}|n\rangle, \tag{3.537}$$

$$E_l^{(n)} = \sum_{k\neq n} a_{k,l-1}^{(n)}\langle n|\hat{V}|k\rangle \qquad l>1. \tag{3.538}$$

The expansion coefficients $a_{m,l}^{(n)}$ are now determined by inserting the ansatz (3.535) into (3.534). This yields

$$a_{m,1}^{(n)} = \frac{\langle m|\hat{V}|n\rangle}{E_0^{(m)}-E_0^{(n)}}, \tag{3.539}$$

and for $l>1$:

$$a_{m,l}^{(n)} = \frac{1}{E_0^{(m)}-E_0^{(n)}}\left[-a_{m,l-1}^{(n)}\langle n|\hat{V}|n\rangle + \sum_{k\neq n} a_{k,l-1}^{(n)}\langle m|\hat{V}|k\rangle - \sum_{l'=1}^{l-2} a_{m,l'}^{(n)}\sum_{k\neq n} a_{k,l-1-l'}^{(n)}\langle n|\hat{V}|k\rangle\right]. \tag{3.540}$$

Using (3.537) and (3.538), this can be simplified to

$$a_{m,l}^{(n)} = \frac{1}{E_0^{(m)}-E_0^{(n)}}\left[\sum_{k\neq n} a_{k,l-1}^{(n)}\langle m|\hat{V}|k\rangle - \sum_{l'=1}^{l-1} a_{m,l'}^{(n)}E_{l-l'}^{(n)}\right]. \tag{3.541}$$

Together with (3.537), (3.538), and (3.539), this is a set of recursion relations for the coefficients $a_{m,l}^{(n)}$ and $E_l^{(n)}$.

The recursion relations allow us to recover the perturbation expansions (3.518) and (3.519) for the energy shift. The second-order result (3.518), for example, follows directly from (3.540) and (3.541), the latter giving

$$E_2^{(n)} = \sum_{k\neq n} a_{k,1}^{(n)}\langle n|\hat{V}|k\rangle = \sum_{k\neq n}\frac{\langle k|\hat{V}|n\rangle\langle n|\hat{V}|k\rangle}{E_0^{(k)}-E_0^{(n)}}. \tag{3.542}$$

If the potential $\hat{V}=V(\hat{x})$ is a polynomial in $\hat{x}$, its matrix elements $\langle n|\hat{V}|k\rangle$ are nonzero only for n in a finite neighborhood of k, and the recursion relations consist of finite sums which can be solved exactly.

3.20 Calculation of Perturbation Series via Feynman Diagrams

The expectation values in formula (3.487) can be evaluated also in another way which can be applied to all potentials which are simple polynomials pf x. Then the partition function can be expanded into a sum of integrals associated with certain *Feynman diagrams*.

The procedure is rooted in the Wick expansion of correlation functions in Section 3.10. To be specific, we assume the anharmonic potential to have the form

$$V(x) = \frac{g}{4}x^4. \tag{3.543}$$

The graphical expansion terms to be found will be typical for all so-called φ^4-theories of quantum field theory.

To calculate the free energy shift (3.487) to first order in g, we have to evaluate the harmonic expectation of $\mathcal{A}_{\rm int,e}$. This is written as

$$\langle \mathcal{A}_{\rm int,e} \rangle_\omega = \frac{g}{4} \int_0^{\hbar\beta} d\tau \langle x^4(\tau) \rangle_\omega. \tag{3.544}$$

The integrand contains the correlation function

$$\langle x(\tau_1)x(\tau_2)x(\tau_3)x(\tau_4) \rangle_\omega = G^{(4)}_{\omega^2}(\tau_1,\tau_2,\tau_3,\tau_4)$$

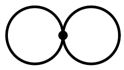
at identical time arguments. According to the Wick rule (3.305), this can be expanded into the sum of three pair terms

$$G^{(2)}_{\omega^2}(\tau_1,\tau_2)G^{(2)}_{\omega^2}(\tau_3,\tau_4) + G^{(2)}_{\omega^2}(\tau_1,\tau_3)G^{(2)}_{\omega^2}(\tau_2,\tau_4) + G^{(2)}_{\omega^2}(\tau_1,\tau_4)G^{(2)}_{\omega^2}(\tau_2,\tau_3),$$

where $G^{(2)}_{\omega^2}(\tau,\tau')$ are the periodic Euclidean Green functions of the harmonic oscillator [see (3.304) and (3.251)]. The expectation (3.544) is therefore equal to the integral

$$\langle \mathcal{A}_{\rm int,e} \rangle_\omega = 3\,\frac{g}{4} \int_0^{\hbar\beta} d\tau G^{(2)}_{\omega^2}(\tau,\tau)^2. \tag{3.545}$$

The right-hand side is pictured by the Feynman diagram

 .

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Because of its shape this is called a two-loop diagram. In general, a Feynman diagram consists of lines meeting at points called *vertices*. A line connecting two points represents the Green function $G^{(2)}_{\omega^2}(\tau_1,\tau_2)$. A vertex indicates a factor $g/4\hbar$ and a variable τ to be integrated over the interval $(0,\hbar\beta)$. The present simple diagram has only one point, and the τ-arguments of the Green functions coincide. The number underneath counts how often the integral occurs. It is called the *multiplicity* of the diagram.

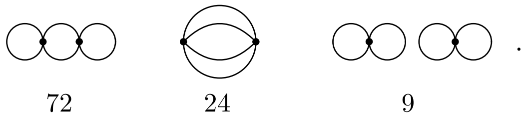
To second order in $V(x)$, the harmonic expectation to be evaluated is

$$\langle \mathcal{A}^2_{\rm int,e} \rangle_\omega = \left(\frac{g}{4}\right)^2 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_1 \langle x^4(\tau_2)x^4(\tau_1) \rangle_\omega. \tag{3.546}$$

The integral now contains the correlation function $G^{(8)}_{\omega^2}(\tau_1,\dots,\tau_8)$ with eight time arguments. According to the Wick rule, it decomposes into a sum of $7!! = 105$ products of four Green functions $G^{(2)}_{\omega^2}(\tau,\tau')$. Due to the coincidence of the time arguments, there are only three different types of contributions to the integral (3.546):

$$\langle \mathcal{A}^2_{\rm int,e} \rangle_\omega = \left(\frac{g}{4}\right)^2 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_1 \Big[72 G^{(2)}_{\omega^2}(\tau_2,\tau_2)G^{(2)}_{\omega^2}(\tau_2,\tau_1)^2 G^{(2)}_{\omega^2}(\tau_1,\tau_1)$$
$$+24 G^{(2)}_{\omega^2}(\tau_2,\tau_1)^4 + 9 G^{(2)}_{\omega^2}(\tau_2,\tau_2)^2 G^{(2)}_{\omega^2}(\tau_1,\tau_1)^2\Big]. \tag{3.547}$$

The integrals are pictured by the following Feynman diagrams composed of three loops:



They contain two vertices indicating two integration variables τ_1, τ_2. The first two diagrams with the shape of three bubbles in a chain and of a watermelon, respectively, are *connected* diagrams, the third is *disconnected*. When going over to the cumulant $\langle \mathcal{A}^2_{\rm int,e} \rangle_{\omega,c}$, the disconnected diagram is eliminated.

To higher orders, the counting becomes increasingly tedious and it is worth developing computer-algebraic techniques for this purpose. Figure 3.7 shows the diagrams for the free-energy shift up to four loops. The cumulants eliminate precisely all disconnected diagrams. This diagram-rearranging property of the logarithm is very general and happens to every order in g, as can be shown with the help of functional differential equations.

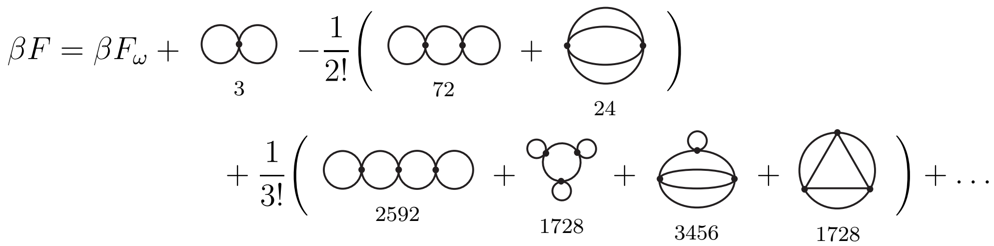


Figure 3.7 Perturbation expansion of free energy up to order g^3 (four loops).

The lowest-order term βF_ω containing the free energy of the harmonic oscillator [recall Eqs. (3.245) and (2.526)]

$$F_\omega = \frac{1}{\beta} \log \left(2 \sinh \frac{\beta \hbar \omega}{2} \right) \tag{3.548}$$

is often represented by the one-loop diagram

$$\beta F_\omega = -\frac{1}{2} \mathrm{Tr} \, \log G^{(2)}_{\omega^2} = -\frac{1}{2\hbar\beta} \int_0^{\hbar\beta} d\tau \left[\log G^{(2)}_{\omega^2} \right] (\tau, \tau) = -\frac{1}{2} \bigcirc \, . \tag{3.549}$$

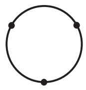
With it, the graphical expansion in Fig. 3.7 starts more systematically with one loop rather than two. The systematics is, however, not perfect since the line in the one-loop diagram does not show that integrand contains a logarithm. In addition, the line is not connected to any vertex.

All τ-variables in the diagrams are integrated out. The diagrams have no open lines and are called *vacuum diagrams*.

The calculation of the diagrams in Fig. 3.7 is simplified with the help of a factorization property: If a diagram consists of two subdiagrams touching each other at a single vertex, its Feynman integral factorizes into those of the subdiagrams. Thanks to this property, we only have to evaluate the following integrals (omitting the factors $g/4\hbar$ for each vertex)

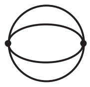
$$= \int_0^{\hbar\beta} d\tau G^{(2)}_{\omega^2}(\tau,\tau) \; = \hbar\beta a^2,$$

$$= \int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2 \; G^{(2)}_{\omega^2}(\tau_1,\tau_2)^2 \equiv \hbar\beta\frac{1}{\omega}a^4_2,$$

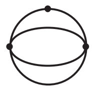


$$= \int_0^{\hbar\beta}\int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2 d\tau_3 \; G^{(2)}_{\omega^2}(\tau_1,\tau_2)G^{(2)}_{\omega^2}(\tau_2,\tau_3)G^{(2)}_{\omega^2}(\tau_3,\tau_1)$$

$$\equiv \hbar\beta\left(\frac{1}{\omega}\right)^2 a^6_3,$$

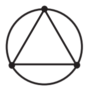


$$= \int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2 \; G^{(2)}_{\omega^2}(\tau_1,\tau_2)^4 \equiv \hbar\beta\frac{1}{\omega}a^8_2,$$



$$= \int_0^{\hbar\beta}\int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2 d\tau_3 \; G^{(2)}_{\omega^2}(\tau_1,\tau_2)G^{(2)}_{\omega^2}(\tau_2,\tau_3)G^{(2)}_{\omega^2}(\tau_3,\tau_1)^3$$

$$\equiv \hbar\beta\left(\frac{1}{\omega}\right)^2 a^{10}_3,$$



$$= \int_0^{\hbar\beta}\int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2 d\tau_3 \; G^{(2)}_{\omega^2}(\tau_1,\tau_2)^2 G^{(2)}_{\omega^2}(\tau_2,\tau_3)^2 G^{(2)}_{\omega^2}(\tau_3,\tau_1)^2$$

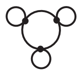
$$\equiv \hbar\beta\left(\frac{1}{\omega}\right)^2 a^{12}_3. \tag{3.550}$$

Note that in each expression, the last τ-integral yields an overall factor $\hbar\beta$, due to the translational invariance along the τ-axis. The others give rise to a factor $1/\omega$, for dimensional reasons. The temperature-dependent quantities a^{2L}_V are labeled by the number of vertices V and lines L of the associated diagrams. Their dimension is length to the nth power [corresponding to the dimension of the n $x(\tau)$-variables in the diagram]. For more than four loops, there can be more than one diagram for each V and L, such that one needs an additional label in a^{2L}_V to specify the diagram uniquely. Each a^{2L}_V may be written as a product of the basic length scale $(\hbar/M\omega)^L$ multiplied by a function of the dimensionless variable $x \equiv \beta\hbar\omega$:

$$a^{2L}_V = \left(\frac{\hbar}{M\omega}\right)^L \alpha^{2L}_V(x). \tag{3.551}$$

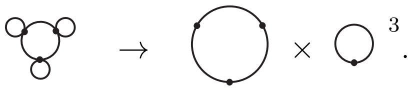
The functions $\alpha^{2L}_V(x)$ are listed in Appendix 3D.

As an example for the application of the factorization property, take the Feynman integral of the second third-order diagram in Fig. 3.7 (called a "daisy" diagram because of its shape):

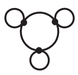


$$= \int_0^{\hbar\beta}\int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2 d\tau_3 G^{(2)}_{\omega^2}(\tau_1,\tau_2)G^{(2)}_{\omega^2}(\tau_2,\tau_3)G^{(2)}_{\omega^2}(\tau_3,\tau_1)$$
$$\times\, G^{(2)}_{\omega^2}(\tau_1,\tau_1)G^{(2)}_{\omega^2}(\tau_2,\tau_2)G^{(2)}_{\omega^2}(\tau_3,\tau_3).$$

It decomposes into a product between the third integral in (3.550) and three powers of the first integral:



Thus we can immediately write



$$= \hbar\beta\left(\frac{1}{\omega}\right)^2 a_3^6(a^2)^3.$$

In terms of a_V^{2L}, the free energy becomes

$$F = F_\omega + \frac{g}{4}\,3a^4 - \frac{1}{2!\hbar\omega}\left(\frac{g}{4}\right)^2\left(72a^2a_2^4a^2 + 24a_2^8\right)$$
$$+\frac{1}{3!\hbar^2\omega^2}\left(\frac{g}{4}\right)^3\left[2592a^2(a_2^4)^2a^2 + 1728a_3^6(a^2)^3 + 3456a_3^{10}a^2 + 1728a_3^{12}\right] + \dots\ . \qquad (3.552)$$

In the limit $T \to 0$, the integrals (3.550) behave like

$$\begin{array}{lllll} a_2^4 & \to & a^4, & a_3^6 & \to \frac{3}{2}a^6, \\ a_2^8 & \to & \frac{1}{2}a^8, & a_3^{10} & \to \frac{5}{8}a^{10}, \\ a_3^{12} & \to & \frac{3}{8}a^{12}, & & \end{array} \qquad (3.553)$$

and the free energy reduces to

$$F = \frac{\hbar\omega}{2} + \frac{g}{4}\,3a^4 - \left(\frac{g}{4}\right)^2 42a^8\frac{1}{\hbar\omega} + \left(\frac{g}{4}\right)^3 4\cdot 333a^{12}\left(\frac{1}{\hbar\omega}\right)^2 + \dots\ . \qquad (3.554)$$

In this limit, it is simpler to calculate the integrals (3.550) directly with the zero-temperature limit of the Green function (3.304), which is $G^{(2)}_{\omega^2}(\tau,\tau') = a^2e^{-\omega|\tau-\tau'|}$ with $a^2 = \hbar/2\omega M$ [see (3.251)]. The limits of integration must, however, be shifted by half a period to $\int_{-\hbar\beta/2}^{\hbar\beta/2} d\tau$ before going to the limit, so that one evaluates $\int_{-\infty}^{\infty} d\tau$ rather than $\int_0^\infty d\tau$ (the latter would give the wrong limit since it misses the left-hand side of the peak at $\tau = 0$). Before integration, the integrals are conveniently split as in Eq. (3D.1).

3.21 Perturbative Definition of Interacting Path Integrals

In Section 2.15 we have seen that it is possible to define a harmonic path integral without time slicing by dimensional regularization. With the techniques developed so far, this definition can trivially be extended to path integrals with interactions, if these can be treated perturbatively. We recall that in Eq. (3.483), the partition function of an interacting system can be expanded in a series of harmonic expectation values of powers of the interaction. The procedure is formulated most conveniently in terms of the generating functional (3.489) using formula (3.490) for the generating functional with interactions and Eq. (3.491) for the associated partition. The harmonic generating functional on the right-hand side of (3.490),

$$Z_\omega[j] = \oint \mathcal{D}x \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}(\dot{x}^2+\omega^2 x^2) - jx\right]\right\}, \tag{3.555}$$

can be evaluated with analytic regularization as described in Section (2.15) and yields, after a quadratic completion [recall (3.246), (3.247)]:

$$Z_\omega[j] = \frac{1}{2\sin(\omega\hbar\beta/2)} \exp\left\{\frac{1}{2M\hbar}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, j(\tau) G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau') j(\tau')\right\}, \tag{3.556}$$

where $G^{\rm p}_{\omega^2,{\rm e}}(\tau)$ is the periodic Green function (3.251)

$$G^{\rm p}_{\omega^2,{\rm e}}(\tau) = \frac{1}{2\omega}\frac{\cosh\omega(\tau-\hbar\beta/2)}{\sinh(\beta\hbar\omega/2)}, \quad \tau\in[0,\hbar\beta]. \tag{3.557}$$

As a consequence, Formula (3.490) for the generating functional of an interacting theory

$$Z[j] = e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau V(\hbar\delta/\delta j(\tau))}\, Z_\omega[j]\,, \tag{3.558}$$

is completely defined by analytic regularization. By expanding the exponential prefactor as in Eq. (3.493), the full generating functional is obtained from the harmonic one without any further path integration. Only functional differentiations are required to find the generating functional of all interacting interacting correlation functions $Z[j]$ from the harmonic one $Z_\omega[j]$.

This procedure yields the perturbative definition of arbitrary path integrals. It is widely used in the quantum field theory of particle physics[15] and critical phenomena[16] It is also the basis for an important extension of the theory of distributions to be discussed in detail in Sections 10.6–10.11.

It must be realized, however, that the perturbative definition is not a complete definition. Important contributions to the path integral may be missing: all those

[15] C. Itzykson and J.-B. Zuber, *Quantum Field Theory*, McGraw-Hill (1985).

[16] H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of ϕ^4-Theories*, World Scientific, Singapore 2001, pp. 1–487 (`www.physik.fu-berlin.de/~kleinert/re.html#b8`).

which are not expandable in powers of the interaction strength g. Such contributions are essential in understanding many physical phenomena, for example, tunneling, to be discussed in Chapter 17. Interestingly, however, information on such phenomena can, with appropriate resummation techniques to be developed in Chapter 5, also be extracted from the large-order behavior of the perturbation expansions, as will be shown in Subsection 17.10.4.

3.22 Generating Functional of Connected Correlation Functions

In Section 3.10 we have seen that the correlation functions obtained from the functional derivatives of $Z[j]$ via relation (3.298) contain many disconnected parts. The physically relevant free energy $F[j] = -k_BT \log Z[j]$, on the other hand, contains only in the connected parts of $Z[j]$. In fact, from statistical mechanics we know that meaningful description of a very large thermodynamic system can only be given in terms of the free energy which is directly proportional to the total volume V. The partition function $Z = e^{-F/k_BT}$ has no meaningful infinite-volume limit, also called the *thermodynamic limit*, since it contains a power series in V. Only the free energy density $f \equiv F/V$ has an infinite-volume limit. The expansion of $Z[j]$ diverges therefore for $V \to \infty$. This is why in thermodynamics we always go over to the free energy density by taking the logarithm of the partition function. This is calculated entirely from the connected diagrams.

Due to this thermodynamic experience we expect the logarithm of $Z[j]$ to provide us with a generating functional for all connected correlation functions. To avoid factors k_BT we define this functional as

$$W[j] = \log Z[j], \tag{3.559}$$

and shall now prove that the functional derivatives of $W[j]$ produce precisely the connected parts of the Feynman diagrams for each correlation function.

Consider the connected correlation functions $G^{(n)}_{\rm c}(\tau_1, \dots, \tau_n)$ defined by the functional derivatives

$$G^{(n)}_{\rm c}(\tau_1, \dots, \tau_n) = \frac{\delta}{\delta j(\tau_1)} \cdots \frac{\delta}{\delta j(\tau_n)} W[j] \,. \tag{3.560}$$

Ultimately, we shall be interested only in these functions with zero external current, where they reduce to the physically relevant connected correlation functions. For the general development in this section, however, we shall consider them as functionals of $j(\tau)$, and set $j = 0$ only at the end.

Of course, given all connected correlation functions $G^{(n)}_{\rm c}(\tau_1, \dots, \tau_n)$, the full correlation functions $G^{(n)}(\tau_1, \dots, \tau_n)$ in Eq. (3.298) can be recovered via simple composition laws from the connected ones. In order to see this clearly, we shall derive the general relationship between the two types of correlation functions in Section 3.22.2. First, we shall prove the connectedness property of the derivatives (3.560).

3.22.1 Connectedness Structure of Correlation Functions

We first prove that the generating functional $W[j]$ collects *only* connected diagrams in its Taylor coefficients $\delta^n W/\delta j(\tau_1)\ldots\delta j(\tau_n)$. Later, after Eq. (3.588), we shall see that these functional derivatives comprise *all* connected diagrams in $G^{(n)}(\tau_1,\ldots,\tau_n)$.

Let us write the path integral for the generating functional $Z[j]$ as follows (here we use natural units with $\hbar=1$):

$$Z[j]=\int\mathcal{D}x\,e^{-\mathcal{A}_{\rm e}[x,j]/\hbar},\tag{3.561}$$

with the action

$$\mathcal{A}_{\rm e}[x,j]=\int_0^{\hbar\beta}d\tau\left[\frac{M}{2}\left(\dot{x}^2+\omega^2x^2\right)+V(x)-j(\tau)x(\tau)\right].\tag{3.562}$$

In the following structural considerations we shall use natural physical units in which $\hbar=1$, for simplicity of the formulas. By analogy with the integral identity

$$\int dx\,\frac{d}{dx}\,e^{-F(x)}=0,$$

which holds by partial integration for any function $F(x)$ which goes to infinity for $x\to\pm\infty$, the functional integral satisfies the identity

$$\int\mathcal{D}x\;\frac{\delta}{\delta x(\tau)}e^{-\mathcal{A}_{\rm e}[x,j]}=0,\tag{3.563}$$

since the action $\mathcal{A}_{\rm e}[x,j]$ goes to infinity for $x\to\pm\infty$. Performing the functional derivative, we obtain

$$\int\mathcal{D}x\;\frac{\delta\mathcal{A}_{\rm e}[x,j]}{\delta x(\tau)}e^{-\mathcal{A}_{\rm e}[x,j]}=0.\tag{3.564}$$

To be specific, let us consider the anharmonic oscillator with potential $V(x)=\lambda x^4/4!$. We have chosen a coupling constant $\lambda/4!$ instead of the previous g in (3.543) since this will lead to more systematic numeric factors. The functional derivative of the action yields the classical equation of motion

$$\frac{\delta\mathcal{A}_{\rm e}[x,j]}{\delta x(\tau)}=M(-\ddot{x}+\omega^2x)+\frac{\lambda}{3!}x^3-j=0,\tag{3.565}$$

which we shall write as

$$\frac{\delta\mathcal{A}_{\rm e}[x,j]}{\delta x(\tau)}=G_0^{-1}x+\frac{\lambda}{3!}x^3-j=0,\tag{3.566}$$

where we have set $G_0(\tau,\tau')\equiv G^{(2)}$ to get free space for upper indices. With this notation, Eq. (3.564) becomes

$$\int\mathcal{D}x\,\left\{G_0^{-1}x(\tau)+\frac{\lambda}{3!}x^3(\tau)-j(\tau)\right\}e^{-\mathcal{A}_{\rm e}[x,j]}=0.\tag{3.567}$$

We now express the paths $x(\tau)$ as functional derivatives with respect to the source current $j(\tau)$, such that we can pull the curly brackets in front of the integral. This leads to the functional differential equation for the generating functional $Z[j]$:

$$\left\{G_0^{-1}\frac{\delta}{\delta j(\tau)}+\frac{\lambda}{3!}\left[\frac{\delta}{\delta j(\tau)}\right]^3-j(\tau)\right\}Z[j]=0. \tag{3.568}$$

With the short-hand notation

$$Z_{j(\tau_1)j(\tau_2)\dots j(\tau_n)}[j]\equiv\frac{\delta}{\delta j(\tau_1)}\frac{\delta}{\delta j(\tau_2)}\cdots\frac{\delta}{\delta j(\tau_n)}Z[j], \tag{3.569}$$

where the arguments of the currents will eventually be suppressed, this can be written as

$$G_0^{-1}Z_{j(\tau)}+\frac{\lambda}{3!}Z_{j(\tau)j(\tau)j(\tau)}-j(\tau)=0. \tag{3.570}$$

Inserting here (3.559), we obtain a functional differential equation for $W[j]$:

$$G_0^{-1}W_j+\frac{\lambda}{3!}\left(W_{jjj}+3W_{jj}W_j+W_j^3\right)-j=0. \tag{3.571}$$

We have employed the same short-hand notation for the functional derivatives of $W[j]$ as in (3.569) for $Z[j]$,

$$W_{j(\tau_1)j(\tau_2)\dots j(\tau_n)}[j]\equiv\frac{\delta}{\delta j(\tau_1)}\frac{\delta}{\delta j(\tau_2)}\cdots\frac{\delta}{\delta j(\tau_n)}W[j], \tag{3.572}$$

suppressing the arguments $\tau_1,\dots,\tau_n$ of the currents, for brevity. Multiplying (3.571) functionally by G_0 gives

$$W_j=-\frac{\lambda}{3!}G_0\left(W_{jjj}+3W_{jj}W_j+W_j^3\right)+G_0\,j. \tag{3.573}$$

We have omitted the integral over the intermediate τ's, for brevity. More specifically, we have written $G_0\,j$ for $\int d\tau'\,G_0(\tau,\tau')j(\tau')$. Similar expressions abbreviate all functional products. This corresponds to a functional version of *Einstein's summation convention*.

Equation (3.573) may now be expressed in terms of the one-point correlation function

$$G_{\rm c}^{(1)}=W_j, \tag{3.574}$$

defined in (3.560), as

$$G_{\rm c}^{(1)} \;=\; -\frac{\lambda}{3!}G_0\left\{G_{{\rm c}\,jj}^{(1)}+3G_{{\rm c}\,j}^{(1)}G_{\rm c}^{(1)}+\left[G_{\rm c}^{(1)}\right]^3\right\}+G_0\,j. \tag{3.575}$$

The solution to this equation is conveniently found by a diagrammatic procedure displayed in Fig. 3.8. To lowest, zeroth, order in λ we have

$$G_{\rm c}^{(1)} = G_0\, j. \tag{3.576}$$

From this we find by functional integration the zeroth order generating functional $W_0[j]$

$$W_0[j] \;=\; \int \mathcal{D}j\, G_{\rm c}^{(1)} = \frac{1}{2} jG_0 j, \tag{3.577}$$

up to a j-independent constant. Subscripts of $W[j]$ indicate the order in the interaction strength λ.

Reinserting (3.576) on the right-hand side of (3.575) gives the first-order expression

$$G_{\rm c}^{(1)} \;=\; -G_0 \frac{\lambda}{3!}\left[3G_0G_0 j + (G_0 j)^3\right] + G_0 j, \tag{3.578}$$

represented diagrammatically in the second line of Fig. 3.8. Equation (3.578) can be integrated functionally in j to obtain $W[j]$ up to first order in λ. Diagrammatically, this process amounts to multiplying each open lines in a diagram by a current j, and dividing the arising j^ns by n. Thus we arrive at

$$W_0[j] + W_1[j] \;=\; \frac{1}{2} jG_0 j - \frac{\lambda}{4} G_0\, (G_0 j)^2 - \frac{\lambda}{24}\, (G_0 j)^4\,, \tag{3.579}$$

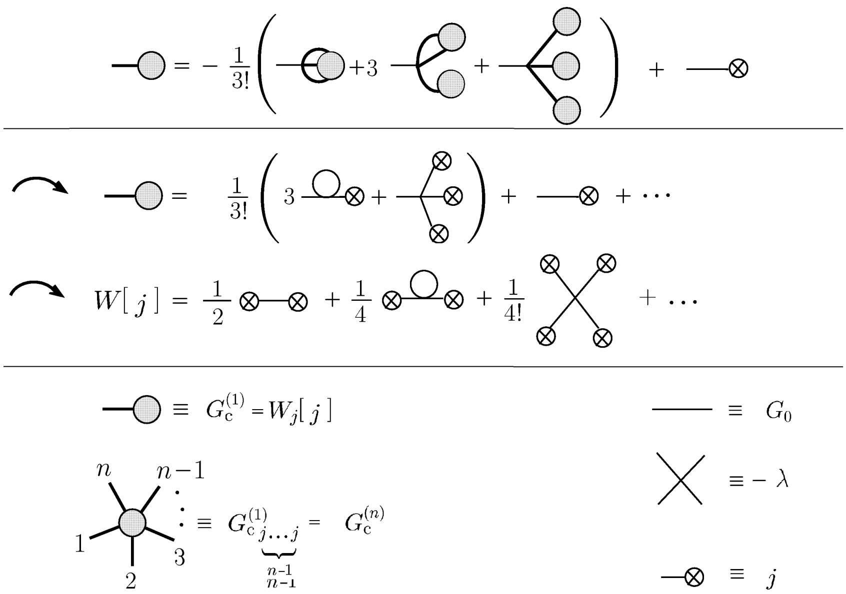


Figure 3.8 Diagrammatic solution of recursion relation (3.573) for the generating functional $W[j]$ of all connected correlation functions. First line represents Eq. (3.575), second (3.578), third (3.579). The remaining lines define the diagrammatic symbols.

as illustrated in the third line of Fig. 3.8. This procedure can be continued to any order in λ.

The same procedure allows us to prove that the generating functional $W[j]$ collects *only* connected diagrams in its Taylor coefficients $\delta^n W/\delta j(x_1)\dots\delta j(x_n)$. For the lowest two orders we can verify the connectedness by inspecting the third line in Fig. 3.8. The diagrammatic form of the recursion relation shows that this topological property remains true for all orders in λ, by induction. Indeed, if we suppose it to be true for some n, then all $G_{\rm c}^{(1)}$ inserted on the right-hand side are connected, and so are the diagrams constructed from these when forming $G_{\rm c}^{(1)}$ to the next, $(n+1)$st, order.

Note that this calculation is unable to recover the value of $W[j]$ at $j=0$ which is an unknown integration constant of the functional differential equation. For the purpose of generating correlation functions, this constant is irrelevant. We have seen in Fig. 3.7 that $W[0]$, which is equal to $-F/k_BT$, consists of the sum of all connected vacuum diagrams contained in $Z[0]$.

3.22.2 Correlation Functions versus Connected Correlation Functions

Using the logarithmic relation (3.559) between $W[j]$ and $Z[j]$ we can now derive general relations between the n-point functions and their connected parts. For the one-point function we find

$$G^{(1)}(\tau) = Z^{-1}[j]\frac{\delta}{\delta j(\tau)}Z[j] = \frac{\delta}{\delta j(\tau)}W[j] = G_{\rm c}^{(1)}(\tau). \tag{3.580}$$

This equation implies that the one-point function representing the ground state expectation value of the path $x(\tau)$ is always connected:

$$\langle x(\tau)\rangle \equiv G^{(1)}(\tau) = G_{\rm c}^{(1)}(\tau) = X. \tag{3.581}$$

Consider now the two-point function, which decomposes as follows:

$$\begin{aligned} G^{(2)}(\tau_1,\tau_2) &= Z^{-1}[j]\frac{\delta}{\delta j(\tau_1)}\frac{\delta}{\delta j(\tau_2)}Z[j] \\ &= Z^{-1}[j]\frac{\delta}{\delta j(\tau_1)}\left\{\left(\frac{\delta}{\delta j(\tau_2)}W[j]\right)Z[j]\right\} \\ &= Z^{-1}[j]\left\{W_{j(\tau_1)j(\tau_2)} + W_{j(\tau_1)}W_{j(\tau_2)}\right\}Z[j] \\ &= G_{\rm c}^{(2)}(\tau_1,\tau_2) + G_{\rm c}^{(1)}(\tau_1)\,G_{\rm c}^{(1)}(\tau_2). \end{aligned} \tag{3.582}$$

In addition to the connected diagrams with two ends there are two connected diagrams ending in a single line. These are absent in a x^4-theory at $j=0$ because of the symmetry of the potential, which makes all odd correlation functions vanish. In that case, the two-point function is automatically connected.

For the three-point function we find

$$
\begin{aligned}
G^{(3)}(\tau_1,\tau_2,\tau_3) \;=\; & Z^{-1}[j]\frac{\delta}{\delta j(\tau_1)}\frac{\delta}{\delta j(\tau_2)}\frac{\delta}{\delta j(\tau_3)}Z[j] \\
&= Z^{-1}[j]\frac{\delta}{\delta j(\tau_1)}\frac{\delta}{\delta j(\tau_2)}\left\{\left[\frac{\delta}{\delta j(\tau_3)}W[j]\right]Z[j]\right\} \\
&= Z^{-1}[j]\frac{\delta}{\delta j(\tau_1)}\left\{\left[W_{j(\tau_3)j(\tau_2)}+W_{j(\tau_2)}W_{j(\tau_3)}\right]Z[j]\right\} \\
&= Z^{-1}[j]\left\{W_{j(\tau_1)j(\tau_2)j(\tau_3)}+\Big(W_{j(\tau_1)}W_{j(\tau_2)j(\tau_3)}+W_{j(\tau_2)}W_{j(\tau_1)j(\tau_3)}\right. \\
&\qquad\qquad \left.+W_{j(\tau_3)}W_{j(\tau_1)j(\tau_2)}\Big)+W_{j(\tau_1)}W_{j(\tau_2)}W_{j(\tau_3)}\right\}Z[j] \\
&= G_{\rm c}^{(3)}(\tau_1,\tau_2,\tau_3)+\left[G_{\rm c}^{(1)}(\tau_1)G_{\rm c}^{(2)}(\tau_2,\tau_3)+2\text{ perm}\right]+G_{\rm c}^{(1)}(\tau_1)G_{\rm c}^{(1)}(\tau_2)G_{\rm c}^{(1)}(\tau_3),
\end{aligned}
\tag{3.583}
$$

and for the four-point function

$$
\begin{aligned}
G^{(4)}(\tau_1,\dots,\tau_4) \;=\; & G_{\rm c}^{(4)}(\tau_1,\dots,\tau_4)+\left[G_{\rm c}^{(3)}(\tau_1,\tau_2,\tau_3)\,G_{\rm c}^{(1)}(\tau_4)+3\text{ perm}\right] \\
&+\left[G_{\rm c}^{(2)}(\tau_1,\tau_2)\,G_{\rm c}^{(2)}(\tau_3,\tau_4)+2\text{ perm}\right] \\
&+\left[G_{\rm c}^{(2)}(\tau_1,\tau_2)\,G_{\rm c}^{(1)}(\tau_3)G_{\rm c}^{(1)}(\tau_4)+5\text{ perm}\right] \\
&+\;G_{\rm c}^{(1)}(\tau_1)\cdots G_{\rm c}^{(1)}(\tau_4).
\end{aligned}
\tag{3.584}
$$

In the pure x^4-theory there are no odd correlation functions, because of the symmetry of the potential.

For the general correlation function $G^{(n)}$, the total number of terms is most easily retrieved by dropping all indices and differentiating with respect to j (the arguments $\tau_1,\dots,\tau_n$ of the currents are again suppressed):

$$
\begin{aligned}
G^{(1)} &= e^{-W}\left(e^W\right)_j &&= W_j = G_{\rm c}^{(1)} \\
G^{(2)} &= e^{-W}\left(e^W\right)_{jj} &&= W_{jj}+{W_j}^2 = G_{\rm c}^{(2)}+G_{\rm c}^{(1)2} \\
G^{(3)} &= e^{-W}\left(e^W\right)_{jjj} &&= W_{jjj}+3W_{jj}W_j+{W_j}^3 = G_{\rm c}^{(3)}+3G_{\rm c}^{(2)}G_{\rm c}^{(1)}+G_{\rm c}^{(1)3} \\
G^{(4)} &= e^{-W}\left(e^W\right)_{jjjj} &&= W_{jjjj}+4W_{jjj}W_j+3{W_{jj}}^2+6W_{jj}{W_j}^2+{W_j}^4 \\
& &&= G_{\rm c}^{(4)}+4G_{\rm c}^{(3)}G_{\rm c}^{(1)}+3G_{\rm c}^{(2)2}+6G_{\rm c}^{(2)}G_{\rm c}^{(1)2}+G_{\rm c}^{(1)4}.
\end{aligned}
\tag{3.585}
$$

All equations follow from the recursion relation

$$
G^{(n)} = G_j^{(n-1)}+G^{(n-1)}G_{\rm c}^{(1)}, \qquad n\geq 2,
\tag{3.586}
$$

if one uses $G_j^{(n-1)} = G_{\rm c}^{(n)}$ and the initial relation $G^{(1)} = G_{\rm c}^{(1)}$. By comparing the first four relations with the explicit expressions (3.582)–(3.584) we see that the numerical factors on the right-hand side of (3.585) refer to the permutations of the arguments $\tau_1,\tau_2,\tau_3,\dots$ of otherwise equal expressions. Since there is no problem in reconstructing the explicit permutations we shall henceforth write all composition laws in the short-hand notation (3.585).

The formula (3.585) and its generalization is often referred to as *cluster decomposition*, or also as the *cumulant expansion*, of the correlation functions.

We can now prove that the connected correlation functions collect precisely all connected diagrams in the n-point functions. For this we observe that the decomposition rules can be inverted by repeatedly differentiating both sides of the equation $W[j] = \log Z[j]$ functionally with respect to the current j:

$$\begin{aligned}
G_{\rm c}^{(1)} &= G^{(1)} \\
G_{\rm c}^{(2)} &= G^{(2)} - G^{(1)}G^{(1)} \\
G_{\rm c}^{(3)} &= G^{(3)} - 3G^{(2)}G^{(1)} + 2G^{(1)3} \\
G_{\rm c}^{(4)} &= G^{(4)} - 4G^{(3)}G^{(1)} + 12G^{(2)}G^{(1)2} - 3G^{(2)2} - 6G^{(1)4}.
\end{aligned} \tag{3.587}$$

Each equation follows from the previous one by one more derivative with respect to j, and by replacing the derivatives on the right-hand side according to the rule

$$G_j^{(n)} = G^{(n+1)} - G^{(n)}G^{(1)}. \tag{3.588}$$

Again the numerical factors imply different permutations of the arguments and the subscript j denotes functional differentiations with respect to j.

Note that Eqs. (3.587) for the connected correlation functions are valid for symmetric as well as asymmetric potentials $V(x)$. For symmetric potentials, the equations simplify, since all terms involving $G^{(1)} = X = \langle x \rangle$ vanish.

It is obvious that any connected diagram contained in $G^{(n)}$ must also be contained in $G_{\rm c}^{(n)}$, since all the terms added or subtracted in (3.587) are products of $G_j^{(n)}$s, and thus necessarily disconnected. Together with the proof in Section 3.22.1 that the correlation functions $G_{\rm c}^{(n)}$ contain *only* the connected parts of $G^{(n)}$, we can now be sure that $G_{\rm c}^{(n)}$ contains precisely the connected parts of $G^{(n)}$.

3.22.3 Functional Generation of Vacuum Diagrams

The functional differential equation (3.573) for $W[j]$ contains all information on the connected correlation functions of the system. However, it does not tell us anything about the vacuum diagrams of the theory. These are contained in $W[0]$, which remains an undetermined constant of functional integration of these equations.

In order to gain information on the vacuum diagrams, we consider a modification of the generating functional (3.561), in which we set the external source j equal to zero, but generalize the source $j(\tau)$ in (3.561) coupled linearly to $x(\tau)$ to a bilocal form $K(\tau,\tau')$ coupled linearly to $x(\tau)x(\tau')$:

$$Z[K] \;=\; \int \mathcal{D}x(\tau)\, e^{-\mathcal{A}_{\rm e}[x,K]}, \tag{3.589}$$

where $\mathcal{A}_{\rm e}[x,K]$ is the Euclidean action

$$\mathcal{A}_{\rm e}[x,K] \equiv \mathcal{A}_0[x] + \mathcal{A}^{\rm int}[x] + \frac{1}{2}\int d\tau \int d\tau'\, x(\tau)K(\tau,\tau')x(\tau'). \tag{3.590}$$

When forming the functional derivative with respect to $K(\tau,\tau')$ we obtain the correlation function in the presence of $K(\tau,\tau')$:

$$G^{(2)}(\tau,\tau') = -2Z^{-1}[K]\frac{\delta Z}{\delta K(\tau,\tau')}. \tag{3.591}$$

At the end we shall set $K(\tau,\tau')=0$, just as previously the source j. When differentiating $Z[K]$ twice, we obtain the four-point function

$$G^{(4)}(\tau_1,\tau_2,\tau_3,\tau_4) = 4Z^{-1}[K]\frac{\delta^2 Z}{\delta K(\tau_1,\tau_2)\delta K(\tau_3,\tau_4)}. \tag{3.592}$$

As before, we introduce the functional $W[K] \equiv \log Z[K]$. Inserting this into (3.591) and (3.592), we find

$$G^{(2)}(\tau,\tau') = 2\frac{\delta W}{\delta K(\tau,\tau')}, \tag{3.593}$$

$$G^{(4)}(\tau_1,\tau_2,\tau_3,\tau_4) = 4\left[\frac{\delta^2 W}{\delta K(\tau_1,\tau_2)\delta K(\tau_3,\tau_4)} + \frac{\delta W}{\delta K(\tau_1,\tau_2)}\frac{\delta W}{\delta K(\tau_3,\tau_4)}\right]. \tag{3.594}$$

With the same short notation as before, we shall use again a subscript K to denote functional differentiation with respect to K, and write

$$G^{(2)} = 2W_K, \qquad G^{(4)} = 4\left[W_{KK} + W_K W_K\right] = 4W_{KK} + G^{(2)}\,G^{(2)}. \tag{3.595}$$

From Eq. (3.585) we know that in the absence of a source j and for a symmetric potential, $G^{(4)}$ has the connectedness structure

$$G^{(4)} = G_{\rm c}^{(4)} + 3G_{\rm c}^{(2)}\,G_{\rm c}^{(2)}. \tag{3.596}$$

This shows that in contrast to W_{jjjj}, the derivative W_{KK} does not directly yield a connected four-point function, but two disconnected parts:

$$4W_{KK} = G_{\rm c}^{(4)} + 2G_{\rm c}^{(2)}\,G_{\rm c}^{(2)}, \tag{3.597}$$

the two-point functions being automatically connected for a symmetric potential. More explicitly, (3.597) reads

$$\frac{4\delta^2 W}{\delta K(\tau_1,\tau_2)\delta K(\tau_3,\tau_4)}$$
$$= G_{\rm c}^{(4)}(\tau_1,\tau_2,\tau_3,\tau_4) + G_{\rm c}^{(2)}(\tau_1,\tau_3)G_{\rm c}^{(2)}(\tau_2,\tau_4) + G_{\rm c}^{(2)}(\tau_1,\tau_4)G_{\rm c}^{(2)}(\tau_2,\tau_3). \tag{3.598}$$

Let us derive functional differential equations for $Z[K]$ and $W[K]$. By analogy with (3.563) we start out with the trivial functional differential equation

$$\int \mathcal{D}x\; x(\tau)\frac{\delta}{\delta x(\tau')}e^{-\mathcal{A}_{\rm e}[x,K]} = -\delta(\tau-\tau')Z[K], \tag{3.599}$$

which is immediately verified by a functional integration by parts. Performing the functional derivative yields

$$\int \mathcal{D}x\, x(\tau)\frac{\delta \mathcal{A}_{\rm e}[x,K]}{\delta x(\tau')} e^{-\mathcal{A}_{\rm e}[x,K]} = \delta(\tau-\tau')Z[K], \tag{3.600}$$

or

$$\int \mathcal{D}x \int d\tau \int d\tau' \left\{ x(\tau)G_0^{-1}(\tau,\tau')x(\tau') + \frac{\lambda}{3!}x(\tau)x^3(\tau')\right\} e^{-\mathcal{A}_{\rm e}[x,K]} = \delta(\tau-\tau')Z[K]. \tag{3.601}$$

For brevity, we have absorbed the source in the free-field correlation function G_0:

$$G_0 \to [G_0^{-1} - K]^{-1}. \tag{3.602}$$

The left-hand side of (3.601) can obviously be expressed in terms of functional derivatives of $Z[K]$, and we obtain the functional differential equation whose short form reads

$$G_0^{-1}Z_K + \frac{\lambda}{3}Z_{KK} = \frac{1}{2}Z. \tag{3.603}$$

Inserting $Z[K]=e^{W[K]}$, this becomes

$$G_0^{-1}W_K + \frac{\lambda}{3}(W_{KK} + W_K W_K) = \frac{1}{2}. \tag{3.604}$$

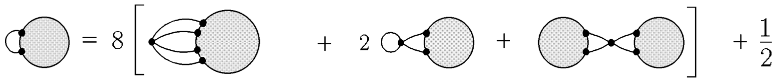
It is useful to reconsider the functional $W[K]$ as a functional $W[G_0]$. Then $\delta G_0/\delta K = G_0^2$, and the derivatives of $W[K]$ become

$$W_K = G_0^2\, W_{G_0}, \quad W_{KK} = 2G_0^3\, W_{G_0} + G_0^4\, W_{G_0G_0}, \tag{3.605}$$

and (3.604) takes the form

$$G_0 W_{G_0} + \frac{\lambda}{3}(G_0^4 W_{G_0G_0} + 2G_0^3 W_{G_0} + G_0^4 W_{G_0}W_{G_0}) = \frac{1}{2}. \tag{3.606}$$

This equation is represented diagrammatically in Fig. 3.9. The zeroth-order solution



$$G_0 W_{G_0} = 8\frac{-1}{4!}\left[\lambda G_0^4 W_{G_0G_0} + 2G_0\lambda G_0^2 W_{G_0} + W_{G_0}G_0^2\lambda G_0^2 W_{G_0}\right] + \frac{1}{2}$$

Figure 3.9 Diagrammatic representation of functional differential equation (3.606). For the purpose of finding the multiplicities of the diagrams, it is convenient to represent here by a vertex the coupling strength $-\lambda/4!$ rather than $g/4$ in Section 3.20.

to this equation is obtained by setting $\lambda = 0$:

$$W^{(0)}[G_0] = \frac{1}{2}\mathrm{Tr}\,\log(G_0). \tag{3.607}$$

Explicitly, the right-hand side is equal to the one-loop contribution to the free energy in Eq. (3.549), apart from a factor $-\beta$.

The corrections are found by iteration. For systematic treatment, we write $W[G_0]$ as a sum of a free and an interacting part,

$$W[G_0] = W^{(0)}[G_0] + W^{\rm int}[G_0], \tag{3.608}$$

insert this into Eq. (3.606), and find the differential equation for the interacting part:

$$G_0 W^{\rm int}_{G_0} + \frac{\lambda}{3}(G_0^4 W^{\rm int}_{G_0 G_0} + 3G_0^3 W^{\rm int}_{G_0} + G_0^4 W^{\rm int}_{G_0} W^{\rm int}_{G_0}) = 6\frac{-\lambda}{4!}G_0^2. \tag{3.609}$$

This equation is solved iteratively. Setting $W^{\rm int}[G_0] = 0$ in all terms proportional to λ, we obtain the first-order contribution to $W^{\rm int}[G_0]$:

$$W^{\rm int}[G_0] = 3\frac{-\lambda}{4!}G_0^2. \tag{3.610}$$

This is precisely the contribution (3.545) of the two-loop Feynman diagram (apart from the different normalization of g).

In order to see how the iteration of Eq. (3.609) may be solved systematically, let us ignore for the moment the functional nature of Eq. (3.609), and treat G_0 as an ordinary real variable rather than a functional matrix. We expand $W[G_0]$ in a Taylor series:

$$W^{\rm int}[G_0] = \sum_{p=1}^{\infty} \frac{1}{p!} W_p \left(\frac{-\lambda}{4!}\right)^p (G_0)^{2p}, \tag{3.611}$$

and find for the expansion coefficients the recursion relation

$$W_{p+1} = 4\left\{[2p\,(2p-1) + 3(2p)]\,W_p + \sum_{q=1}^{p-1}\left(\begin{array}{c} p \\ q \end{array}\right) 2q\,W_q \times 2(p-q)W_{p-q}\right\}. \tag{3.612}$$

Solving this with the initial number $W_1 = 3$, we obtain the multiplicities of the connected vacuum diagrams of pth order:

$$\begin{array}{l} 3,\ 96,\ 9504,\ 1880064,\ 616108032,\ 301093355520,\ 205062331760640, \\ 185587468924354560,\ 215430701800551874560,\ 312052349085504377978880. \end{array} \tag{3.613}$$

To check these numbers, we go over to $Z[G] = e^{W[G_0]}$, and find the expansion:

$$\begin{aligned} Z[G_0] &= \exp\left[\frac{1}{2}\mathrm{Tr}\,\log G_0 + \sum_{p=1}^{\infty}\frac{1}{p!}W_p\left(\frac{-\lambda}{4!}\right)^p (G_0)^{2p}\right] \\ &= \mathrm{Det}^{1/2}[G_0]\left[1 + \sum_{p=1}^{\infty}\frac{1}{p!}z_p\left(\frac{-\lambda}{4!}\right)^p (G_0)^{2p}\right]. \end{aligned} \tag{3.614}$$

The expansion coefficients z_p count the total number of vacuum diagrams of order p. The exponentiation (3.614) yields $z_p = (4p-1)!!$, which is the correct number of Wick contractions of p interactions x^4.

In fact, by comparing coefficients in the two expansions in (3.614), we may derive another recursion relation for W_p:

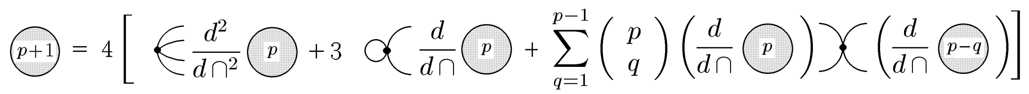
$$W_p + 3\binom{p-1}{1} W_{p-1} + 7\cdot 5\cdot 3\binom{p-1}{2} + \ldots + (4p-5)!!\binom{p-1}{p-1} = (4p-1)!!, \quad (3.615)$$

which is fulfilled by the solutions of (3.612).

In order to find the associated Feynman diagrams, we must perform the differentiations in Eq. (3.609) functionally. The numbers W_p become then a sum of diagrams, for which the recursion relation (3.612) reads

$$W_{p+1} = 4\left[G_0^4 \frac{d^2}{d\cap^2} W_p + 3\cdot G_0^3 \frac{d}{d\cap} W_p + \sum_{q=1}^{p-1}\binom{p}{q}\left(\frac{d}{d\cap}W_q\right)G_0^2\cdot G_0^2\left(\frac{d}{d\cap}W_{p-q}\right)\right], \quad (3.616)$$

where the differentiation $d/d\cap$ removes one line connecting two vertices in all possible ways. This equation is solved diagrammatically, as shown in Fig. 3.10.



$$W_{p+1} = 4\left[G_0^4 \frac{d^2}{d\cap^2} W_p + 3\cdot G_0^3 \frac{d}{d\cap} W_p + \sum_{q=1}^{p-1}\binom{p}{q}\left(\frac{d}{d\cap}W_q\right)G_0^2\cdot G_0^2\left(\frac{d}{d\cap}W_{p-q}\right)\right]$$

Figure 3.10 Diagrammatic representation of recursion relation (3.612). A vertex represents the coupling strength $-\lambda$.

Starting the iteration with $W_1 = 3$, we have $dW_p/d\cap = 6$ and $d^2W_p/d\cap^2 = 6$. Proceeding to order five loops and going back to the usual vertex notation $-\lambda$, we find the vacuum diagrams with their weight factors as shown in Fig. 3.11. For more than five loops, the reader is referred to the paper quoted in Notes and References, and to the internet address from which Mathematica programs can be downloaded which solve the recursion relations and plot all diagrams of $W[0]$ and the resulting two- and four-point functions.

3.22.4 Correlation Functions from Vacuum Diagrams

The vacuum diagrams contain information on all correlation functions of the theory. One may rightly say that the vacuum is the world. The two- and four-point functions are given by the functional derivatives (3.595) of the vacuum functional $W[K]$. Diagrammatically, a derivative with respect to K corresponds to cutting one line of a vacuum diagram in all possible ways. Thus, all diagrams of the two-point function

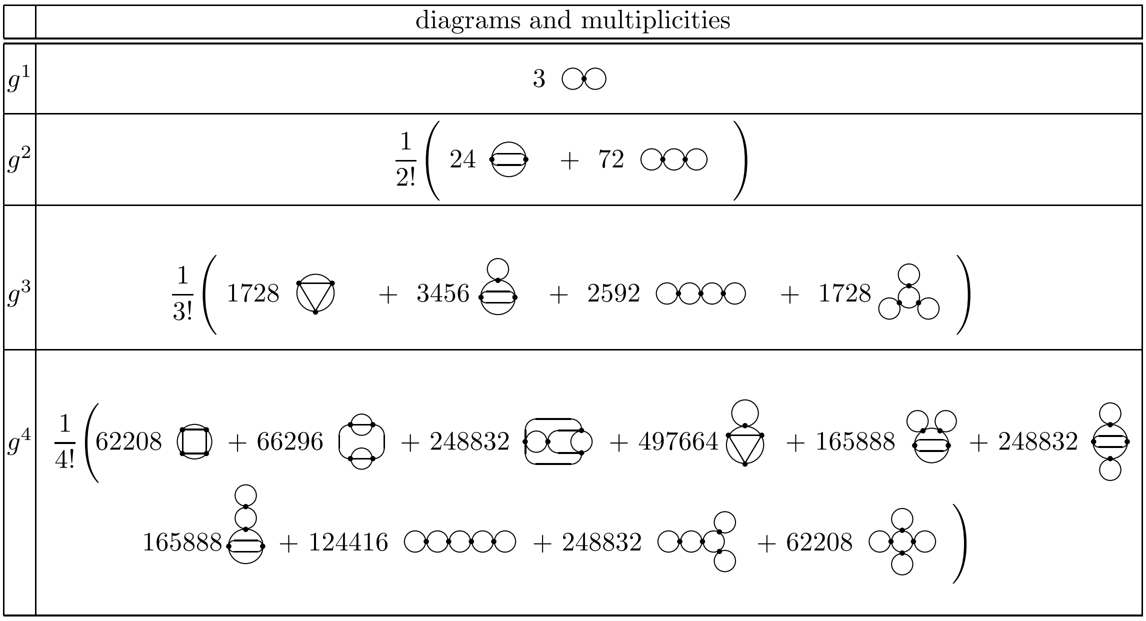
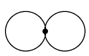
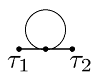
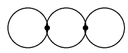
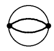


Figure 3.11 Vacuum diagrams up to five loops and their multiplicities. The total numbers to orders g^n are 3, 96, 9504, 1880064, respectively. In contrast to Fig. 3.10, and to the previous diagrammatic notation in Fig. 3.7, a vertex stands here for $-\lambda/4!$ for brevity. For more than five loops see the tables on the internet (`http://users.physik.fu-berlin/~kleinert/b3/programs`).

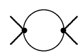
$G^{(2)}$ can be derived from such cuts, multiplied by a factor 2. As an example, consider the first-order vacuum diagram of $W[K]$ in Fig. 3.11. Cutting one line, which is possible in two ways, and recalling that in Fig. 3.11 a vertex stands for $-\lambda/4!$ rather than $-\lambda$, as in the other diagrams, we find

$$W_1[0] = \frac{1}{8}$$  $$\longrightarrow \quad G_1^{(2)}(\tau_1, \tau_2) = 2 \times \frac{1}{8}\, 2$$  $$. \tag{3.617}$$

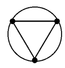
The second equation in (3.595) tells us that all connected contributions to the four-point function $G^{(4)}$ may be obtained by cutting two lines in all combinations, and multiplying the result by a factor 4. As an example, take the second-order vacuum diagrams of $W[0]$ with the proper translation of vertices by a factor 4!, which are

$$W_2[0] = \frac{1}{16}$$  $$+ \frac{1}{48}$$  $$. \tag{3.618}$$

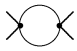
Cutting two lines in all possible ways yields the following contributions to the connected diagrams of the two-point function:

$$G^{(4)} = 4 \times \left(2 \cdot 1 \cdot \frac{1}{16} + 4 \cdot 3 \cdot \frac{1}{48}\right)$$  $$. \tag{3.619}$$

It is also possible to find all diagrams of the four-point function from the vacuum diagrams by forming a derivative of $W[0]$ with respect to the coupling constant $-\lambda$, and multiplying the result by a factor 4!. This follows directly from the fact that this differentiation applied to $Z[0]$ yields the correlation function $\int d\tau \langle x^4 \rangle$. As an example, take the first diagram of order g^3 in Table 3.11 (with the same vertex convention as in Fig. 3.11):

$$W_2[0] = \frac{1}{48}$$  . (3.620)

Removing one vertex in the three possible ways and multiplying by a factor 4! yields

$$G^{(4)} = 4! \times \frac{1}{48}\, 3$$  . (3.621)

3.22.5 Generating Functional for Vertex Functions. Effective Action

Apart from the connectedness structure, the most important step in economizing the calculation of Feynman diagrams consists in the decomposition of higher connected correlation functions into *one-particle irreducible* vertex functions and one-particle irreducible two-particle correlation functions, from which the full amplitudes can easily be reconstructed. A diagram is called one-particle irreducible if it cannot be decomposed into two disconnected pieces by cutting a single line.

There is, in fact, a simple algorithm which supplies us in general with such a decomposition. For this purpose let us introduce a new generating functional $\Gamma[X]$, to be called the *effective action* of the theory. It is defined via a Legendre transformation of $W[j]$:

$$-\Gamma[X] \equiv W[j] - W_j\, j. \tag{3.622}$$

Here and in the following, we use a short-hand notation for the functional multiplication, $W_j\, j = \int d\tau\, W_j(\tau) j(\tau)$, which considers fields as vectors with a continuous index τ. The new variable X is the functional derivative of $W[j]$ with respect to $j(\tau)$ [recall (3.572)]:

$$X(\tau) \equiv \frac{\delta W[j]}{\delta j(\tau)} \equiv W_{j(\tau)} = \langle x \rangle_{j(\tau)}, \tag{3.623}$$

and thus gives the ground state expectation of the field operator in the presence of the current j. When rewriting (3.622) as

$$-\Gamma[X] \equiv W[j] - X\, j, \tag{3.624}$$

and functionally differentiating this with respect to X, we obtain the equation

$$\Gamma_X[X] = j. \tag{3.625}$$

This equation shows that the physical path expectation $X(\tau) = \langle x(\tau)\rangle$, where the external current is zero, extremizes the effective action:

$$\Gamma_X[X] = 0. \tag{3.626}$$

We shall study here only physical systems for which the path expectation value is a constant $X(\tau) \equiv X_0$. Thus we shall not consider systems which possess a time-dependent $X_0(\tau)$, although such systems can also be described by x^4-theories by admitting more general types of gradient terms, for instance $x(\partial^2 - k_0^2)^2 x$. The ensuing τ-dependence of $X_0(\tau)$ may be oscillatory.[17] Thus we shall assume a constant

$$X_0 = \langle x\rangle|_{j=0}, \tag{3.627}$$

which may be zero or non-zero, depending on the phase of the system.

Let us now demonstrate that the effective action contains all the information on the proper vertex functions of the theory. These can be found directly from the functional derivatives:

$$\Gamma^{(n)}(\tau_1, \dots, \tau_n) \equiv \frac{\delta}{\delta X(\tau_1)} \cdots \frac{\delta}{\delta X(\tau_n)} \Gamma[X]\,. \tag{3.628}$$

We shall see that the proper vertex functions are obtained from these functions by a Fourier transform and a simple removal of an overall factor $(2\pi)^D \delta\left(\sum_{i=1}^n \omega_i\right)$ to ensure momentum conservation. The functions $\Gamma^{(n)}(\tau_1, \dots, \tau_n)$ will therefore be called *vertex functions*, without the adjective *proper* which indicates the absence of the δ-function. In particular, the Fourier transforms of the vertex functions $\Gamma^{(2)}(\tau_1, \tau_2)$ and $\Gamma^{(4)}(\tau_1, \tau_2, \tau_3, \tau_4)$ are related to their proper versions by

$$\Gamma^{(2)}(\omega_1, \omega_2) = 2\pi\delta(\omega_1 + \omega_2)\, \bar{\Gamma}^{(2)}(\omega_1), \tag{3.629}$$

$$\Gamma^{(4)}(\omega_1, \omega_2, \omega_3, \omega_4) = 2\pi\delta\left(\sum_{i=1}^{4} \omega_i\right) \bar{\Gamma}^{(4)}(\omega_1, \omega_2, \omega_3, \omega_4). \tag{3.630}$$

For the functional derivatives (3.628) we shall use the same short-hand notation as for the functional derivatives (3.572) of $W[j]$, setting

$$\Gamma_{X(\tau_1)\dots X(\tau_n)} \equiv \frac{\delta}{\delta X(\tau_1)} \cdots \frac{\delta}{\delta X(\tau_n)} \Gamma[X]\,. \tag{3.631}$$

The arguments $\tau_1, \dots, \tau_n$ will usually be suppressed.

In order to derive relations between the derivatives of the effective action and the connected correlation functions, we first observe that the connected one-point function $G_c^{(1)}$ at a nonzero source j is simply the path expectation X [recall (3.581)]:

$$G_c^{(1)} = X. \tag{3.632}$$

[17] In higher dimensions there can be crystal- or quasicrystal-like modulations. See, for example, H. Kleinert and K. Maki, Fortschr. Phys. **29**, 1 (1981) (`http://www.physik.fu-berlin.de/~kleinert/75`). This paper was the first to investigate in detail icosahedral quasicrystalline structures discovered later in aluminum.

Second, we see that the connected two-point function at a nonzero source j is given by

$$G_{\rm c}^{(2)} = G_j^{(1)} = W_{jj} = \frac{\delta X}{\delta j} = \left(\frac{\delta j}{\delta X}\right)^{-1} = \Gamma_{XX}^{-1}. \tag{3.633}$$

The inverse symbols on the right-hand side are to be understood in the functional sense, i.e., Γ_{XX}^{-1} denotes the functional matrix:

$$\Gamma^{\;-1}_{X(\tau)X(\mathbf{y})} \equiv \left[\frac{\delta^2\Gamma}{\delta X(\tau)\delta X(\tau')}\right]^{-1}, \tag{3.634}$$

which satisfies

$$\int d\tau'\, \Gamma^{-1}_{X(\tau)X(\tau')}\Gamma_{X(\tau')X(\tau''} = \delta(\tau-\tau''). \tag{3.635}$$

Relation (3.633) states that the second derivative of the effective action determines directly the connected correlation function $G_{\rm c}^{(2)}(\omega)$ of the interacting theory in the presence of the external source j. Since j is an auxiliary quantity, which eventually be set equal to zero thus making X equal to X_0, the actual physical propagator is given by

$$G_{\rm c}^{(2)}\Big|_{j=0} = \Gamma^{\;-1}_{XX}\Big|_{X=X_0}. \tag{3.636}$$

By Fourier-transforming this relation and removing a δ-function for the overall momentum conservation, the full propagator $G_{\omega^2}(\omega)$ is related to the vertex function $\Gamma^{(2)}(\omega)$, defined in (3.629) by

$$G_{\omega^2}(\omega) \equiv \bar G^{(2)}(\mathrm{k}) = \frac{1}{\bar\Gamma^{(2)}(\omega)}. \tag{3.637}$$

The third derivative of the generating functional $W[j]$ is obtained by functionally differentiating W_{jj} in Eq. (3.633) once more with respect to j, and applying the chain rule:

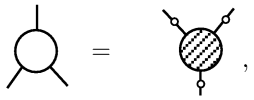
$$W_{jjj} = -\Gamma_{XX}^{-2}\Gamma_{XXX}\frac{\delta X}{\delta j} = -\Gamma_{XX}^{-3}\Gamma_{XXX} = -{G_c^{(2)}}^3\,\Gamma_{XXX}. \tag{3.638}$$

This equation has a simple physical meaning. The third derivative of $W[j]$ on the left-hand side is the full three-point function at a nonzero source j, so that

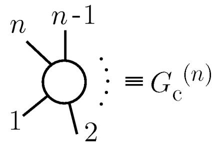
$$G_{\rm c}^{(3)} = W_{jjj} = -{G_c^{(2)}}^3\Gamma_{XXX}. \tag{3.639}$$

This equation states that the full three-point function arises from a third derivative of $\Gamma[X]$ by attaching to each derivation a full propagator, apart from a minus sign.

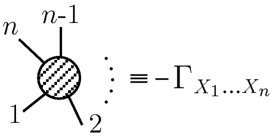
We shall express Eq. (3.639) diagrammatically as follows:



where



denotes the connected n-point function, and

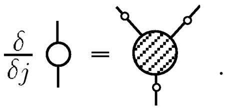


the negative n-point vertex function.

For the general analysis of the diagrammatic content of the effective action, we observe that according to Eq. (3.638), the functional derivative of the correlation function G with respect to the current j satisfies

$$G_c^{(2)}{}_j = W_{jjj} = G_c^{(3)} = -G_c^{(2)^3}\Gamma_{XXX}. \tag{3.640}$$

This is pictured diagrammatically as follows:

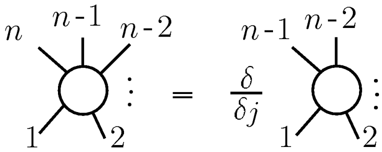


(3.641)

This equation may be differentiated further with respect to j in a diagrammatic way. From the definition (3.560) we deduce the trivial recursion relation

$$G_{\rm c}^{(n)}(\tau_1, \dots, \tau_n) = \frac{\delta}{\delta j(\tau_n)} G_{\rm c}^{(n-1)}(\tau_1, \dots, \tau_{n-1}), \tag{3.642}$$

which is represented diagrammatically as

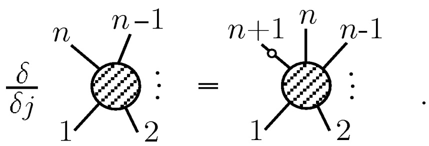


$n > 2$.

By applying $\delta/\delta j$ repeatedly to the left-hand side of Eq. (3.640), we generate all higher connected correlation functions. On the right-hand side of (3.640), the chain rule leads to a derivative of all correlation functions $G = G_c^{(2)}$ with respect to j, thereby changing a line into a line with an extra three-point vertex as indicated in the diagrammatic equation (3.641). On the other hand, the vertex function Γ_{XXX} must be differentiated with respect to j. Using the chain rule, we obtain for any n-point vertex function:

$$\Gamma_{X \dots Xj} = \Gamma_{X \dots XX} \frac{\delta X}{\delta j} = \Gamma_{X \dots XX} G_c^{(2)}, \tag{3.643}$$

which may be represented diagrammatically as



With these diagrammatic rules, we can differentiate (3.638) any number of times, and derive the diagrammatic structure of the connected correlation functions with an arbitrary number of external legs. The result up to $n = 5$ is shown in Fig. 3.12.

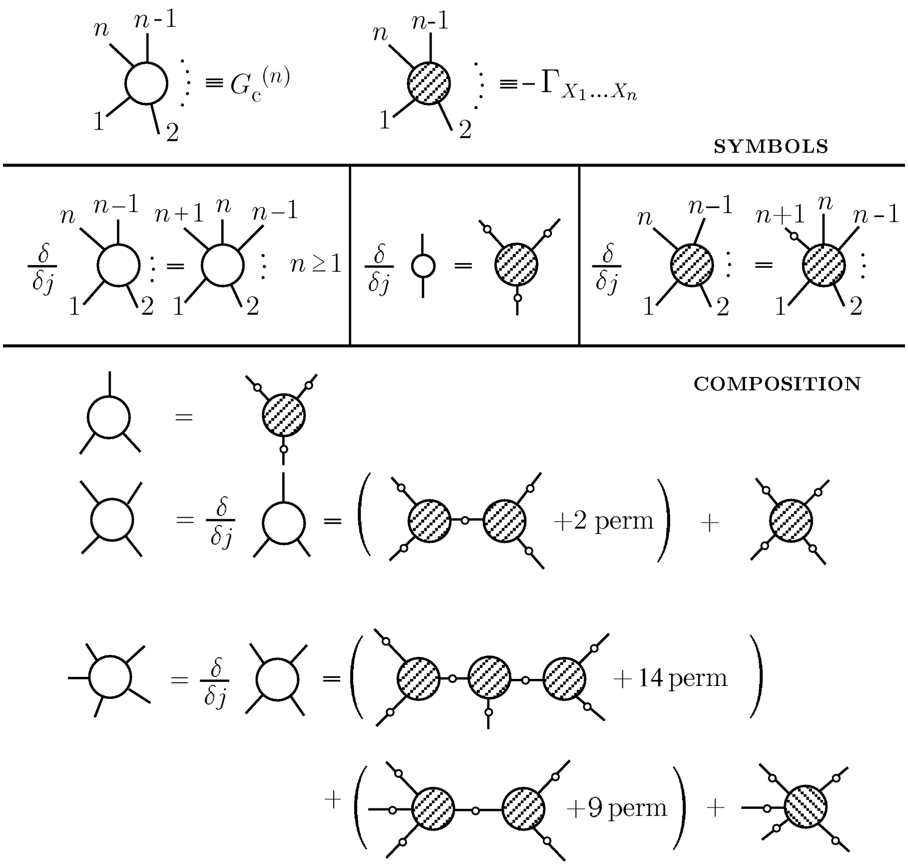


Figure 3.12 Diagrammatic differentiations for deriving tree decomposition of connected correlation functions. The last term in each decomposition yields, after amputation and removal of an overall δ-function of momentum conservation, precisely all one-particle irreducible diagrams.

The diagrams generated in this way have a tree-like structure, and for this reason they are called *tree diagrams*. The tree decomposition reduces all diagrams to their one-particle irreducible contents.

The effective action $\Gamma[X]$ can be used to prove an important composition theorem: The full propagator G can be expressed as a geometric series involving the so-called *self-energy*. Let us decompose the vertex function as

$$\bar{\Gamma}^{(2)} = G_0^{-1} + \bar{\Gamma}^{\text{int}}_{XX}, \tag{3.644}$$

such that the full propagator (3.636) can be rewritten as

$$G = \left(1 + G_0\bar{\Gamma}^{\text{int}}_{XX}\right)^{-1} G_0. \tag{3.645}$$

Expanding the denominator, this can also be expressed in the form of an integral equation:

$$G = G_0 - G_0\bar{\Gamma}^{\text{int}}_{XX}G_0 + G_0\bar{\Gamma}^{\text{int}}_{XX}G_0\bar{\Gamma}^{\text{int}}_{XX}G_0 - \dots\ . \tag{3.646}$$

The quantity $-\bar{\Gamma}^{\text{int}}_{XX}$ is called the self-energy, commonly denoted by Σ:

$$\Sigma \equiv -\bar{\Gamma}^{\text{int}}_{XX}, \tag{3.647}$$

i.e., the self-energy is given by the interacting part of the second functional derivative of the effective action, except for the opposite sign.

According to Eq. (3.646), all diagrams in G can be obtained from a repetition of self-energy diagrams connected by a single line. In terms of Σ, the full propagator reads, according to Eq. (3.645):

$$G \equiv [G_0^{-1} - \Sigma]^{-1}. \tag{3.648}$$

This equation can, incidentally, be rewritten in the form of an integral equation for the correlation function G:

$$G = G_0 + G_0\Sigma G. \tag{3.649}$$

3.22.6 Ginzburg-Landau Approximation to Generating Functional

Since the vertex functions are the functional derivatives of the effective action [see (3.628)], we can expand the effective action into a functional Taylor series

$$\Gamma[X] = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tau_1 \dots d\tau_n \Gamma^{(n)}(\tau_1, \dots, \tau_n) X(\tau_1) \dots X(\tau_n). \tag{3.650}$$

The expansion in the number of loops of the generating functional $\Gamma[X]$ collects systematically the contributions of fluctuations. To zeroth order, all fluctuations are neglected, and the effective action reduces to the initial action, which is the mean-field approximation to the effective action. In fact, in the absence of loop diagrams, the vertex functions contain only the lowest-order terms in $\Gamma^{(2)}$ and $\Gamma^{(4)}$:

$$\Gamma_0^{(2)}(\tau_1, \tau_2) = M\left(-\partial_{\tau_1}^2 + \omega^2\right)\delta(\tau_1 - \tau_2), \tag{3.651}$$

$$\Gamma_0^{(4)}(\tau_1, \tau_2, \tau_3, \tau_4) = \lambda\,\delta(\tau_1 - \tau_2)\delta(\tau_1 - \tau_3)\delta(\tau_1 - \tau_4). \tag{3.652}$$

Inserted into (3.650), this yields the zero-loop approximation to $\Gamma[X]$:

$$\Gamma_0[X] = \frac{M}{2!}\int d\tau\, [(\partial_\tau X)^2 + \omega^2 X^2] + \frac{\lambda}{4!}\int d\tau\, X^4. \tag{3.653}$$

This is precisely the original action functional (3.562). By generalizing $X(\tau)$ to be a magnetization vector field, $X(\tau) \to \mathbf{M}(\mathbf{x})$, which depends on the three-dimensional space variables $\mathbf{x}$ rather than the Euclidean time, the functional (3.653) coincides with the phenomenological energy functional set up by Ginzburg and Landau to describe the behavior of magnetic materials near the Curie point, which they wrote as[18]

$$\Gamma[\mathbf{M}] = \int d^3x \left[\frac{1}{2}\sum_{i=1}^{3}(\partial_i \mathbf{M})^2 + \frac{m^2}{2!}\mathbf{M}^2 + \frac{\lambda}{4!}\mathbf{M}^4\right]. \tag{3.654}$$

The use of this functional is also referred to as *mean-field theory* or *mean-field approximation* to the full theory.

3.22.7 Composite Fields

Sometimes it is of interest to study also correlation functions in which two fields coincide at one point, for instance

$$G^{(1,n)}(\tau,\tau_1,\dots,\tau_n) = \frac{1}{2}\langle x^2(\tau)x(\tau_1)\cdots x(\tau_n)\rangle. \tag{3.655}$$

If multiplied by a factor $M\omega^2$, the composite operator $M\omega^2 x^2(\tau)/2$ is precisely the frequency term in the action energy functional (3.562). For this reason one speaks of a *frequency insertion*, or, since in the Ginzburg-Landau action (3.654) the frequency ω is denoted by the mass symbol m, one speaks of a *mass insertion* into the correlation function $G^{(n)}(\tau_1,\dots,\tau_n)$.

Actually, we shall never make use of the full correlation function (3.655), but only of the integral over τ in (3.655). This can be obtained directly from the generating functional $Z[j]$ of all correlation functions by differentiation with respect to the square mass in addition to the source terms

$$\int d\tau\, G^{(1,n)}(\tau,\tau_1,\dots,\tau_n) = -\, Z^{-1}\frac{\partial}{M\partial\omega^2}\frac{\delta}{\delta j(\tau_1)}\cdots\frac{\delta}{\delta j(\tau_n)}Z[j]\bigg|_{j=0}. \tag{3.656}$$

By going over to the generating functional $W[j]$, we obtain in a similar way the connected parts:

$$\int d\tau\, G_{\rm c}^{(1,n)}(\tau,\tau_1,\dots,\tau_n) = -\frac{\partial}{M\partial\omega^2}\frac{\delta}{\delta j(\tau_1)}\cdots\frac{\delta}{\delta j(\tau_n)}W[j]\bigg|_{j=0}. \tag{3.657}$$

[18] L.D. Landau, J.E.T.P. *7*, 627 (1937).

The right-hand side can be rewritten as

$$\int d\tau\, G_{\rm c}^{(1,n)}(\tau,\tau_1,\dots,\tau_n) = -\frac{\partial}{M\partial\omega^2} G_{\rm c}^{(n)}(\tau_1,\dots,\tau_n). \tag{3.658}$$

The connected correlation functions $G_{\rm c}^{(1,n)}(\tau,\tau_1,\dots,\tau_n)$ can be decomposed into tree diagrams consisting of lines and one-particle irreducible vertex functions $\Gamma^{(1,n)}(\tau,\tau_1,\dots,\tau_n)$. If integrated over τ, these are defined from Legendre transform (3.622) by a further differentiation with respect to $M\omega^2$:

$$\int d\tau\, \Gamma^{(1,n)}(\tau,\tau_1,\dots,\tau_n) = -\frac{\partial}{M\partial\omega^2}\frac{\delta}{\delta X(\tau_1)}\cdots\frac{\delta}{\delta X(\tau_n)}\Gamma[X]\bigg|_{X_0}, \tag{3.659}$$

implying the relation

$$\int d\tau\, \Gamma^{(1,n)}(\tau,\tau_1,\dots,\tau_n) = -\frac{\partial}{M\partial\omega^2}\Gamma^{(n)}(\tau_1,\dots,\tau_n). \tag{3.660}$$

3.23 Path Integral Calculation of Effective Action by Loop Expansion

Path integrals give the most direct access to the effective action of a theory avoiding the cumbersome Legendre transforms. The derivation will proceed diagrammatically loop by loop, which will turn out to be organized by the powers of the Planck constant $\hbar$. This will now be kept explicit in all formulas. For later applications to quantum mechanics we shall work with real time.

3.23.1 General Formalism

Consider the generating functional of all Green functions

$$Z[j] = e^{iW[j]/\hbar}, \tag{3.661}$$

where $W[j]$ is the generating functional of all *connected* Green functions. The vacuum expectation of the field, the average

$$X(t) \equiv \langle x(t)\rangle, \tag{3.662}$$

is given by the first functional derivative

$$X(t) = \delta W[j]/\delta j(t). \tag{3.663}$$

This can be inverted to yield $j(t)$ as a functional of $X(t)$:

$$j(t) = j[X](t), \tag{3.664}$$

which leads to the Legendre transform of $W[j]$:

$$\Gamma[X] \equiv W[j] - \int dt\, j(t)X(t), \tag{3.665}$$

where the right-hand side is replaced by (3.664). This is the *effective action* of the theory. The effective action for time independent $\mathbf{X}(t) \equiv \mathbf{X}$ defines the *effective potential*

$$V^{\text{eff}}(X) \equiv -\frac{1}{t_b - t_a}\Gamma[X]. \tag{3.666}$$

The first functional derivative of the effective action gives back the current

$$\frac{\delta\Gamma[X]}{\delta X(t)} = -j(t). \tag{3.667}$$

The generating functional of all connected Green functions can be recovered from the effective action by the inverse Legendre transform

$$W[j] = \Gamma[X] + \int dt\, j(t)X(t). \tag{3.668}$$

We now calculate these quantities from the path integral formula (3.561) for the generating functional $Z[j]$:

$$Z[j] = \int \mathcal{D}x(t)e^{(i/\hbar)\left\{\mathcal{A}[x]+\int dt\, j(t)x(t)\right\}}. \tag{3.669}$$

With (3.661), this amounts to the path integral formula for $\Gamma[X]$:

$$e^{\frac{i}{\hbar}\left\{\Gamma[X]+\int dt\, j(t)X(t)\right\}} = \int \mathcal{D}x(t)e^{(i/\hbar)\left\{\mathcal{A}[x]+\int dt\, j(t)x(t)\right\}}. \tag{3.670}$$

The action quantum $\hbar$ is a measure for the size of quantum fluctuations. Under many physical circumstances, quantum fluctuations are small, which makes it desirable to develop a method of evaluating (3.670) as an expansion in powers of $\hbar$.

3.23.2 Mean-Field Approximation

For $\hbar \to 0$, the path integral over the path $x(t)$ in (3.669) is dominated by the classical solution $x_{\text{cl}}(t)$ which extremizes the exponent

$$\left.\frac{\delta\mathcal{A}[x]}{\delta x(t)}\right|_{x=x_{\text{cl}}(t)} = -j(t), \tag{3.671}$$

and is a functional of $j(t)$ which may be written, more explicitly, as $x_{\text{cl}}(t)[j]$. At this level we can identify

$$W[j] = \Gamma[X] + \int dt\, j(t)X(t) \;\;\approx\;\; \mathcal{A}[x_{\text{cl}}[j]] + \int dt\, j(t)x_{\text{cl}}(t)[j]. \tag{3.672}$$

By differentiating $W[j]$ with respect to j, we have from the general first part of Eq. (3.662):

$$X = \frac{\delta W}{\delta j} = \frac{\delta\Gamma}{\delta X}\frac{\delta X}{\delta j} + X + j\frac{\delta X}{\delta j}. \tag{3.673}$$

Inserting the classical equation of motion (3.671), this becomes

$$X = \frac{\delta \mathcal{A}}{\delta x_{\rm cl}} \frac{\delta x_{\rm cl}}{\delta j} + x_{\rm cl} + j \frac{\delta x_{\rm cl}}{\delta j} = x_{\rm cl}. \tag{3.674}$$

Thus, to this approximation, $X(t)$ coincides with the classical path $x_{\rm cl}(t)$. Replacing $x_{\rm cl}(t) \to X(t)$ on the right-hand side of Eq. (3.672), we obtain the lowest-order result, which is of zeroth order in $\hbar$, the classical approximation to the effective action:

$$\Gamma_0[X] = \mathcal{A}[X]. \tag{3.675}$$

For an anharmonic oscillator in N dimensions with unit mass and an interaction $\mathbf{x}^4$, where $\mathbf{x} = (x_1, \dots, x_N)$, which is symmetric under N-dimensional rotations O(N), the lowest-order effective action reads

$$\Gamma_0[\mathbf{X}] = \int dt \left[\frac{1}{2} \left(\dot{X}_a^2 - \omega^2 X_a^2 \right) - \frac{g}{4!} \left(X_a^2 \right)^2 \right], \tag{3.676}$$

where repeated indices $a, b, \dots$ are summed from 1 to N following Einstein's summation convention. The effective potential (3.666) is simply the initial potential

$$V_0^{\rm eff}(\mathbf{X}) = V(\mathbf{X}) = \frac{\omega^2}{2} X_a^2 + \frac{g}{4!} \left(X_a^2 \right)^2. \tag{3.677}$$

For $\omega^2 > 0$, this has a minimum at $\mathbf{X} \equiv \mathbf{0}$, and there are only two non-vanishing vertex functions $\Gamma^{(n)}(t_1, \dots, t_n)$:

For $n = 2$:

$$\begin{aligned} \Gamma^{(2)}(t_1, t_2)_{ab} &\equiv \left. \frac{\delta^2 \Gamma}{\delta X_a(t_1) \delta X_b(t_2)} \right|_{X_a=0} = \left. \frac{\delta^2 \mathcal{A}}{x_a(t_1) x_b(t_2)} \right|_{x_a=X_a=0} \\ &= (-\partial_t^2 - \omega^2) \delta_{ab} \delta(t_1 - t_2). \end{aligned} \tag{3.678}$$

This determines the inverse of the propagator:

$$\Gamma^{(2)}(t_1, t_2)_{ab} = [i\hbar G^{-1}]_{ab}(t_1, t_2). \tag{3.679}$$

Thus we find to this zeroth-order approximation that $G_{ab}(t_1, t_2)$ is equal to the free propagator:

$$G_{ab}(t_1, t_2) = G_{0ab}(t_1, t_2). \tag{3.680}$$

For $n = 4$:

$$\Gamma^{(4)}(t_1, t_2, t_3, t_4)_{abcd} \equiv \frac{\delta^4 \Gamma}{\delta X_a(t_1) \delta X_b(t_2) \delta X_c(t_3) \delta X_d(t_4)} = g T_{abcd}, \tag{3.681}$$

with

$$T_{abcd} = \frac{1}{3} (\delta_{ab} \delta_{cd} + \delta_{ac} \delta_{bd} + \delta_{ad} \delta_{bc}). \tag{3.682}$$

According to the definition of the effective action, all diagrams of the theory can be composed from the propagator $G_{ab}(t_1, t_2)$ and this vertex via tree diagrams. Thus we see that in this lowest approximation, we recover precisely the subset of all original Feynman diagrams with a tree-like topology. These are all diagrams which do not involve any loops. Since the limit $\hbar \to 0$ corresponds to the classical equations of motion with no quantum fluctuations we conclude: Classical theory corresponds to tree diagrams.

For $\omega^2 < 0$ the discussion is more involved since the minimum of the potential (3.677) lies no longer at $\mathbf{X} = \mathbf{0}$, but at a nonzero vector $\mathbf{X}_0$ with an arbitrary direction, and a length

$$|\mathbf{X}_0| = \sqrt{-6\omega^2/g}. \tag{3.683}$$

The second functional derivative (3.678) at $\mathbf{X}$ is anisotropic and reads

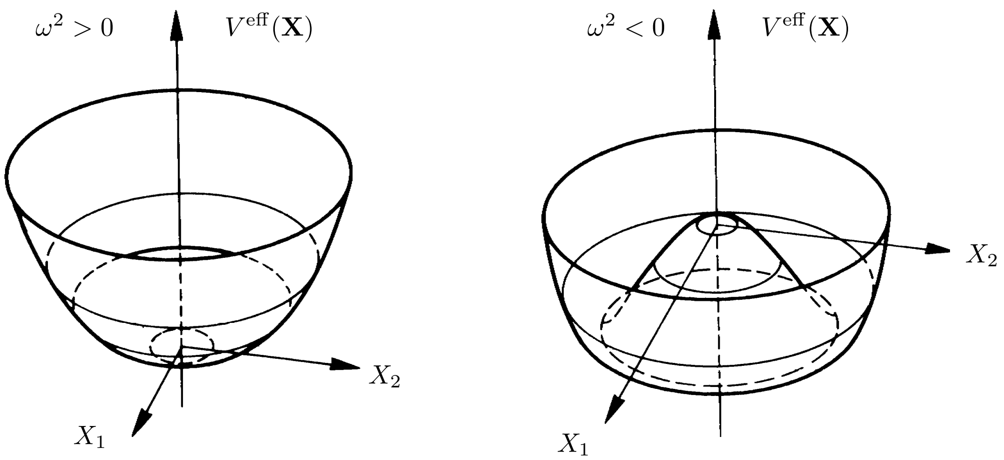


Figure 3.13 Effective potential for $\omega^2 > 0$ and $\omega^2 < 0$ in mean-field approximation, pictured for the case of two components X_1, X_2. The right-hand figure looks like a Mexican hat or the bottom of a champaign bottle..

$$\begin{aligned}\Gamma^{(2)}(t_1, t_2)_{ab} &\equiv \left.\frac{\delta^2\Gamma}{\delta X_a(t_1)\delta X_b(t_2)}\right|_{X_a\neq 0} = \left.\frac{\delta^2\mathcal{A}}{x_a(t_1)x_b(t_2)}\right|_{x_a=X_a\neq 0}\\ &= \left[-\partial_t^2 - \omega^2 - \frac{g}{6}\left(\delta_{ab}X_c^2 + 2X_aX_b\right)\right]\delta(t_1-t_2).\end{aligned} \tag{3.684}$$

This is conveniently separated into longitudinal and transversal derivatives with respect to the direction $\hat{\mathbf{X}} = \mathbf{X}/|\mathbf{X}|$. We introduce associated projection matrices:

$$P_{Lab}(\hat{\mathbf{X}}) = \hat{X}_a\hat{X}_b, \qquad P_{Tab}(\hat{\mathbf{X}}) = \delta_{ab} - \hat{X}_a\hat{X}_b, \tag{3.685}$$

and decompose

$$\Gamma^{(2)}(t_1, t_2)_{ab} = \Gamma_L^{(2)}(t_1, t_2)_{ab}P_{Lab}(\hat{\mathbf{X}}) + \Gamma_T^{(2)}(t_1, t_2)_{ab}P_{Tab}(\hat{\mathbf{X}}), \tag{3.686}$$

where

$$\Gamma_T^{(2)}(t_1,t_2)_{ab} = \left[-\partial_t^2 - \left(\omega^2 + \frac{g}{6}\mathbf{X}^2\right)\right]\delta(t_1-t_2), \tag{3.687}$$

and

$$\Gamma_L^{(2)}(t_1,t_2)_{ab} = \left[-\partial_t^2 - \left(\omega^2 + 3\frac{g}{6}\mathbf{X}^2\right)\right]\delta(t_1-t_2). \tag{3.688}$$

This can easily be inverted to find the propagator

$$\mathcal{G}(t_1,t_2)_{ab} = i\hbar\left[\Gamma^{(2)}(t_1,t_2)\right]^{-1}_{ab} = \mathcal{G}_L(t_1,t_2)_{ab}P_{Lab}(\hat{\mathbf{X}}) + \mathcal{G}_T(t_1,t_2)_{ab}P_{Tab}(\hat{\mathbf{X}}), \tag{3.689}$$

where

$$\begin{aligned}
\mathcal{G}_L(t_1,t_2)_{ab} &= \frac{i\hbar}{\Gamma_L(t_1,t_2)} = \frac{i\hbar}{-\partial_t^2 - \omega_L^2(\mathbf{X})}, && (3.690)\\
\mathcal{G}_T(t_1,t_2)_{ab} &= \frac{i\hbar}{\Gamma_T^{(2)}(t_1,t_2)} = \frac{i\hbar}{-\partial_t^2 - \omega_T^2(\mathbf{X})} && (3.691)
\end{aligned}$$

are the longitudinal and transversal parts of the Green function. For convenience, we have introduced the $\mathbf{X}$-dependent frequencies of the longitudinal and transversal Green functions:

$$\omega_L^2(\mathbf{X}) \equiv \omega^2 + 3\,\frac{g}{6}\mathbf{X}^2, \quad \omega_T^2(\mathbf{X}) \equiv \omega^2 + \frac{g}{6}\mathbf{X}^2. \tag{3.692}$$

To emphasize the fact that this propagator is a functional of $\mathbf{X}$ we represent it by the calligraphic letter $\mathcal{G}$. For $\omega^2 > 0$, we perform the fluctuation expansion around the minimum of the potential (3.666) at $\mathbf{X} = 0$, where the two Green functions coincide, both having the same frequency ω:

$$\mathcal{G}_L(t_1,t_2)_{ab}\,|_{\mathbf{X}=\mathbf{0}} = \mathcal{G}_T(t_1,t_2)_{ab}\,|_{\mathbf{X}=\mathbf{0}} = \mathcal{G}(t_1,t_2)_{ab}\,|_{\mathbf{X}=\mathbf{0}} = \frac{i\hbar}{-\partial_t^2 - \omega^2}, \tag{3.693}$$

For $\omega^2 < 0$, however, where the minimum lies at the vector $\mathbf{X}_0$ of length (3.683), they are different:

$$\mathcal{G}_L(t_1,t_2)_{ab}\,|_{\mathbf{X}=\mathbf{X}_0} = \frac{i\hbar}{-\partial_t^2 + 2\omega^2}, \quad \mathcal{G}_T(t_1,t_2)_{ab}\,|_{\mathbf{X}=\mathbf{X}_0} = \frac{i\hbar}{-\partial_t^2}. \tag{3.694}$$

Since the curvature of the potential at the minimum in radial direction of $\mathbf{X}$ is positive at the minimum, the longitudinal part has now the positive frequency $-2\omega^2$. The movement along the valley of the minimum, on the other hand, does not increase the energy. For this reason, the transverse part has zero frequency. This feature, observed here in lowest order of the fluctuation expansion, is a very general one, and can be found in the effective action to any loop order. In quantum field theory, there exists a theorem asserting this called *Nambu-Goldstone theorem*. It states that if a quantum field theory without long-range interactions has a continuous symmetry which is broken by a nonzero expectation value of the field corresponding to the present $\mathbf{X}$ [recall (3.662)], then the fluctuations transverse to it have a zero mass. They are called *Nambu-Goldstone modes* or, because of their bosonic nature, *Nambu-Goldstone bosons*. The exclusion of long-range interactions is necessary, since these can mix with the zero-mass modes and make it massive. This happens, for example, in a superconductor where they make the magnetic field massive, giving it a finite penetration depth, the famous *Meissner effect*. One expresses this pictorially by saying that the long-range mode can eat up the Nambu-Goldstone modes and become massive. The same mechanism is used in elementary particle physics to explain the mass of the $W^{\pm}$ and Z^0 vector bosons as a consequence of having eaten up a would be Nambu-Goldstone boson of an auxiliary Higgs-field theory.

In quantum-mechanical systems, however, a nonzero expectation value with the associated zero frequency mode in the transverse direction is found only as an artifact of perturbation theory. If all fluctuation corrections are summed, the minimum of the effective potential lies always at the origin. For example, it is well known, that the ground state wave functions of a particle in a double-well potential is symmetric, implying a zero expectation value of the particle position. This symmetry is caused by quantum-mechanical tunneling, a phenomenon which will be discussed in detail in Chapter 17. This phenomenon is of a nonperturbative nature which cannot be described by an effective potential calculated order by order in the fluctuation expansion. Such a potential does, in general, posses a nonzero minimum at some $\mathbf{X}_0$ somewhere near the zero-order minimum (3.683). Due to this shortcoming, it is possible to derive the Nambu-Goldstone theorem from the quantum-mechanical effective action in the loop expansion, even though the nonzero expectation value $\mathbf{X}_0$ assumed in the derivation of the zero-frequency mode does not really exist in quantum mechanics. The derivation will be given in Section 3.24.

The use of the initial action to approximate the effective action neglecting corrections caused by the fluctuations is referred to as *mean-field approximation*.

3.23.3 Corrections from Quadratic Fluctuations

In order to find the first $\hbar$-correction to the mean-field approximation we expand the action in powers of the fluctuations of the paths around the classical solution

$$\delta x(t) \equiv x(t) - x_{\rm cl}(t), \tag{3.695}$$

and perform a perturbation expansion. The quadratic term in $\delta x(t)$ is taken to be the free-particle action, the higher powers in $\delta x(t)$ are the interactions. Up to second order in the fluctuations $\delta x(t)$, the action is expanded as follows:

$$\begin{aligned}
&\mathcal{A}[x_{\rm cl}+\delta x] + \int dt\, j(t)\, [x_{\rm cl}(t)+\delta x(t)] \\
&\quad = \mathcal{A}[x_{\rm cl}] + \int dt\, j(t)\, x_{\rm cl}(t) + \int dt\, \left\{ j(t) + \left.\frac{\delta \mathcal{A}}{\delta x(t)}\right|_{x=x_{\rm cl}} \right\} \delta x(t) \\
&\quad + \frac{1}{2}\int dt\, dt'\; \delta x(t) \left.\frac{\delta^2 \mathcal{A}}{\delta x(t)\delta x(t')}\right|_{x=x_{\rm cl}} \delta x(t') + \mathcal{O}\left((\delta x)^3\right).
\end{aligned}\tag{3.696}$$

The curly bracket multiplying the linear terms in the variation $\delta x(t)$ vanish due to the extremality property of the classical path $x_{\rm cl}$ expressed by the equation of motion (3.671). Inserting this expansion into (3.670), we obtain the approximate expression

$$Z[j] \approx e^{(i/\hbar)\left\{\mathcal{A}[x_{\rm cl}]+\int dt\, j(t)x_{\rm cl}(t)\right\}} \int \mathcal{D}\delta x \exp\left\{\frac{i}{\hbar}\int dt\, dt'\;\, \delta x(t)\frac{\delta^2\mathcal{A}}{\delta x(t)\delta x(t')}\bigg|_{x=x_{\rm cl}} \delta x(t')\right\}. \tag{3.697}$$

We now observe that the fluctuations $\delta x(t)$ will be of average size $\sqrt{\hbar}$ due to the $\hbar$-denominator in the Fresnel exponent. Thus the fluctuations $(\delta x)^n$ are of average size $\sqrt{\hbar}^{\,n}$. The approximate path integral (3.697) is of the Fresnel type and my be integrated to yield

$$\begin{aligned} & e^{(i/\hbar)\left\{\mathcal{A}[x_{\rm cl}]+\int dt\, j(t)x_{\rm cl}(t)\right\}} \left[\det \frac{\delta^2\mathcal{A}}{\delta x(t)\delta x(t')}\right]^{-1/2}_{x=x_{\rm cl}} \\ &\quad = e^{(i/\hbar)\left\{\mathcal{A}[x_{\rm cl}]+\int dt\, j(t)x_{\rm cl}(t)+i(\hbar/2){\rm Tr}\log[\delta^2\mathcal{A}/\delta x(t)\delta x(t')|_{x=x_{\rm cl}}\right\}}. \end{aligned} \tag{3.698}$$

Comparing this with the left-hand side of (3.670), we find that to first order in $\hbar$, the effective action may be recovered by equating

$$\Gamma[X]+\int dt\, j(t)X(t) = \mathcal{A}[x_{\rm cl}[j]] + \int dt\, j(t)\, x_{\rm cl}(t)[j] + \frac{i\hbar}{2}{\rm Tr}\log\frac{\delta^2\mathcal{A}\left[x_{\rm cl}[j]\right]}{\delta x(t)\delta x(t')}. \tag{3.699}$$

In the limit $\hbar \to 0$, the tracelog term disappears and (3.699) reduces to the classical expression (3.672).

To include the $\hbar$-correction into $\Gamma[X]$, we expand $W[j]$ as

$$W[j] = W_0[j] + \hbar W_1[j] + \mathcal{O}(\hbar^2). \tag{3.700}$$

Correspondingly, the path X differs from $X_{\rm cl}$ by a correction term of order $\hbar$:

$$X = x_{\rm cl} + \hbar\, X_1 + \mathcal{O}(\hbar^2). \tag{3.701}$$

Inserting this into (3.699), we find

$$\begin{aligned} \Gamma[X]+\int dt\, jX &= \mathcal{A}\left[X-\hbar X_1\right] + \int dt\, jX - \hbar\int dt\, jX_1 \\ &\quad + \frac{i}{2}\hbar\,{\rm Tr}\log\frac{\delta^2\mathcal{A}}{\delta x_a\delta x_b}\bigg|_{x=X-\hbar X_1} + \mathcal{O}\left(\hbar^2\right). \end{aligned} \tag{3.702}$$

Expanding the action up to the same order in $\hbar$ gives

$$\Gamma[X] = \mathcal{A}[X] - \hbar\int dt\left\{\frac{\delta\mathcal{A}[X]}{\delta X}+j\right\}X_1 + \frac{i}{2}\hbar\,{\rm Tr}\log\frac{\delta^2\mathcal{A}}{\delta x_a\delta x_b}\bigg|_{x=X} + \mathcal{O}\left(\hbar^2\right). \tag{3.703}$$

Due to (3.671), the curly-bracket term is only of order $\hbar^2$, so that we find the one-loop form of the effective action

$$\begin{aligned}\Gamma[X] = \Gamma_0[X] + \hbar\Gamma_1[X] &= \int dt \left[\frac{1}{2}\dot{X}^2 - \frac{\omega^2}{2}X_a^2 - \frac{g}{4!}\left(X_a^2\right)^2\right] \\ &+ \frac{i}{2}\hbar \operatorname{Tr}\log\left[-\partial_t^2 - \omega^2 - \frac{g}{6}\left(\delta_{ab}X_c^2 + 2X_aX_b\right)\right]. \quad (3.704)\end{aligned}$$

Using the decomposition (3.686), the tracelog term can be written as a sum of transversal and longitudinal parts

$$\begin{aligned}\hbar\Gamma_1[X] &= \frac{i}{2}\hbar \operatorname{Tr}\log\Gamma_L^{(2)}(t_1,t_2)_{ab} + \frac{i}{2}(N-1)\hbar\operatorname{Tr}\log\Gamma_T^{(2)}(t_1,t_2)_{ab} \quad (3.705)\\ &= \frac{i}{2}\hbar\operatorname{Tr}\log\left(-\partial_t^2 - \omega_L^2(\mathbf{X})\right) + \frac{i}{2}(N-1)\hbar\operatorname{Tr}\log\left(-\partial_t^2 - \omega_T^2(\mathbf{X})\right).\end{aligned}$$

What is the graphical content in the Green functions at this level of approximation? Assuming $\omega^2 > 0$, we find for $\mathbf{j} = 0$ that the minimum lies at $\bar{\mathbf{X}} = \mathbf{0}$, as in the mean-field approximation. Around this minimum, we may expand the tracelog in powers of $\mathbf{X}$. For the simplest case of a single X-variable, we obtain

$$\begin{aligned}\frac{i}{2}\hbar\operatorname{Tr}\log\left(-\partial_t^2-\omega^2-\frac{g}{2}X^2\right) &= \frac{i}{2}\hbar\operatorname{Tr}\log\left(-\partial_t^2-\omega^2\right) + \frac{i}{2}\hbar\operatorname{Tr}\log\left(1+\frac{i}{-\partial_t^2-\omega^2}ig\frac{X^2}{2}\right)\\ &= i\frac{\hbar}{2}\operatorname{Tr}\log\left(-\partial_t^2-\omega^2\right) - i\frac{\hbar}{2}\sum_{n=1}^{\infty}\left(-i\frac{g}{2}\right)^n\frac{1}{n}\operatorname{Tr}\left(\frac{i}{-\partial_t^2-\omega^2}X^2\right)^n. \quad (3.706)\end{aligned}$$

If we insert

$$G_0 = \frac{i}{-\partial_t^2 - \omega^2}, \quad (3.707)$$

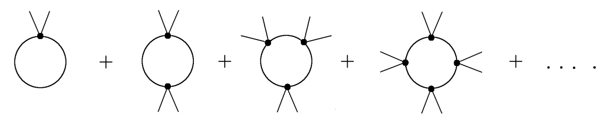
this can be written as

$$i\frac{\hbar}{2}\operatorname{Tr}\log\left(-\partial_t^2-\omega^2\right) - i\frac{\hbar}{2}\sum_{n=1}^{\infty}\left(-i\frac{g}{2}\right)^n\frac{1}{n}\operatorname{Tr}\left(G_0X^2\right)^n. \quad (3.708)$$

More explicitly, the terms with $n = 1$ and $n = 2$ read:

$$\begin{aligned}&-\frac{\hbar}{4}g\int dt\,dt'\,\delta(t-t')G_0(t,t')X^2(t')\\ &+i\hbar\frac{g^2}{16}\int dt\,dt'\,dt''\,\delta^4(t-t'')G_0(t,t')X^2(t')G_0(t',t'')X^2(t'') + \dots \quad . \quad (3.709)\end{aligned}$$

The expansion terms of (3.708) for $n \geq 1$ correspond obviously to the Feynman diagrams (omitting multiplicity factors)

$\mathcal{A}[x_{\rm cl}] =$  (3.710)

The series (3.708) is therefore a sum of all diagrams with one loop and any number of fundamental X^4-vertices

To systematize the entire expansion (3.708), the tracelog term is [compare (3.549)] pictured by a single-loop diagram

$$i\frac{\hbar}{2}\mathrm{Tr}\log\left(-\partial_t^2-\omega^2\right)=\frac{1}{2}\bigcirc\ . \tag{3.711}$$

The first two diagrams in (3.710) contribute corrections to the vertices $\Gamma^{(2)}$ and $\Gamma^{(4)}$. The remaining diagrams produce higher vertex functions and lead to more involved tree diagrams. In Fourier space we find from (3.709)

$$\Gamma^{(2)}(q) \;=\; q^2-\omega^2-\hbar\frac{g}{2}\int\frac{dk}{2\pi}\frac{i}{k^2-\omega^2+i\eta} \tag{3.712}$$

$$\Gamma^{(4)}(q_i) \;=\; g-i\frac{g^2}{2}\left[\int\frac{dk}{2\pi}\frac{i}{k^2-\omega^2+i\eta}\frac{i}{\left(q_1+q_2-k\right)^2-\omega^2+i\eta}+2\text{ perm}\right]. \tag{3.713}$$

We may write (3.712) in Euclidean form as

$$\begin{aligned}\Gamma^{(2)}(q) &= -q^2-\omega^2-\hbar\,\frac{g}{2}\int\frac{dk}{2\pi}\frac{1}{k^2+\omega^2}\\ &= -\left(q^2+\omega^2+\hbar\frac{g}{2}\frac{1}{2\omega}\right),\end{aligned} \tag{3.714}$$

$$\Gamma^{(4)}(q_i) \;=\; g-\hbar\frac{g^2}{2}\left[I\left(q_1+q_2\right)+2\text{ perm}\right], \tag{3.715}$$

with the Euclidean two-loop integral

$$I(q_1+q_2)=\int\frac{dk}{2\pi}\frac{1}{k^2+\omega^2}\frac{i}{\left(q_1+q_2-k\right)^2+\omega^2}, \tag{3.716}$$

to be calculated explicitly in Chapter 10. It is equal to $J((q_1+q_2)^2)/2\pi$ with the functions $J(z)$ of Eq. (10.259).

For $\omega^2<0$ where the minimum of the effective action lies at $\bar{\mathbf{X}}\neq\mathbf{0}$, the expansion of the trace of the logarithm in (3.704) must distinguish longitudinal and transverse parts.

3.23.4 Effective Action to Order $\hbar^2$

Let us now find the next correction to the effective action.[19] Instead of truncating the expansion (3.696), we keep all terms, reorganizing only the linear and quadratic terms as in (3.697). This yields

$$e^{(i/\hbar)\{\Gamma[X]+jX\}}=e^{i(\hbar/2)W[j]}=e^{(i/\hbar)\{(\mathcal{A}[x_{\rm cl}]+jx_{\rm cl})+(i\hbar/2)\mathrm{Tr}\log\mathcal{A}_{xx}[x_{\rm cl}]\}}\,e^{(i/\hbar)\hbar^2W_2[x_{\rm cl}]}. \tag{3.717}$$

[19]R. Jackiw, Phys. Rev. D *9*, 1687 (1976)

The functional $W_2[x_{\rm cl}]$ is defined by the path integral over the fluctuations

$$e^{(i/\hbar)\hbar^2 W_2[x_{\rm cl}]} = \frac{\int \mathcal{D}x \exp\frac{i}{\hbar}\left\{\frac{1}{2}\delta x \mathcal{D}[x_{\rm cl}]\delta x + \mathcal{R}[x_{\rm cl},\delta x]\right\}}{\int \mathcal{D}\delta x \exp\frac{i}{\hbar}\left\{\frac{1}{2}\delta x \mathcal{A}_{xx}[x_{\rm cl}]\delta x\right\}}, \tag{3.718}$$

where $\mathcal{D}[x_{\rm cl}] \equiv \mathcal{A}_{xx}[x_{\rm cl}]$ is the second functional derivative of the action at $x = x_{\rm cl}$. The subscripts x of $\mathcal{A}_{xx}$ denote functional differentiation. For the anharmonic oscillator:

$$\mathcal{D}[x_{\rm cl}] \equiv \mathcal{A}_{xx}[x_{\rm cl}] = -\partial_t^2 - \omega^2 - \frac{g}{2}x_{\rm cl}^2. \tag{3.719}$$

The functional $\mathcal{R}$ collects all unharmonic terms:

$$\mathcal{R}[x_{\rm cl},\delta x] = \mathcal{A}[x_{\rm cl}+\delta x] - \mathcal{A}[x_{\rm cl}] - \int dt\, \mathcal{A}_x[x_{\rm cl}](t)\delta x(t) - \frac{1}{2}\int dt dt'\, \delta x(t)\mathcal{A}_{xx}[x_{\rm cl}](t,t')\delta x(t'). \tag{3.720}$$

In condensed functional vector notation, we shall write expressions like the last term as

$$\frac{1}{2}\int dtdt'\, \delta x(t)\mathcal{A}_{xx}[x_{\rm cl}](t,t')\delta x(t') \to \frac{1}{2}\delta x \mathcal{A}_{xx}[x_{\rm cl}]\delta x. \tag{3.721}$$

By construction, $\mathcal{R}$ is at least cubic in δx. The path integral (3.718) may thus be considered as the generating functional $Z^{\rm fl}$ of a fluctuating variable $\delta x(\tau)$ with a propagator

$$\mathcal{G}[x_{\rm cl}] = i\hbar\{\mathcal{A}_{xx}[x_{\rm cl}]\}^{-1} \equiv i\hbar\mathcal{D}^{-1}[x_{\rm cl}],$$

and an interaction $\mathcal{R}[x_{\rm cl},\dot{x}]$, both depending on j via $x_{\rm cl}$. We know from the previous sections, and will immediately see this explicitly, that $\hbar^2 W_2[x_{\rm cl}]$ is of order $\hbar^2$. Let us write the full generating functional $W[j]$ in the form

$$W[j] = \mathcal{A}[x_{\rm cl}] + x_{\rm cl}j + \hbar\Delta_1[x_{\rm cl}], \tag{3.722}$$

where the last term collects one- and two-loop corrections (in higher-order calculations, of course, also higher loops):

$$\Delta_1[x_{\rm cl}] = \frac{i}{2}{\rm Tr}\log\mathcal{D}[x_{\rm cl}] + \hbar W_2[x_{\rm cl}]. \tag{3.723}$$

From (3.722) we find the vacuum expectation value $X = \langle x\rangle$ as the functional derivative

$$X = \frac{\delta W[j]}{\delta j} = x_{\rm cl} + \hbar\Delta_{1x_{\rm cl}}[x_{\rm cl}]\frac{\delta x_{\rm cl}}{\delta j}, \tag{3.724}$$

implying the correction term X_1:

$$X_1 = \Delta_{1x_{\rm cl}}[x_{\rm cl}]\frac{\delta x_{\rm cl}}{\delta j}. \tag{3.725}$$

The only explicit dependence of $W[j]$ on j comes from the second term in (3.722). In all others, the j-dependence is due to $x_{\rm cl}[j]$. We may use this fact to express j as a function of $x_{\rm cl}$. For this we consider $W[j]$ for a moment as a functional of $x_{\rm cl}$:

$$W[x_{\rm cl}] = \mathcal{A}[x_{\rm cl}] + x_{\rm cl}\, j[x_{\rm cl}] + \hbar\Delta_1[x_{\rm cl}]. \tag{3.726}$$

The combination $W[x_{\rm cl}] - jX$ gives us the effective action $\Gamma[X]$ [recall (3.665)]. We therefore express $x_{\rm cl}$ in (3.726) as $X - \hbar X_1 - \mathcal{O}(\hbar^2)$ from (3.701), and re-expand everything around X rather than $x_{\rm cl}$, yields

$$\begin{aligned}\Gamma[X] \;&=\; \mathcal{A}[X] - \hbar\mathcal{A}_X[X]X_1 - \hbar X_1\, j[X] + \hbar^2 X_1\, j_X[X]X_1 + \frac{1}{2}\hbar^2 X_1\,\mathcal{D}[X]X_1\\ &\qquad + \;\hbar\Delta_1[X] - \hbar^2\Delta_{1X}[X]X_1 + \mathcal{O}(\hbar^3).\end{aligned} \tag{3.727}$$

Since the action is extremal at $x_{\rm cl}$, we have

$$\mathcal{A}_X[X - \hbar X_1] = -j[X] + \mathcal{O}(\hbar^2), \tag{3.728}$$

and thus

$$\mathcal{A}_X[X] = -j[X] + \hbar\mathcal{A}_{XX}[X]X_1 + \mathcal{O}(\hbar^2) = -j[X] + \hbar\mathcal{D}[X]X_1 + \mathcal{O}(\hbar^2), \tag{3.729}$$

and therefore:

$$\Gamma[X] \;=\; \mathcal{A}[X] + \hbar\Delta_1[X] + \hbar^2\left\{-\frac{1}{2}X_1\mathcal{D}[X]X_1 + X_1 j_X[X]X_1 - \Delta_{1X}X_1\right\}. \tag{3.730}$$

From (3.725) we see that

$$\frac{\delta j}{\delta x_{\rm cl}}X_1 = \Delta_{1x_{\rm cl}}[x_{\rm cl}]. \tag{3.731}$$

Replacing $x_{\rm cl} \to X$ with an error of order $\hbar$, this implies

$$\frac{\delta j}{\delta X}X = \Delta_{1X}[X] + \mathcal{O}(\hbar). \tag{3.732}$$

Inserting this into (3.730), the last two terms in the curly brackets cancel, and the only remaining $\hbar^2$-terms are

$$-\frac{\hbar^2}{2}X_1\mathcal{D}[X]X_1 + \hbar^2 W_2[X] + \mathcal{O}(\hbar^3). \tag{3.733}$$

From the classical equation of motion (3.671) one has a further equation for $\delta j/\delta x_{\rm cl}$:

$$\frac{\delta j}{\delta x_{\rm cl}} = -\mathcal{A}_{xx}[x_{\rm cl}] = -\mathcal{D}[x_{\rm cl}]. \tag{3.734}$$

Inserting this into (3.725) and replacing again $x_{\rm cl} \to X$, we find

$$X_1 = -\mathcal{D}^{-1}[X]\Delta_{1X}[X] + \mathcal{O}(\hbar). \tag{3.735}$$

We now express $\Delta_{1X}[X]$ via (3.723). This yields

$$\Delta_{1X}[X] = \frac{i}{2}\mathrm{Tr}\left(\mathcal{D}^{-1}[X]\frac{\delta}{\delta X}\mathcal{D}[X]\right) + \hbar W_{2X}[X] + \mathcal{O}(\hbar^2). \tag{3.736}$$

Inserting this into (3.735) and further into (3.730), we find for the effective action the expansion up to the order $\hbar^2$:

$$\begin{aligned}\Gamma[X] &= \mathcal{A}[X] + \hbar\Gamma_1[X] + \hbar^2\Gamma_2[X] \\ &= \mathcal{A}[X] + i\frac{\hbar}{2}\mathrm{Tr}\log\mathcal{D}[X] + \hbar^2 W_2[X] \\ &+ \frac{\hbar^2}{2}\frac{1}{2}\mathrm{Tr}\left(\mathcal{D}^{-1}[X]\frac{\delta}{\delta X}\mathcal{D}[X]\right)\mathcal{D}^{-1}[X]\,\frac{1}{2}\mathrm{Tr}\left(\mathcal{D}^{-1}[X]\frac{\delta}{\delta X}\mathcal{D}[X]\right).\end{aligned} \tag{3.737}$$

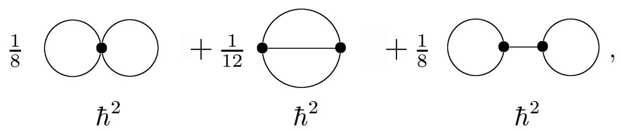
We now calculate $W_2[X]$ to lowest order in $\hbar$. The remainder $\mathcal{R}[X;x]$ in (3.720) has the expansion

$$\mathcal{R}[X;\delta x] = \frac{1}{3!}\mathcal{A}_{XXX}[X]\delta x\,\delta x\,\delta x + \frac{1}{4!}\mathcal{A}_{XXXX}[X]\delta x\,\delta x\,\delta x\,\delta x + \ldots\,. \tag{3.738}$$

Being interested only in the $\hbar^2$-corrections, we have simply replaced $x_{\rm cl}$ by X. In order to obtain $W_2[X]$, we have to calculate all connected vacuum diagrams for the interaction terms in $\mathcal{R}[X;\delta x]$ with a $\delta x(t)$-propagator

$$\mathcal{G}[X] = i\hbar\{\mathcal{A}_{XX}[X]\}^{-1} \equiv i\hbar\mathcal{D}^{-1}[X].$$

Since every contraction brings in a factor $\hbar$, we can truncate the expansion (3.738) after δx^4. Thus, the only contributions to $i\hbar W_2[X]$ come from the connected vacuum diagrams



(3.739)

where a line stands now for $\mathcal{G}[X]$, a four-vertex for

$$(i/\hbar)\mathcal{A}_{XXXX}[X] = (i/\hbar)\mathcal{D}_{XX}[X], \tag{3.740}$$

and a three-vertex for

$$(i/\hbar)\mathcal{A}_{XXX}[X] = (i/\hbar)\mathcal{D}_X[X]. \tag{3.741}$$

Only the first two diagrams are one-particle irreducible. As a pleasant result, the third diagram which is one-particle reducible cancels with the last term in (3.737). To see this we write that term more explicitly as

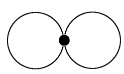
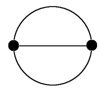
$$\frac{\hbar^2}{8}\mathcal{D}^{-1}_{X_1X_2}\mathcal{A}_{X_1X_2X_3}\mathcal{D}^{-1}_{X_3X_{3'}}\mathcal{A}_{X_{3'}X_{1'}X_{2'}}\mathcal{D}^{-1}_{X_{1'}X_{2'}}, \tag{3.742}$$

which corresponds precisely to the third diagram in $\Gamma_2[X]$, except for an opposite sign. Note that the diagram has a multiplicity 9.

Thus, at the end, only the one-particle irreducible vacuum diagrams contribute to the $\hbar^2$-correction to $\Gamma[X]$:

$$i\Gamma_2[X] = i\frac{3}{4!}\mathcal{D}_{12}^{-1}\mathcal{A}_{X_1X_2X_3X_4}\mathcal{D}_{34}^{-1} + i\frac{1}{4!2}\mathcal{A}_{X_1X_2X_3}\mathcal{D}_{X_1X_{1'}}^{-1}\mathcal{D}_{X_2X_{2'}}^{-1}\mathcal{D}_{X_3X_{3'}}^{-1}\mathcal{A}_{X_1X_2X_3}. \tag{3.743}$$

Their diagrammatic representation is

$\frac{i}{\hbar}\hbar^2\Gamma_2[X] = \frac{1}{8}$  $+\frac{1}{12}$  . (3.744)

$\hbar^2$ $\hbar^2$

The one-particle irreducible nature of the diagrams is found to all orders in $\hbar$.

3.23.5 Finite-Temperature Two-Loop Effective Action

At finite temperature, and in D dimensions, the expansion proceeds with the imaginary-time versions of the **X**-dependent Green functions (3.690) and (3.691)

$$\mathcal{G}_L(\tau_1,\tau_2) = \frac{\hbar}{2M\omega_L}\frac{\cosh(\omega_L|\tau_1-\tau_2| - \hbar\beta\omega_L/2)}{\sinh(\hbar\beta\omega_L/2)}, \tag{3.745}$$

and

$$\mathcal{G}_T(\tau_1,\tau_2) = \frac{\hbar}{2M\omega_T}\frac{\cosh(\omega_T|\tau_1-\tau_2| - \hbar\beta\omega_T/2)}{\sinh(\hbar\beta\omega_T/2)}, \tag{3.746}$$

where we have omitted the argument $\mathbf{X}$ in $\omega_L(\mathbf{X})$ and $\omega_T(\mathbf{X})$. Treating here the general rotationally symmetric potential $V(\mathbf{x}) = v(x)$, $x = \sqrt{\mathbf{x}^2}$, the two frequencies are

$$\omega_L^2(\mathbf{X}) \equiv \frac{1}{M}v''(X), \quad \omega_T^2(\mathbf{X}) \equiv \frac{1}{MX}v'(X). \tag{3.747}$$

We also decompose the vertex functions into longitudinal and transverse parts. The three-point vertex is a sum

$$\frac{\partial^3 v(X)}{\partial X_i \partial X_j \partial X_k} = P^L_{ijk}v'''(X) + P^T_{ijk}\left[\frac{v''(X)}{X} - \frac{v'(X)}{X^2}\right], \tag{3.748}$$

with the symmetric tensors

$$P^L_{ijk} \equiv \frac{X_iX_jX_k}{X^3} \quad \text{and} \quad P^T_{ijk} \equiv \delta_{ij}\frac{X_k}{X} + \delta_{ik}\frac{X_j}{X} + \delta_{jk}\frac{X_i}{X} - 3P^L_{ijk}. \tag{3.749}$$

The four-point vertex reads

$$\frac{\partial^4 v(X)}{\partial X_i \partial X_j \partial X_k \partial X_l} = P^L_{ijkl}v^{(4)}(X) + P^T_{ijkl}\frac{v'''(X)}{X} + P^S_{ijkl}\left[\frac{v''(X)}{X^2} - \frac{v'(X)}{X^3}\right], \tag{3.750}$$

with the symmetric tensors

$$P^L_{ijkl} = \frac{X_iX_jX_kX_l}{X^4}, \tag{3.751}$$

$$P^T_{ijkl} = \delta_{ij}\frac{X_kX_l}{X^2} + \delta_{ik}\frac{X_jX_l}{X^2} + \delta_{il}\frac{X_jX_k}{X^2} + \delta_{jk}\frac{X_iX_l}{X^2} + \delta_{jl}\frac{X_iX_k}{X^2} + \delta_{kl}\frac{X_iX_k}{X^2} - 6P^L_{ijkl}, \tag{3.752}$$

$$P^S_{ijkl} = \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - 3P^L_{ijkl} - 3P^T_{ijkl}. \tag{3.753}$$

The tensors obey the following relations:

$$\frac{X_i}{X}P^L_{ijk} = P^L_{jk}\,, \qquad \frac{X_i}{X}P^T_{ijk} = P^T_{jk}\,, \tag{3.754}$$

$$P^L_{ij}P^L_{ikl} = P^L_{jkl},\;\; P^T_{ij}P^T_{ikl} = \frac{X_k}{X}P^T_{jl} + \frac{X_l}{X}P^T_{jk},\;\; P^L_{ij}P^T_{ikl} = \frac{X_j}{X}P^T_{kl},\;\; P^T_{ij}P^L_{ikl} = 0, \tag{3.755}$$

$$P^L_{hij}P^L_{hkl} = P^L_{ijkl}, \quad P^T_{hij}P^T_{hkl} = P^T_{ij}P^T_{kl} + P^L_{ik}P^T_{jl} + P^L_{il}P^T_{jk} + P^L_{jk}P^T_{il} + P^L_{jl}P^T_{ik}, \tag{3.756}$$

$$P^L_{hij}P^T_{hkl} = P^L_{ij}P^T_{kl},\;\; P^T_{hij}P^L_{hkl} = P^T_{ij}P^L_{kl},\;\; P^L_{ij}P^L_{ijkl} = P^L_{kl},\;\; P^T_{ij}P^T_{ijkl} = (D-1)P^L_{kl}, \tag{3.757}$$

$$P^L_{ij}P^T_{ijkl} = P^T_{kl}, \qquad P^T_{ij}P^L_{ijkl} = 0\,, \tag{3.758}$$

$$P^L_{ij}P^S_{ijkl} = -2P^T_{kl},\;\; P^T_{ij}P^S_{ijkl} = (D+1)P^T_{kl} - 2(D-1)P^L_{kl}. \tag{3.759}$$

Instead of the effective action, the diagrammatic expansion (3.744) yields now the free energy

$$(i/\hbar)\Gamma[\mathbf{X}] \to -\beta F(\mathbf{X}). \tag{3.760}$$

Using the above formulas we obtain immediately the mean field contribution to the free energy

$$-\beta F_{\rm MF} = -\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{\mathbf{X}}^2 + v(X)\right], \tag{3.761}$$

and the one-loop contribution [from the trace-log term in Eq. (3.737)]:

$$-\beta F_{1-\rm loop} = -\log\left[2\sinh(\hbar\beta\omega_L/2)\right] - (D-1)\log\left[2\sinh(\hbar\beta\omega_T/2)\right]. \tag{3.762}$$

The first of the two-loop diagrams in (3.744) yields the contribution to the free energy

$$\begin{aligned}-\beta\Delta_1 F_{2-\rm loop} = -\beta\Bigg\{&\mathcal{G}^2_L(\tau,\tau)v^{(4)}(X) + (D^2-1)\,\mathcal{G}^2_T(\tau,\tau)\left[\frac{v''(X)}{X^2} - \frac{v'(X)}{X^3}\right]\\ &+ 2(D-1)\mathcal{G}_L(\tau,\tau)\mathcal{G}_T(\tau,\tau)\left[\frac{v'''(X)}{X} - \frac{2v''(X)}{X^2} + \frac{2v'(X)}{X^3}\right]\Bigg\}.\end{aligned} \tag{3.763}$$

From the second diagram we obtain the contribution

$$\begin{aligned}-\beta\Delta_2 F_{2-\rm loop} = \frac{1}{\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \Bigg\{&\mathcal{G}^3_L(\tau_1,\tau_2)\left[v'''(X)\right]^2\\ &+ 3(D-1)\mathcal{G}_L(\tau_1,\tau_2)\mathcal{G}^2_T(\tau_1,\tau_2)\left[\frac{v''(X)}{X} - \frac{v'(X)}{X^2}\right]^2\Bigg\}.\end{aligned} \tag{3.764}$$

The explicit evaluation yields

$$\begin{aligned}-\beta\Delta_1 F_{2-\rm loop} = -\frac{\hbar^2\beta}{(2M)^2}\Bigg\{&\frac{1}{\omega_L^2}\coth^2(\hbar\beta\omega_L/2)v^{(4)}(X)\\ &+\frac{D^2-1}{\omega_T^2}\coth^2(\hbar\beta\omega_T/2)\left[\frac{v''(X)}{X^2} - \frac{v'(X)}{X^3}\right]\\ &+\frac{2(D-1)}{\omega_L\omega_T}\coth(\hbar\beta\omega_L/2)\coth(\hbar\beta\omega_T/2)\left[\frac{v'''(X)}{X} - \frac{2v''(X)}{X^2} + \frac{2v'(X)}{X^3}\right]\Bigg\}.\end{aligned} \tag{3.765}$$

and

$$\begin{aligned}-\beta\Delta_2 F_{2-\rm loop} = &\frac{2\hbar^2\beta}{\omega_L}\frac{1}{(2M\omega_L)^3}\left[v'''(X)\right]^2\left[\frac{1}{3} + \frac{1}{\sinh^2(\hbar\beta\omega_L/2)}\right]\\ &+\frac{6\hbar^2\beta(D-1)}{2\omega_T+\omega_L}\frac{1}{2M\omega_L}\frac{1}{(2M\omega_T)^2}\left[\frac{v''(X)}{X} - \frac{v'(X)}{X^2}\right]^2\\ &\times\left[\coth^2(\hbar\beta\omega_T/2) + \frac{\omega_T}{\omega_L}\frac{1}{\sinh^2(\hbar\beta\omega_T/2)} + \frac{\omega_T}{2\omega_T-\omega_L}\frac{\sinh[\hbar\beta(2\omega_T-\omega_L)/2]}{\sinh(\hbar\beta\omega_L/2)\sinh^2(\hbar\beta\omega_T/2)}\right].\end{aligned} \tag{3.766}$$

In the limit of zero temperature, the effective potential in the free energy becomes

$$
\begin{aligned}
V_{\rm eff}(X) \underset{T\to 0}{=} & \; v(X) + \frac{\hbar\omega_L}{2} + (D-1)\frac{\hbar\omega_T}{2} + \frac{\hbar^2}{8(2M)^2}\left\{\frac{1}{\omega_L^2}v^{(4)}(X)\right. \\
& \left. + \frac{D^2-1}{\omega_T^2}\left[\frac{v''(X)}{X^2} - \frac{v'(X)}{X^3}\right] + \frac{2(D-1)}{\omega_L\omega_T}\left[\frac{v'''(X)}{X} - \frac{2v''(X)}{X^2} + \frac{2v'(X)}{X^3}\right]\right\} \\
& - \frac{\hbar^2}{6(2M)^3}\left\{\frac{1}{3\omega_L^4}[v'''(X)]^2 + \frac{3(D-1)}{2\omega_T+\omega_L}\frac{1}{\omega_L\omega_T^2}\left[\frac{v''(X)}{X} - \frac{v'(X)}{X^2}\right]^2\right\} + \mathcal{O}(\hbar^3). \qquad (3.767)
\end{aligned}
$$

For the one-dimensional potential

$$
V(x) = \frac{M}{2}\omega^2 x^2 + \frac{g_3}{3!}x^3 + \frac{g_4}{4!}x^4\,, \qquad (3.768)
$$

the effective potential becomes, up to two loops,

$$
\begin{aligned}
V_{\rm eff}(X) = & \; \frac{M}{2}\omega^2X^2 + g_3X^3 + g_4X^4 + \frac{1}{\beta}\log\left(2\sinh\hbar\beta\omega/2\right) + \hbar^2\frac{g_4}{8(2M\omega)^2}\frac{1}{\tanh^2(\hbar\beta\omega/2)} \\
& - \frac{\hbar^2}{6\omega}\frac{(g_3+g_4X)^2}{(2M\omega)^3}\left[\frac{1}{3} + \frac{1}{\sinh^2(\hbar\beta\omega/2)}\right] + \mathcal{O}(\hbar^3)\,, \qquad (3.769)
\end{aligned}
$$

whose $T \to 0$ limit is

$$
\begin{aligned}
V_{\rm eff}(X) \underset{T\to 0}{=} & \; \frac{M}{2}\omega^2X^2 + \frac{g_3}{3!}X^3 + \frac{g_4}{4!}X^4 + \frac{\hbar\omega}{2} + \hbar^2\frac{g_4}{8(2M\omega)^2} \\
& - \frac{\hbar^2}{18\omega}\frac{(g_3+g_4X)^2}{(2M\omega)^3} + \mathcal{O}(\hbar^3)\,. \qquad (3.770)
\end{aligned}
$$

If the potential is a polynomial in $\mathbf{X}$, the effective potential at zero temperature can be solved more efficiently than here and to much higher loop orders with the help of recursion relations. This will be shown in Appendix 3C.5.

3.23.6 Background Field Method for Effective Action

In order to find the rules for the loop expansion to any order, let us separate the total effective action into a sum of the classical action $\mathcal{A}[\mathbf{X}]$ and a term $\Gamma^{\rm fl}[\mathbf{X}]$ which collects the contribution of all quantum fluctuations:

$$
\Gamma[\mathbf{X}] = \mathcal{A}[\mathbf{X}] + \Gamma^{\rm fl}[\mathbf{X}]. \qquad (3.771)
$$

To calculate the fluctuation part $\Gamma^{\rm fl}[\mathbf{X}]$, we expand the paths $\mathbf{x}(t)$ around some arbitrarily chosen background path $\mathbf{X}(t)$:[20]

$$
\mathbf{x}(t) = \mathbf{X}(t) + \delta\mathbf{x}(t), \qquad (3.772)
$$

and calculate the generating functional $W[\mathbf{j}]$ by performing the path integral over the fluctuations:

$$
\exp\left\{\frac{i}{\hbar}W[\mathbf{j}]\right\} = \int \mathcal{D}\delta\mathbf{x}\,\exp\left\{\frac{i}{\hbar}\Big(\mathcal{A}\left[\mathbf{X}+\delta\mathbf{x}\right] + \mathbf{j}[\mathbf{X}](\mathbf{X}+\delta\mathbf{x})\Big)\right\}. \qquad (3.773)
$$

[20]In the theory of fluctuating fields, this is replaced by a more general *background field* which explains the name of the method.

From $W[\mathbf{j}]$ we find a $\mathbf{j}$-dependent expectation value $\mathbf{X}^{\mathbf{j}} = \langle \mathbf{x} \rangle^{\mathbf{j}}$ as $\mathbf{X}^{\mathbf{j}} = \delta W[\mathbf{j}]/\delta \mathbf{j}$, and the Legendre transform $\Gamma[\mathbf{X}] = W[\mathbf{j}] - \mathbf{j}\mathbf{X}^{\mathbf{j}}$. In terms of $\mathbf{X}^{\mathbf{j}}$, Eq. (3.773) can be rewritten as

$$\exp\left\{\frac{i}{\hbar}\left(\Gamma[\mathbf{X}^{\mathbf{j}}] + \mathbf{j}[\mathbf{X}^{\mathbf{j}}]\,\mathbf{X}^{\mathbf{j}}\right)\right\} = \int \mathcal{D}\delta\mathbf{x}\,\exp\left\{\frac{i}{\hbar}\Big(\mathcal{A}\,[\mathbf{X}+\delta\mathbf{x}] + \mathbf{j}[\mathbf{X}](\mathbf{X}+\delta\mathbf{x})\Big)\right\}. \quad (3.774)$$

The expectation value $\mathbf{X}^{\mathbf{j}}$ has the property of extremizing $\Gamma[\mathbf{X}]$, i.e., it satisfies the equation

$$\mathbf{j} = -\left.\frac{\delta\Gamma[\mathbf{X}]}{\partial\mathbf{X}}\right|_{\mathbf{X}=\mathbf{X}^{\mathbf{j}}} = -\Gamma_{\mathbf{X}}[\mathbf{X}^{\mathbf{j}}]. \quad (3.775)$$

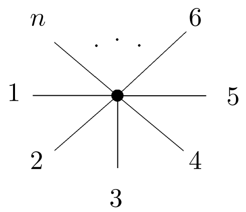
We now choose $\mathbf{j}$ in such a way that $\mathbf{X}^{\mathbf{j}}$ equals the initially chosen $\mathbf{X}$, and find

$$\exp\left\{\frac{i}{\hbar}\Gamma[\mathbf{X}]\right\} = \int \mathcal{D}\delta\mathbf{x}\,\exp\left(\frac{i}{\hbar}\Big\{\mathcal{A}\,[\mathbf{X}+\delta\mathbf{x}] - \Gamma_{\mathbf{X}}[\mathbf{X}]\delta\mathbf{x}\Big\}\right). \quad (3.776)$$

This is a functional integro-differential equation for the effective action $\Gamma[\mathbf{X}]$ which we can solve perturbatively order by order in $\hbar$. This is done diagrammatically. The diagrammatic elements are lines representing the propagator (3.689)

$$\text{———} = \mathcal{G}_{ab}[\mathbf{X}] \equiv i\hbar\left[\frac{\delta^2\mathcal{A}[\mathbf{X}]}{\delta X_a \delta X_b}\right]^{-1}_{ab}, \quad (3.777)$$

and vertices



$$= \frac{\delta^n \mathcal{A}[\mathbf{X}]}{\delta X_{a_1}\delta X_{a_2}\dots\delta X_{a_n}}. \quad (3.778)$$

From the explicit calculations in the last two subsections we expect the effective action to be the sum of all one-particle irreducible vacuum diagrams formed with these propagators and vertices. This will now be proved to all orders in perturbation theory.

We introduce an auxiliary generating functional $\tilde{W}\left[\mathbf{X}, \tilde{\mathbf{j}}\right]$ which governs the correlation functions of the fluctuations $\delta\mathbf{x}$ around the above fixed backgound $\mathbf{X}$:

$$\exp\left\{i\tilde{W}\left[\mathbf{X},\tilde{\mathbf{j}}\right]/\hbar\right\} \equiv \int \mathcal{D}\delta\mathbf{x}\,\exp\left(\frac{i}{\hbar}\left\{\tilde{\mathcal{A}}\,[\mathbf{X},\delta\mathbf{x}] + \int dt\,\tilde{\mathbf{j}}(t)\,\delta\mathbf{x}(t)\right\}\right), \quad (3.779)$$

with the action of fluctuations

$$\tilde{\mathcal{A}}[\mathbf{X},\delta\mathbf{x}] = \mathcal{A}[\mathbf{X}+\delta\mathbf{x}] - \mathcal{A}[\mathbf{X}] - \mathcal{A}_{\mathbf{X}}[\mathbf{X}]\delta\mathbf{x}, \quad (3.780)$$

whose expansion in powers of $\delta\mathbf{x}(t)$ starts out with a quadratic term. A source $\tilde{\mathbf{j}}(t)$ is coupled to the fluctuations $\delta\mathbf{x}(t)$. By comparing (3.779) with (3.776) we see that for the special choice of the current

$$\tilde{\mathbf{j}} = -\Gamma_{\mathbf{X}}[\mathbf{X}] + \mathcal{A}_{\mathbf{X}}[\mathbf{X}] = -\tilde{\Gamma}_{\mathbf{X}}[\mathbf{X}], \tag{3.781}$$

the right-hand sides coincide, such that the auxiliary functional $\tilde{W}[\mathbf{X},\tilde{\mathbf{j}}]$ contains precisely the diagrams in $\Gamma^{\mathrm{fl}}[\mathbf{X}]$ which we want to calculate. We now form the Legendre transform of $\tilde{W}[\mathbf{X},\tilde{\mathbf{j}}]$, which is an auxiliary effective action with two arguments:

$$\tilde{\Gamma}\left[\mathbf{X},\tilde{\mathbf{X}}\right] \equiv \tilde{W}[\mathbf{X},\tilde{\mathbf{j}}] - \int dt\,\tilde{\mathbf{j}}\,\tilde{\mathbf{X}}, \tag{3.782}$$

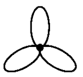
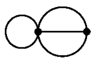
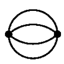
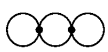
with the auxiliary conjugate variable

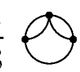
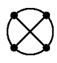
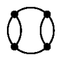
$$\tilde{\mathbf{X}} = \frac{\delta \tilde{W}[\mathbf{X},\tilde{\mathbf{j}}]}{\delta\tilde{\mathbf{j}}} = \tilde{\mathbf{X}}[\mathbf{X},\tilde{\mathbf{j}}]. \tag{3.783}$$

This is the expectation value of the fluctuations $\langle\delta\mathbf{x}\rangle$ in the path integral (3.779). If $\tilde{\mathbf{j}}$ has the value (3.781), this expectation vanishes, i.e. $\tilde{\mathbf{X}} = 0$. The auxiliary action $\tilde{\Gamma}\left[\mathbf{X},\mathbf{0}\right]$ coincides with the fluctuating part $\Gamma^{\mathrm{fl}}[\mathbf{X}]$ of the effective action which we want to calculate.

The functional derivatives of $\tilde{W}[\mathbf{X},\tilde{\mathbf{j}}]$ with respect to $\tilde{\mathbf{j}}$ yield all connected correlation functions of the fluctuating variables $\delta\mathbf{x}(t)$. The functional derivatives of $\tilde{\Gamma}\left[\mathbf{X},\tilde{\mathbf{X}}\right]$ with respect to $\tilde{\mathbf{X}}$ select from these the one-particle irreducible correlation functions. For $\tilde{\mathbf{X}} = 0$, only vacuum diagrams survive.

Thus we have proved that the full effective action is obtained from the sum of the classical action $\Gamma_0[\mathbf{X}] = \mathcal{A}[\mathbf{X}]$, the one-loop contribution $\Gamma_1[\mathbf{X}]$ given by the trace of the logarithm in Eq. (3.705), the two-loop contribution $\Gamma_2[\mathbf{X}]$ in (3.744), and the sum of all connected one-particle irreducible vacuum diagrams with more than two loops

$\frac{i}{\hbar}\sum_{n\geq 3} i\hbar^n\Gamma_n[\mathbf{X}] = \frac{1}{8}$  $+\frac{1}{12}$  $+\frac{1}{48}$  $+\frac{1}{16}$ 

$+\frac{1}{8}$  $+\frac{1}{8}$  $+\frac{1}{24}$  $+\frac{1}{16}$  $.$ (3.784)

Observe that in the expansion of $\Gamma[X]/\hbar$, each line carries a factor $\hbar$, whereas each n-point vertex contributes a factor $\hbar^{-1}$. The contribution of an n-loop diagram to $\Gamma[X]$ is therefore of order $\hbar^n$. The higher-loop diagrams are most easily generated by a recursive treatment of the type developed in Subsection 3.22.3.

For a harmonic oscillator, the expansion stops after the trace of the logarithm (3.705), and reads simply, in one dimension:

$$\begin{aligned}\Gamma[X] &= \mathcal{A}[X] + \frac{i}{2}\hbar\,\mathrm{Tr}\log\Gamma^{(2)}(t_b,t_a)\\ &= \int_{t_a}^{t_b} dt\left[\frac{M}{2}\dot{X}^2 - \frac{M\omega^2}{2}X^2\right] + \frac{i}{2}\hbar\,\mathrm{Tr}\log\left(-\partial_t^2-\omega^2\right).\end{aligned} \tag{3.785}$$

Evaluating the trace of the logarithm we find for a constant X the effective potential (3.666):

$$V^{\rm eff}(X) = V(X) - \frac{i}{2(t_b - t_a)} \log\{2\pi i \sin[\omega(t_b - t_a)] / M\omega\}. \tag{3.786}$$

If the boundary conditions are periodic, so that the analytic continuation of the result can be used for quantum statistical calculations, the result is

$$V^{\rm eff}(X) = V(X) - \frac{i}{(t_b - t_a)} \log\{2i \sin[\omega(t_b - t_a)/2]\}. \tag{3.787}$$

It is important to keep in mind that a line in the above diagrams contains an infinite series of fundamental Feynman diagrams of the original perturbation expansion, as can be seen by expanding the denominators in the propagator $\mathcal{G}_{ab}$ in Eqs. (3.689)–(3.691) in powers of $\mathbf{X}^2$. This expansion produces a sum of diagrams which can be obtained from the loop diagrams in the expansion of the trace of the logarithm in (3.710) by cutting the loop.

If the potential is a polynomial in $\mathbf{X}$, the effective potential at zero temperature can be solved most efficiently to high loop orders with the help of recursion relations. This is shown in detail in Appendix 3C.5.

3.24 Nambu-Goldstone Theorem

The appearance of a zero-frequency mode as a consequence of a nonzero expectation value $\mathbf{X}$ can easily be proved for any continuous symmetry and to all orders in perturbation theory by using the full effective action. To be more specific we consider as before the case of O(N)-symmetry, and perform infinitesimal symmetry transformations on the currents $\mathbf{j}$ in the generating functional $W[\mathbf{j}]$:

$$j_a \to j_a - i\epsilon_{cd} \left(L_{cd}\right)_{ab} j_b, \tag{3.788}$$

where L_{cd} are the $N(N-1)/2$ generators of O(N)-rotations with the matrix elements

$$(L_{cd})_{ab} = i\left(\delta_{ca}\delta_{db} - \delta_{da}\delta_{cb}\right), \tag{3.789}$$

and ϵ_{ab} are the infinitesimal angles of the rotations. Under these, the generating functional is assumed to be invariant:

$$\delta W[\mathbf{j}] = 0 = \int dt\, \frac{\delta W[\mathbf{j}]}{\delta j_a(x)} i \left(L_{cd}\right)_{ab} j_b \epsilon_{cd} = 0. \tag{3.790}$$

Expressing the integrand in terms of Legendre-transformed quantities via Eqs. (3.623) and (3.625), we obtain

$$\int dt X_a(t) i \left(L_{cd}\right)_{ab} \frac{\delta\Gamma[\mathbf{X}]}{\delta X_b(t)} \epsilon_{cd} = 0. \tag{3.791}$$

This expresses the infinitesimal invariance of the effective action $\Gamma[\mathbf{X}]$ under infinitesimal rotations

$$X_a \to X_a - i\epsilon_{cd} \left(L_{cd}\right)_{ab} X_b.$$

The invariance property (3.791) is called the *Ward-Takakashi identity* for the functional $\Gamma[\mathbf{X}]$. It can be used to find an infinite set of equally named identities for all vertex functions by forming all $\Gamma[\mathbf{X}]$ functional derivatives of $\Gamma[\mathbf{X}]$ and setting $\mathbf{X}$ equal to the expectation value at the minimum of $\Gamma[\mathbf{X}]$. The first derivative of $\Gamma[\mathbf{X}]$ gives directly from (3.791) (dropping the infinitesimal parameter ϵ_{cd})

$$\begin{aligned} \left(L_{cd}\right)_{ab} j_b(t) &= \left(L_{cd}\right)_{ab} \frac{\delta\Gamma[\mathbf{X}]}{\delta X(t)_b} \\ &= -\int dt' X_{a'}(t') \left(L_{cd}\right)_{a'b} \frac{\delta^2\Gamma[\mathbf{X}]}{\delta X_b(t')\delta X_n(t)}. \end{aligned} \tag{3.792}$$

Denoting the expectation value at the minimum of the effective potential by $\bar{\mathbf{X}}$, this yields

$$\int dt' \bar{X}_{a'}(t') \left(L_{cd}\right)_{a'b} \left. \frac{\delta^2\Gamma[\mathbf{X}]}{\delta X_b(t')\delta X_a(t)} \right|_{\mathbf{X}(t)=\bar{\mathbf{X}}} = 0. \tag{3.793}$$

Now the second derivative is simply the vertex function $\Gamma^{(2)}(t',t)$ which is the functional inverse of the correlation function $G^{(2)}(t',t)$. The integral over t selects the zero-frequency component of the Fourier transform

$$\tilde{\Gamma}^{(2)}(\omega') \equiv \int dt'\, e^{i\omega' t}\Gamma^{(2)}(t',t). \tag{3.794}$$

If we define the Fourier components of $\Gamma^{(2)}(t',t)$ accordingly, we can write (3.793) in Fourier space as

$$X^0_{a'} \left(L_{cd}\right)_{a'b} \tilde{G}^{-1}_{ba}(\omega' = 0) = 0. \tag{3.795}$$

Inserting the matrix elements (3.789) of the generators of the rotations, this equation shows that for $\bar{\mathbf{X}} \neq 0$, the fully interacting transverse propagator has to possess a singularity at $\omega' = 0$. In quantum field theory, this implies the existence of $N-1$ massless particles, the Nambu-Goldstone boson. The conclusion may be drawn only if there are no massless particles in the theory from the outset, which may be "eaten up" by the Nambu-Goldstone boson, as explained earlier in the context of Eq. (3.691).

As mentioned before at the end of Subsection 3.23.1, the Nambu-Goldstone theorem does not have any consequences for quantum mechanics since fluctuations are too violent to allow for the existence of a nonzero expectation value $\mathbf{X}$. The effective action calculated to any finite order in perturbation theory, however, is incapable of reproducing this physical property and does have a nonzero extremum and ensuing transverse zero-frequency modes.

3.25 Effective Classical Potential

The loop expansion of the effective action $\Gamma[X]$ in (3.771), consisting of the trace of the logarithm (3.705) and the one-particle irreducible diagrams (3.744), (3.784) and the associated effective potential $V(X)$ in Eq. (3.666), can be continued in a straightforward way to imaginary times setting $t_b - t_a \to -i\hbar\beta$ to form the Euclidean effective potential $\Gamma_{\rm e}[X]$. For the harmonic oscillator, where the expansion stops after the trace of the logarithm and the effective potential reduces to the simple expression (3.785), we find the imaginary-time version

$$V^{\rm eff}(X) = V(X) + \frac{1}{\beta}\log\left(2\sinh\frac{\beta\hbar\omega}{2}\right). \tag{3.796}$$

Since the effective action contains the effect of all fluctuations, the minimum of the effective potential $V(X)$ should yield directly the full quantum statistical partition function of a system:

$$Z = \exp[-\beta V(X)\Big|_{\rm min}]. \tag{3.797}$$

Inserting the harmonic oscillator expression (3.796) we find indeed the correct result (2.407).

For anharmonic systems, we expect the loop expansion to be able to approximate $V(X)$ rather well to yield a good approximation for the partition function via Eq. (3.797). It is easy to realize that this cannot be true. We have shown in Section 2.9 that for high temperatures, the partition function is given by the integral [recall (2.353)]

$$Z_{\rm cl} = \int_{-\infty}^{\infty}\frac{dx}{l_{\rm e}(\hbar\beta)}e^{-V(x)/k_BT}. \tag{3.798}$$

This integral can in principle be treated by the same background field method as the path integral, albeit in a much simpler way. We may write $x = X + \delta x$ and find a loop expansion for an effective potential. This expansion evaluated at the extremum will yield a good approximation to the integral (3.798) only if the potential is very close to a harmonic one. For any more complicated shape, the integral at small β will cover the entire range of x and can therefore only be evaluated numerically. Thus we can never expect a good result for the partition function of anharmonic systems at high temperatures, if it is calculated from Eq. (3.797).

It is easy to find the culprit for this problem. In a one-dimensional system, the correlation functions of the fluctuations around X are given by the correlation function [compare (3.304), (3.251), and (3.690)]

$$\begin{aligned}\langle\delta x(\tau)\delta x(\tau')\rangle &= G^{(2)}_{\Omega^2(X)}(\tau,\tau') = \frac{\hbar}{M}G^{\rm p}_{\Omega^2(X),{\rm e}}(\tau-\tau')\\ &= \frac{\hbar}{M}\frac{1}{2\Omega(X)}\frac{\cosh\Omega(X)(|\tau-\tau'|-\hbar\beta/2)}{\sinh[\Omega(X)\hbar\beta/2]}, \quad |\tau-\tau'|\in[0,\hbar\beta], \end{aligned}\tag{3.799}$$

with the X-dependent frequency given by

$$\Omega^2(X) = \omega^2 + 3\,\frac{g}{6}X^2. \tag{3.800}$$

At equal times $\tau = \tau'$, this specifies the square width of the fluctuations $\delta x(\tau)$:

$$\left\langle [\delta x(\tau)]^2 \right\rangle = \frac{\hbar}{M}\frac{1}{2\Omega(X)}\coth\frac{\Omega(X)\hbar\beta}{2}. \tag{3.801}$$

The point is now that for large temperatures T, this width grows linearly in T

$$\left\langle [\delta x(\tau)]^2 \right\rangle \xrightarrow{T\to\infty} \frac{k_BT}{M\Omega^2}. \tag{3.802}$$

The linear behavior follows the historic *Dulong-Petit law* for the classical fluctuation width of a harmonic oscillator [compare with the Dulong-Petit law (2.603) for the thermodynamic quantities]. It is a direct consequence of the *equipartition theorem* for purely thermal fluctuations, according to which the potential energy has an average $k_BT/2$:

$$\frac{M\Omega^2}{2}\left\langle x^2 \right\rangle = \frac{k_BT}{2}. \tag{3.803}$$

If we consider the spectral representation (3.248) of the correlation function,

$$G^{\rm p}_{\Omega^2,{\rm e}}(\tau-\tau') = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\frac{1}{\omega_m^2+\Omega^2}e^{-i\omega_m(\tau-\tau')}, \tag{3.804}$$

we see that the linear growth is entirely due to term with zero Matsubara frequency.

The important observation is now that if we remove this zero frequency term from the correlation function and form the *subtracted correlation function* [recall (3.253)]

$$G^{\rm p\prime}_{\Omega^2,{\rm e}}(\tau) \equiv G^{\rm p}_{\Omega^2,{\rm e}}(\tau) - \frac{1}{\hbar\beta\Omega^2} = \frac{1}{2\Omega}\frac{\cosh\Omega(|\tau|-\hbar\beta/2)}{\sinh[\Omega\hbar\beta/2]} - \frac{1}{\hbar\beta\Omega^2}, \tag{3.805}$$

we see that the subtracted square width

$$a_\Omega^2 \equiv G^{\rm p\prime}_{\Omega^2,{\rm e}}(0) = \frac{1}{2\Omega}\coth\frac{\Omega\hbar\beta}{2} - \frac{1}{\hbar\beta\Omega^2} \tag{3.806}$$

decrease for large T. This is shown in Fig. 3.14. Due to this decrease, there exists a method to substantially improve perturbation expansions with the help of the so-called effective classical potential.

3.25.1 Effective Classical Boltzmann Factor

The above considerations lead us to the conclusion that a useful approximation for partition function can be obtained only by expanding the path integral in powers of

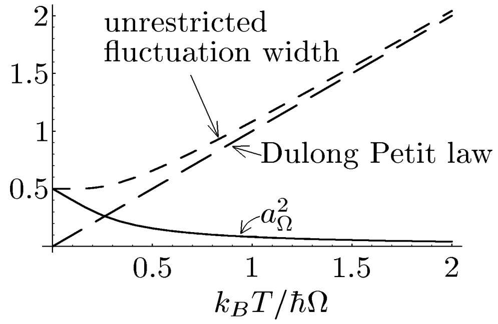


Figure 3.14 Local fluctuation width compared with the unrestricted fluctuation width of harmonic oscillator and its linear Dulong-Petit approximation. The vertical axis shows units of $\hbar/M\Omega$, a quantity of dimension length^2.

the subtracted fluctuations $\delta' x(\tau)$ which possess no zero Matsubara frequency. The quantity which is closely related to the effective potential $V^{\rm eff}(X)$ in Eq. (3.666) but allows for a more accurate evaluation of the partition function is the *effective classical potential* $V^{\rm eff\,cl}(x_0)$. Just as $V^{\rm eff}(X)$, it contains the effects of *all* quantum fluctuations, but it keeps separate track of the thermal fluctuations which makes it a convenient tool for numerical treatment of the partition function. The definition starts out similar to the background method in Subsection 3.23.6 in Eq. (3.772). We split the paths as in Eq. (2.443) into a time-independent constant background x_0 and a fluctuation $\eta(\tau)$ with zero temporal average $\bar\eta = 0$:

$$x(\tau) = x_0 + \eta(\tau) \equiv x_0 + \sum_{m=1}^{\infty} \left(x_m e^{i\omega_m \tau} + \text{c.c.} \right), \qquad x_0 = \text{real}, \qquad x_{-m} \equiv x_m^*, \tag{3.807}$$

and write the partition function using the measure (2.448) as

$$Z = \oint \mathcal{D}x\, e^{-\mathcal{A}_{\rm e}/\hbar} = \int_{-\infty}^{\infty} \frac{dx_0}{l_{\rm e}(\hbar\beta)} \oint \mathcal{D}'x\, e^{-\mathcal{A}_{\rm e}/\hbar}, \tag{3.808}$$

where

$$\oint \mathcal{D}'x\, e^{-\mathcal{A}_{\rm e}/\hbar} = \prod_{m=1}^{\infty} \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\,{\rm Re}\, x_m\, d\,{\rm Im}\, x_m}{\pi k_B T / M\omega_m^2} \right] e^{-\mathcal{A}_{\rm e}/\hbar}. \tag{3.809}$$

Comparison of (2.447) with the integral expression (2.352) for the classical partition function $Z_{\rm cl}$ suggests writing the path integral over the components with nonzero Matsubara frequencies as a Boltzmann factor

$$B(x_0) \equiv e^{-V^{\rm eff\,cl}(x_0)/k_B T} \tag{3.810}$$

and defined the quantity $V^{\rm eff\,cl}(x_0)$ as the effective classical potential. The full partition function is then given by the integral

$$Z = \int_{-\infty}^{\infty} \frac{dx_0}{l_{\rm e}(\hbar\beta)} e^{-V^{\rm eff\,cl}(x_0)/k_B T}, \tag{3.811}$$

where the *effective classical Boltzmann factor* $B(x_0)$ contains all information on the quantum fluctuations of the system and allows to calculate the full quantum statistical partition function from a single classically looking integral. At high-temperature, the partition function (3.811) takes the classical limit (2.462). Thus, by construction, the effective classical potential $V^{\rm eff\,cl}(x_0)$ will approach the initial potential $V(x_0)$:

$$V^{\rm eff\,cl}(x_0) \xrightarrow{T\to\infty} V(x_0). \tag{3.812}$$

This is a direct consequence of the shrinking fluctuation width (3.806) for growing temperature.

The path integral representation of the effective classical Boltzmann factor

$$B(x_0) \equiv \oint \mathcal{D}'x \, e^{-\mathcal{A}_{\rm e}/\hbar} \tag{3.813}$$

can also be written as a path integral in which one has inserted a δ-function to ensure the path average

$$\bar{x} \equiv \frac{1}{\hbar\beta}\int_0^{\hbar\beta} d\tau\, x(\tau). \tag{3.814}$$

Let us introduce the slightly modified δ-function [recall (2.353)]

$$\tilde{\delta}(\bar{x}-x_0) \equiv l_{\rm e}(\hbar\beta)\delta(\bar{x}-x_0) = \sqrt{\frac{2\pi\hbar^2\beta}{M}}\,\delta(\bar{x}-x_0). \tag{3.815}$$

Then we can write

$$\begin{aligned} B(x_0) \equiv e^{-V^{\rm eff\,cl}(x_0)/k_BT} &= \oint \mathcal{D}'x\, e^{-\mathcal{A}_{\rm e}/\hbar} = \oint \mathcal{D}x\, \tilde{\delta}(\bar{x}-x_0)\, e^{-\mathcal{A}_{\rm e}/\hbar} \\ &= \oint \mathcal{D}\eta\, \tilde{\delta}(\bar{\eta})\, e^{-\mathcal{A}_{\rm e}/\hbar}. \end{aligned} \tag{3.816}$$

As a check we evaluate the effective classical Boltzmann factor for the harmonic action (2.445). With the path splitting (3.807), it reads

$$\mathcal{A}_{\rm e}[x_0+\eta] = \hbar\beta\,\frac{M\omega^2}{2}x_0^2 + \frac{M}{2}\int_0^{\hbar\beta} d\tau\, \left[\dot{\eta}^2(\tau)+\omega^2\eta^2(\tau)\right]. \tag{3.817}$$

After representing the δ function by a Fourier integral

$$\tilde{\delta}(\bar{\eta}) = l_{\rm e}(\hbar\beta)\int_{-i\infty}^{i\infty}\frac{d\lambda}{2\pi i}\exp\left(\lambda\frac{1}{\hbar\beta}\int d\tau\,\eta(\tau)\right), \tag{3.818}$$

we find the path integral

$$\begin{aligned} B_\omega(x_0) = \oint \mathcal{D}\eta\, \tilde{\delta}(\bar{\eta})\, e^{-\mathcal{A}_{\rm e}/\hbar} &= e^{-\beta M\omega^2 x_0^2/2} l_{\rm e}(\hbar\beta)\int_{-i\infty}^{i\infty}\frac{d\lambda}{2\pi i} \\ &\times \oint \mathcal{D}\eta\, \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\left[\frac{M}{2}\dot{\eta}^2(\tau)-\frac{\lambda}{\beta}\eta(\tau)\right]\right\}. \end{aligned} \tag{3.819}$$

The path integral over $\eta(\tau)$ in the second line can now be performed without the restriction $\hbar\beta = 0$ and yields, recalling (3.555), (3.556), and inserting there $j(\tau) = \lambda/\beta$, we obtain for the path integral over $\eta(\tau)$ in the second line of (3.819):

$$\frac{1}{2\sinh(\beta\hbar\omega/2)} \exp\left\{\frac{\lambda^2}{2M\hbar\beta^2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau')\right\}. \tag{3.820}$$

The integrals over τ, τ' are most easily performed on the spectral representation (3.248) of the correlation function:

$$\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' G^{\rm p}_{\omega^2,{\rm e}}(\tau-\tau') = \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \,\frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\frac{1}{\omega_m^2+\omega^2}e^{-i\omega_m(\tau-\tau')} = \frac{\hbar\beta}{\omega^2}. \tag{3.821}$$

The expression (3.820) has to be integrated over λ and yields

$$\frac{1}{2\sinh(\beta\hbar\omega/2)}\int_{-i\infty}^{i\infty}\frac{d\lambda}{2\pi i}\exp\left(\frac{\lambda^2}{2M\omega^2\beta}\right) = \frac{1}{2\sinh(\beta\hbar\omega/2)}\frac{1}{l_{\rm e}(\hbar\beta)}\,\omega\hbar\beta. \tag{3.822}$$

Inserting this into (3.819) we obtain the local Boltzmann factor

$$B_\omega(x_0) \equiv e^{-V^{\rm eff\,cl}_\omega(x_0)/k_BT} = \oint \mathcal{D}\eta\, \tilde{\delta}(\bar{\eta})\, e^{-\mathcal{A}_{\rm e}/\hbar} \;=\; \frac{\beta\hbar\omega/2}{\sinh(\beta\hbar\omega/2)}e^{-\beta M\omega^2 x_0^2}. \tag{3.823}$$

The final integral over x_0 in (3.808) reproduces the correct partition function (2.409) of the harmonic oscillator.

3.25.2 Effective Classical Hamiltonian

It is easy to generalize the expression (3.816) to phase space, where we define the *effective classical Hamiltonian* $H^{\rm eff\,cl}(p_0,x_0)$ and the associated Boltzmann factor $B(p_0,x_0)$ by the path integral

$$B(p_0,x_0) \equiv \exp\left[-\beta H^{\rm eff\,cl}(p_0,x_0)\right] \equiv \oint \mathcal{D}x \oint \frac{\mathcal{D}p}{2\pi\hbar}\,\delta(x_0-\overline{x})2\pi\hbar\delta(p_0-\overline{p})\, e^{-\mathcal{A}_{\rm e}[p,x]/\hbar}, \tag{3.824}$$

where $\overline{x} = \int_0^{\hbar\beta} d\tau\, x(\tau)/\hbar\beta$ and $\overline{p} = \int_0^{\hbar\beta} d\tau\, p(\tau)/\hbar\beta$ are the temporal averages of position and momentum, and $\mathcal{A}_{\rm e}[p,x]$ is the Euclidean action in phase space

$$\mathcal{A}_{\rm e}[p,x] = \int_0^{\hbar\beta} d\tau\,[-ip(\tau)\dot{x}(\tau) + H(p(\tau),x(\tau))]. \tag{3.825}$$

The full quantum-mechanical partition function is obtained from the classical-looking expression [recall (2.346)]

$$Z = \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty}\frac{dp_0}{2\pi\hbar}e^{-\beta H^{\rm eff\,cl}(p_0,x_0)}. \tag{3.826}$$

The definition is such that in the classical limit, $H^{\text{eff cl}}(p_0, x_0))$ becomes the ordinary Hamiltonian $H(p_0, x_0)$.

For a harmonic oscillator, the effective classical Hamiltonian can be directly deduced from Eq. (3.823) by "undoing" the p_0-integration:

$$B_\omega(p_0, x_0) \equiv e^{-H^{\text{eff cl}}_\omega(p_0,x_0)/k_BT} = l_{\rm e}(\hbar\beta)\frac{\beta\hbar\omega/2}{\sinh(\beta\hbar\omega/2)}e^{-\beta(p_0^2/2M+M\omega^2x_0^2)}. \tag{3.827}$$

Indeed, inserting this into (3.826), we recover the harmonic partition function (2.409).

Consider a particle in three dimensions moving in a constant magnetic field B along the z-axis. For the sake of generality, we allow for an additional harmonic oscillator centered at the origin with frequencies $\omega_\parallel$ in z-direction and $\omega_\perp$ in the xy-plane (as in Section 2.19). It is then easy to calculate the effective classical Boltzmann factor for the Hamiltonian [recall (2.689)]

$$H(\mathbf{p}, \mathbf{x}) = \frac{1}{2M}\mathbf{p}^2 + \frac{M}{2}\omega_\perp^2\mathbf{x}_\perp^2(\tau) + \frac{M}{2}\omega_\parallel^2 z^2(\tau) + \omega_B l_z(\mathbf{p}(\tau), \mathbf{x}(\tau)), \tag{3.828}$$

where $l_z(\mathbf{p}, \mathbf{x})$ is the z-component of the angular momentum defined in Eq. (2.647). We have shifted the center of momentum integration to $\mathbf{p}_0$, for later convenience (see Subsection 5.11.2). The vector $\mathbf{x}^\perp = (x, y)$ denotes the orthogonal part of $\mathbf{x}$. As in the generalized magnetic field action (2.689), we have chosen different frequencies in front of the harmonic oscillator potential and of the term proportional to l_z, for generality. The effective classical Boltzmann factor follows immediately from (2.703) by "undoing" the momentum integrations in p_x, p_y, and using (3.827) for the motion in the z-direction:

$$B(\mathbf{p}_0, \mathbf{x}_0) = e^{-\beta H^{\text{eff cl}}(\mathbf{p}_0,\mathbf{x}_0)} = l_{\rm e}^3(\hbar\beta)\frac{\hbar\beta\omega_+/2}{\sinh\hbar\beta\omega_+/2}\,\frac{\hbar\beta\omega_-/2}{\sinh\hbar\beta\omega_-/2}\,\frac{\hbar\beta\omega_\parallel/2}{\sinh\hbar\beta\omega_\parallel/2}e^{-\beta H(\mathbf{p}_0,\mathbf{x}_0)}, \tag{3.829}$$

where $\omega_\pm \equiv \omega_B \pm \omega_\perp$, as in (2.699). As in Eq. (3.823), the restrictions of the path integrals over $\mathbf{x}$ and $\mathbf{p}$ to the fixed averages $\mathbf{x}_0 = \bar{\mathbf{x}}$ and $\mathbf{p}_0 = \bar{\mathbf{p}}$ give rise to the extra numerators in comparison to (2.703).

3.25.3 High- and Low-Temperature Behavior

We have remarked before in Eq. (3.812) that in the limit $T \to \infty$, the effective classical potential $V^{\text{eff cl}}(x_0)$ converges by construction against the initial potential $V(x_0)$. There exists, in fact, a well-defined power series in $\hbar\omega/k_BT$ which describes this approach. Let us study this limit explicitly for the effective classical potential of the harmonic oscillator calculated in (3.823), after rewriting it as

$$\begin{aligned} V^{\text{eff cl}}_\omega(x_0) &= k_BT\log\frac{\sinh(\hbar\omega/2k_BT)}{\hbar\omega/2k_BT} + \frac{M}{2}\omega^2x_0^2 \qquad (3.830)\\ &= \frac{M}{2}\omega^2x_0^2 + \frac{\hbar\omega}{2} + k_BT\left[\log(1-e^{-\hbar\omega/k_BT}) - \log\frac{\hbar\omega}{k_BT}\right]. \end{aligned}$$

Due to the subtracted logarithm of ω in the brackets, the effective classical potential has a power series

$$V_\omega^{\rm eff\,cl}(x_0) = \frac{M}{2}\omega^2 x_0^2 + \hbar\omega \left[\frac{1}{24}\frac{\hbar\omega}{k_BT} - \frac{1}{2880}\left(\frac{\hbar\omega}{k_BT}\right)^3 + \dots\right]. \qquad (3.831)$$

This pleasant high-temperature behavior is in contrast to that of the effective potential which reads for the harmonic oscillator

$$\begin{aligned} V_\omega^{\rm eff}(x_0) &= k_BT \log\left[2\sinh(\hbar\omega/2k_BT)\right] + \frac{M}{2}\omega^2 x_0^2 \\ &= \frac{M}{2}\omega^2 x_0^2 + \frac{\hbar\omega}{2} + k_BT\log(1-e^{-\hbar\omega/k_BT}), \qquad (3.832) \end{aligned}$$

as we can see from (3.796). The logarithm of ω prevents this from having a power series expansion in $\hbar\omega/k_BT$, reflecting the increasing width of the unsubtracted fluctuations.

Consider now the opposite limit $T \to 0$, where the final integral over the Boltzmann factor $B(x_0)$ can be calculated exactly by the saddle-point method. In this limit, the effective classical potential $V^{\rm eff\,cl}(x_0)$ coincides with the Euclidean version of the effective potential:

$$V^{\rm eff\,cl}(x_0) \underset{T\to 0}{\to} V^{\rm eff}(x_0) \equiv \Gamma_{\rm e}[X]/\beta\Big|_{X=x_0}, \qquad (3.833)$$

whose real-time definition was given in Eq. (3.666).

Let us study this limit again explicitly for the harmonic oscillator, where it becomes

$$V_\omega^{\rm eff\,cl}(x_0) \xrightarrow{T\to 0} \frac{\hbar\omega}{2} + \frac{M}{2}\omega^2 x_0^2 - k_BT\log\frac{\hbar\omega}{k_BT}, \qquad (3.834)$$

i.e., the additional constant tends to $\hbar\omega/2$. This is just the quantum-mechanical zero-point energy which guarantees the correct low-temperature limit

$$\begin{aligned} Z_\omega &\xrightarrow{T\to 0} e^{-\hbar\omega/2k_BT}\frac{\hbar\omega}{k_BT}\int_{-\infty}^{\infty}\frac{dx_0}{l_{\rm e}(\hbar\beta)}e^{-M\omega^2x_0^2/2k_BT} \\ &= e^{-\hbar\omega/2k_BT}. \qquad (3.835) \end{aligned}$$

The limiting partition function is equal to the Boltzmann factor with the zero-point energy $\hbar\omega/2$.

3.25.4 Alternative Candidate for Effective Classical Potential

It is instructive to compare this potential with a related expression which can be defined in terms of the partition function density defined in Eq. (2.332):

$$\tilde V_\omega^{\rm eff\,cl}(x) \equiv k_BT\,\log\left[l_{\rm e}(\hbar\beta)\,z(x)\right]. \qquad (3.836)$$

This quantity shares with $V_\omega^{\text{eff cl}}(x_0)$ the property that it also yields the partition function by forming the integral [compare (2.331)]:

$$Z = \int_{-\infty}^{\infty} \frac{dx_0}{l_{\text{e}}(\hbar\beta)} e^{-\tilde{V}^{\text{eff cl}}(x_0)/k_BT}. \tag{3.837}$$

It may therefore be considered as an alternative candidate for an effective classical potential.

For the harmonic oscillator, we find from Eq. (2.333) the explicit form

$$\tilde{V}_\omega^{\text{eff cl}}(x) = -\frac{k_BT}{2}\log\frac{2\hbar\omega}{k_BT} + \frac{\hbar\omega}{2} + k_BT\left[\log\left(1-e^{-2\hbar\omega/k_BT}\right) + \frac{M\omega}{\hbar}\tanh\frac{\hbar\omega}{k_BT}\,x^2\right]. \tag{3.838}$$

This shares with the effective potential $V^{\text{eff}}(X)$ in Eq. (3.832) the unpleasant property of possessing no power series representation in the high-temperature limit.

The low-temperature limit of $\tilde{V}_\omega^{\text{eff cl}}(x)$ looks at first sight quite similar to (3.834):

$$\tilde{V}^{\text{eff cl}}(x_0) \xrightarrow{T\to 0} \frac{\hbar\omega}{2} + k_BT\,\frac{M\omega}{\hbar}\,x^2 - \frac{k_BT}{2}\log\frac{2\hbar\omega}{k_BT}, \tag{3.839}$$

and the integration leads to the same result (3.835) in only a slightly different way:

$$\begin{aligned} Z_\omega \quad &\xrightarrow{T\to 0} \quad e^{-\hbar\omega/2k_BT}\sqrt{\frac{2\hbar\omega}{k_BT}}\int_{-\infty}^{\infty}\frac{dx}{l_{\text{e}}(\hbar\beta)}e^{-M\omega x^2/\hbar} \\ &= e^{-\hbar\omega/2k_BT}. \end{aligned} \tag{3.840}$$

There is, however, an important difference of (3.839) with respect to (3.834). The width of a local Boltzmann factor formed from the partition function density (2.332):

$$\tilde{B}(x) \equiv l_{\text{e}}(\hbar\beta)\,z(x) = e^{-\tilde{V}^{\text{eff cl}}(x)/k_BT} \tag{3.841}$$

is much wider than that of the effective classical Boltzmann factor $B(x_0) = e^{-V^{\text{eff cl}}(x_0)/k_BT}$. Whereas $B(x_0)$ has a finite width for $T \to 0$, the Boltzmann factor $\tilde{B}(x)$ has a width growing to infinity in this limit. Thus the integral over x in (3.840) converges much more slowly than that over x_0 in (3.835). This is the principal reason for introducing $V^{\text{eff cl}}(x_0)$ as an effective classical potential rather than $\tilde{V}^{\text{eff cl}}(x_0)$.

3.25.5 Harmonic Correlation Function without Zero Mode

By construction, the correlation functions of $\eta(\tau)$ have the desired subtracted form (3.805):

$$\langle\eta(\tau)\eta(\tau')\rangle_\omega = \frac{\hbar}{M}G^{\text{p}\prime}_{\omega^2,\text{e}}(\tau-\tau') = \frac{\hbar}{2M\omega}\frac{\cosh\omega(|\tau-\tau'|-\hbar\beta/2)}{\sinh(\beta\hbar\omega/2)} - \frac{1}{\hbar\beta\omega^2}, \tag{3.842}$$

with the square width as in (3.806):

$$\langle\eta^2(\tau)\rangle_\omega \equiv a_\omega^2 = G^{\mathrm{p}\prime}_{\omega^2,\mathrm{e}}(0) = \frac{1}{2\omega}\coth\frac{\beta\hbar\omega}{2} - \frac{1}{\hbar\beta\omega^2}, \tag{3.843}$$

which decreases with increasing temperature. This can be seen explicitly by adding a current term $-\int d\tau\, j(\tau)\eta(\tau)$ to the action (3.817) which winds up in the exponent of (3.819), replacing λ/β by $j(\tau)+\lambda/\beta$ and multiplies the exponential in (3.820) by a factor

$$\frac{1}{2M\hbar\beta^2}\left\{\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \left[\lambda^2 + \lambda\beta j(\tau) + \lambda\beta j(\tau')\right] G^{\mathrm{p}}_{\omega^2,\mathrm{e}}(\tau-\tau')\right\}$$
$$\times \exp\left\{\frac{1}{2M\hbar}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, j(\tau) G^{\mathrm{p}}_{\omega^2,\mathrm{e}}(\tau-\tau') j(\tau')\right\}. \tag{3.844}$$

In the first exponent, one of the τ-integrals over $G^{\mathrm{p}}_{\omega^2,\mathrm{e}}(\tau-\tau')$, say τ', produces a factor $1/\omega^2$ as in (3.821), so that the first exponent becomes

$$\frac{1}{2M\hbar\beta^2}\left\{\lambda^2\frac{\hbar\beta}{\omega^2} + 2\frac{\lambda\beta}{\omega^2}\int_0^{\hbar\beta} d\tau\, j(\tau)\right\}. \tag{3.845}$$

If we now perform the integral over λ, the linear term in λ yields, after a quadratic completion, a factor

$$\exp\left\{-\frac{1}{2M\beta\hbar^2\omega^2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' j(\tau) j(\tau')\right\}. \tag{3.846}$$

Combined with the second exponential in (3.844) this leads to a generating functional for the subtracted correlation functions (3.842):

$$Z_\omega^{x_0}[j] = \frac{\beta\hbar\omega/2}{\sin(\beta\hbar\omega/2)} e^{-\beta M\omega^2 x_0^2/2} \exp\left\{\frac{1}{2M\hbar}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, j(\tau) G^{\mathrm{p}\prime}_{\omega^2,\mathrm{e}}(\tau-\tau') j(\tau')\right\}. \tag{3.847}$$

For $j(\tau) \equiv 0$, this reduces to the local Boltzmann factor (3.823).

3.25.6 Perturbation Expansion

We can now apply the perturbation expansion (3.483) to the path integral over $\eta(\tau)$ in Eq. (3.816) for the effective classical Boltzmann factor $B(x_0)$. We take the action

$$\mathcal{A}_\mathrm{e}[x] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}^2 + V(x)\right], \tag{3.848}$$

and rewrite it as

$$\mathcal{A}_\mathrm{e} = \hbar\beta V(x_0) + \mathcal{A}^{(0)}_\mathrm{e}[\eta] + \mathcal{A}_{\mathrm{int},\mathrm{e}}[x_0;\eta], \tag{3.849}$$

with an unperturbed action

$$\mathcal{A}_{\rm e}^{(0)}[\eta] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{\eta}^2(\tau) + \frac{M}{2}\Omega^2(x_0)\eta^2(\tau)\right], \quad \Omega^2(x_0) \equiv V''(x_0)/M, \tag{3.850}$$

and an interaction

$$\mathcal{A}_{\rm int,e}[x_0;\eta] = \int_0^{\hbar\beta} d\tau\, V^{\rm int}(x_0;\eta(\tau)), \tag{3.851}$$

containing the subtracted potential

$$V^{\rm int}(x_0;\eta(\tau)) = V(x_0+\eta(\tau)) - V(x_0) - V'(x_0)\eta(\tau) - \frac{1}{2}V''(x_0)\eta^2(\tau). \tag{3.852}$$

This has a Taylor expansion starting with the cubic term

$$V^{\rm int}(x_0;\eta) = \frac{1}{3!}V'''(x_0)\eta^3 + \frac{1}{4!}V^{(4)}(x_0)\eta^4 + \dots\ . \tag{3.853}$$

Since $\eta(\tau)$ has a zero temporal average, the linear term $\int_0^{\hbar\beta} d\tau\, V'(x_0)\eta(\tau)$ is absent in (3.850). The effective classical Boltzmann factor $B(x_0)$ in (3.816) has then the perturbation expansion [compare (3.483)]

$$B(x_0) = \left(1 - \frac{1}{\hbar}\left\langle \mathcal{A}_{\rm int,e}\right\rangle_\Omega^{x_0} + \frac{1}{2!\hbar^2}\left\langle \mathcal{A}_{\rm int,e}^2\right\rangle_\Omega^{x_0} - \frac{1}{3!\hbar^3}\left\langle \mathcal{A}_{\rm int,e}^3\right\rangle_\Omega^{x_0} + \dots\right) B_\Omega(x_0). \tag{3.854}$$

The harmonic expectation values are defined with respect to the harmonic path integral

$$B_\Omega(x_0) = \int \mathcal{D}\eta\, \tilde{\delta}(\bar{\eta})\, e^{-\mathcal{A}_{\rm e}^{(0)}[\eta]//\hbar}. \tag{3.855}$$

For an arbitrary functional $F[x]$ one has to calculate

$$\langle F[x]\rangle_\Omega^{x_0} = B_\Omega^{-1}(x_0)\int \mathcal{D}\eta\, \tilde{\delta}(\bar{\eta})\, F[x]\, e^{-\mathcal{A}_{\rm e}^{(0)}[\eta]/\hbar}. \tag{3.856}$$

Some calculations of local expectation values are conveniently done with the explicit Fourier components of the path integral. Recalling (3.809) and expanding the action (3.817) in its Fourier components using (3.807), they are given by the product of integrals

$$\langle F[x]\rangle_\Omega^{x_0} = [Z_\Omega^{x_0}]^{-1}\prod_{m=1}^{\infty}\left[\int \frac{dx_m^{\rm re}dx_m^{\rm im}}{\pi k_BT/M\omega_m^2}\right] e^{-\frac{M}{k_BT}\Sigma_{m=1}^\infty[\omega_m^2+\Omega^2(x_0)]|x_m|^2}\, F[x]. \tag{3.857}$$

This implies the correlation functions for the Fourier components

$$\left\langle x_m x_{m'}^*\right\rangle_\Omega^{x_0} = \delta_{mm'}\frac{k_BT}{M}\frac{1}{\omega_m^2+\Omega^2(x_0)}. \tag{3.858}$$

From these we can calculate once more the correlation functions of the fluctuations $\eta(\tau)$ as follows:

$$\langle\eta(\tau)\eta(\tau')\rangle_\Omega^{x_0} = \left\langle \sum_{m,m'\neq 0}^{\infty} x_m x_{m'}^* e^{-i(\omega_m-\omega_{m'})\tau}\right\rangle_\Omega^{x_0} = 2\frac{1}{M\beta}\sum_{m=1}\frac{1}{\omega_m^2+\Omega^2(x_0)}. \quad (3.859)$$

Performing the sum gives once more the subtracted correlation function Eq. (3.842), whose generating functional was calculated in (3.847).

The calculation of the harmonic averages in (3.854) leads to a similar loop expansion as for the effective potential in Subsection 3.23.6 using the background field method. The path average x_0 takes over the role of the background X and the nonzero Matsubara frequency part of the paths $\eta(\tau)$ corresponds to the fluctuations. The only difference with respect to the earlier calculations is that the correlation functions of $\eta(\tau)$ contain no zero-frequency contribution. Thus they are obtained from the subtracted Green functions $G^{\mathrm{p}\,\prime}_{\Omega^2(x_0),\mathrm{e}}(\tau)$ defined in Eq. (3.805).

All Feynman diagrams in the loop expansion are one-particle irreducible, just as in the loop expansion of the effective potential. The reducible diagrams are absent since there is no linear term in the interaction (3.853). This trivial absence is an advantage with respect to the somewhat involved proof required for the effective action in Subsection 3.23.6. The diagrams in the two expansions are therefore precisely the same and can be read off from Eqs. (3.744) and (3.784). The only difference lies in the replacement $X \to x_0$ in the analytic expressions for the lines and vertices. In addition, there is the final integral over x_0 to obtain the partition function Z in Eq. (3.811). This is in contrast to the partition function expressed in terms of the effective potential $V^{\mathrm{eff}}(X)$, where only the extremum has to be taken.

3.25.7 Effective Potential and Magnetization Curves

The effective classical potential $V^{\mathrm{eff\,cl}}(x_0)$ in the Boltzmann factor (3.810) allows us to estimate the *effective potential* defined in Eq. (3.666). It can be derived from the generating functional $Z[j]$ restricted to time-independent external source $j(\tau) \equiv j$, in which case $Z[j]$ reduces to a mere function of j:

$$Z(j) = \int \mathcal{D}x(\tau)\exp\left\{-\int_0^\beta d\tau\left[\frac{1}{2}\dot{x}^2 + V(x(\tau))\right] + \beta j\bar{x}\right\}, \quad (3.860)$$

where $\bar{x}$ is the path average of $x(\tau)$. The function $Z(j)$ is obtained from the effective classical potential by a simple integral over x_0:

$$Z(j) = \int_{-\infty}^{\infty}\frac{dx_0}{\sqrt{2\pi\beta}}e^{-\beta[V^{\mathrm{eff\,cl}}(x_0)-jx_0]}. \quad (3.861)$$

The effective potential $V^{\mathrm{eff}}(X)$ is equal to the Legendre transform of $W(j) = \log Z(j)$:

$$V^{\mathrm{eff}}(X) = -\frac{1}{\beta}W(j) + Xj, \quad (3.862)$$

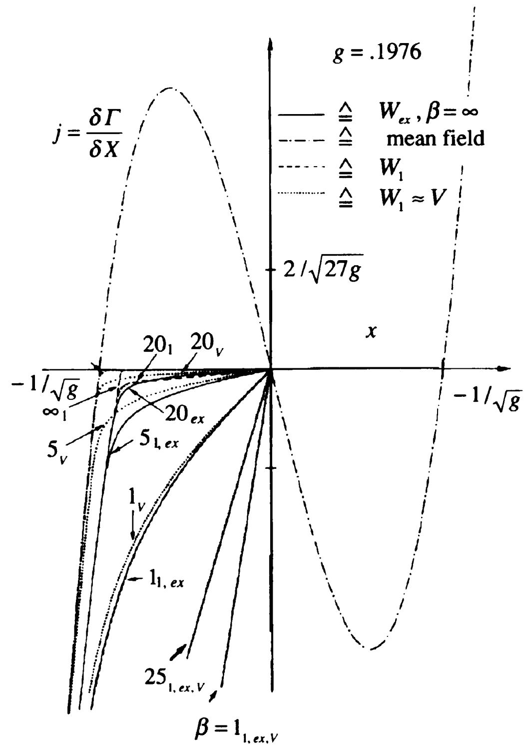


Figure 3.15 Magnetization curves in double-well potential $V(x) = -x^2/2 + gx^4/4$ with $g = 0.4$, at various inverse temperatures β. The integral over these curves returns the effective potential $V^{\rm eff}(X)$. The curves arising from the approximate effective potential $W_1(x_0)$ are labeled by β_1 (- - -) and the exact curves (found by solving the Schrödinger equation numerically) by $\beta_{\rm ex}$ (—). For comparison we have also drawn the classical curves ($\cdots$) obtained by using the potential $V(x_0)$ in Eqs. (3.864) and (3.861) rather than $W_1(x_0)$. They are labeled by β_V. Our approximation $W_1(x_0)$ is seen to render good magnetization curves for all temperatures above $T = 1/\beta \sim 1/10$. The label β carries several subscripts if the corresponding curves are indistinguishable on the plot. Note that all approximations are monotonous, as they should be (except for the mean field, of course).

where the right-hand side is to be expressed in terms of X using

$$X = X(j) = \frac{1}{\beta}\frac{d}{dj}W(j). \tag{3.863}$$

To picture the effective potential, we calculate the average value of $x(\tau)$ from the integral

$$X = Z(j)^{-1}\int_{-\infty}^{\infty}\frac{dx_0}{\sqrt{2\pi\beta}}\,x_0\,\exp\left\{-\beta[V^{\rm eff\,cl}(x_0) - jx_0]\right\} \tag{3.864}$$

and plot $X = X(j)$. By exchanging the axes we display the inverse $j = j(X)$ which is the slope of the effective potential:

$$j(X) = \frac{dV^{\rm eff}(X)}{dX}. \tag{3.865}$$

The curves $j(X)$ are shown in Fig. 3.15 for the double-well potential with a coupling strength $g = 0.4$ at various temperatures.

Note that the x_0-integration makes $j(X)$ necessarily a monotonous function of X. The effective potential is therefore always a convex function of X, no matter what the classical potential looks like. This is in contrast to $j(X)$ *before* fluctuations are taken into account, the *mean-field approximation* to (3.865) [recall the discussion in Subsection 3.23.1], which is given by

$$j = dV(X)/dX. \tag{3.866}$$

For the double-well potential, this becomes

$$j = -X + gX^3. \tag{3.867}$$

Thus, the mean-field effective potential coincides with the classical potential $V(X)$, which is obviously not convex.

In magnetic systems, j is a constant magnetic field and X its associated magnetization. For this reason, plots of $j(X)$ are referred to as *magnetization curves*.

3.25.8 First-Order Perturbative Result

To first order in the interaction $V^{\rm int}(x_0;\eta)$, the perturbation expansion (3.854) becomes

$$B(x_0) = \left(1 - \frac{1}{\hbar}\,\langle \mathcal{A}_{\rm int,e}\rangle_\Omega^{x_0} + \ldots\right) B_\Omega(x_0), \tag{3.868}$$

and we have to calculate the harmonic expectation value of $\mathcal{A}_{\rm int,e}$. Let us assume that the interaction potential possesses a Fourier transform

$$V^{\rm int}(x_0;\eta(\tau)) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x_0+\eta(\tau))}\tilde{V}^{\rm int}(k). \tag{3.869}$$

Then we can write the expectation of (3.851) as

$$\langle \mathcal{A}_{\rm int,e}[x_0;\eta]\rangle_\Omega^{x_0} = \int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} \frac{dk}{2\pi}\,\tilde{V}^{\rm int}(k) e^{ikx_0}\,\left\langle e^{ik\eta(\tau)}\right\rangle_\Omega^{x_0}. \tag{3.870}$$

We now use Wick's rule in the form (3.307) to calculate

$$\left\langle e^{ik\eta(\tau)}\right\rangle_\Omega^{x_0} = e^{-k^2\left\langle \eta^2(\tau)\right\rangle_\Omega^{x_0}/2}. \tag{3.871}$$

We now use Eq. (3.843) to write this as

$$\left\langle e^{ik\eta(\tau)}\right\rangle_\Omega^{x_0} = e^{-k^2 a^2_{\Omega(x_0)}/2}. \tag{3.872}$$

Thus we find for the expectation value (3.870):

$$\langle \mathcal{A}_{\rm int,e}[x_0;\eta]\rangle_\Omega^{x_0} = \int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} \frac{dk}{2\pi}\,\tilde{V}^{\rm int}(k) e^{ikx_0 - k^2 a^2_{\Omega(x_0)}/2}. \tag{3.873}$$

Due to the periodic boundary conditions satisfied by the correlation function and the associated invariance under time translations, this result is independent of τ, so that the τ-integral can be performed trivially, yielding simply a factor $\hbar\beta$. We now reinsert the Fourier coefficients of the potential

$$\tilde{V}^{\rm int}(k) = \int_{-\infty}^{\infty} dx\, V^{\rm int}(x_0;\eta)\, e^{-ik(x_0+\eta)}, \tag{3.874}$$

perform the integral over k via a quadratic completion, and obtain

$$\left\langle V^{\rm int}(x(\tau))\right\rangle_{\Omega}^{x_0} \equiv V^{\rm int}_{a^2_\Omega}(x_0) = \int_{-\infty}^{\infty} \frac{dx_0'}{\sqrt{2\pi a^2_{\Omega(x_0)}}} e^{-\eta^2/2a^2_{\Omega(x_0)}}\, V^{\rm int}(x_0;\eta). \tag{3.875}$$

The expectation $\left\langle V^{\rm int}(x(\tau))\right\rangle_{\Omega}^{x_0} \equiv V^{\rm int}_{a^2_\Omega}(x_0)$ of the potential arises therefore from a convolution integral of the original potential with a Gaussian distribution of square width $a^2_{\Omega(x_0)}$. The convolution integral smears the original interaction potential $V^{\rm int}_{a^2_\Omega}(x_0)$ out over a length scale $a_{\Omega(x_0)}$. In this way, the approximation accounts for the quantum-statistical path fluctuations of the particle.

As a result, we can write the first-order Boltzmann factor (3.868) as follows:

$$B(x_0) \approx \frac{\Omega(x_0)\hbar\beta}{2\sin[\Omega(x_0)\hbar\beta/2]} \exp\left\{-\beta M\Omega(x_0)^2 x_0^2/2 - \beta V^{\rm int}_{a^2_\Omega}(x_0)\right\}. \tag{3.876}$$

Recalling the harmonic effective classical potential (3.834), this may be written as a Boltzmann factor associated with the first-order effective classical potential

$$V^{\rm eff\,cl}(x_0) \approx V^{\rm eff\,cl}_{\Omega(x_0)}(x_0) + V^{\rm int}_{a^2_\Omega}(x_0). \tag{3.877}$$

Given the power series expansion (3.853) of the interaction potential

$$V^{\rm int}(x_0;\eta) = \sum_{k=3}^{\infty} \frac{1}{k!} V^{(k)}(x_0)\hbar^k, \tag{3.878}$$

we may use the integral formula

$$\int_{-\infty}^{\infty} \frac{d\eta}{\sqrt{2\pi a^2}} e^{-\eta^2/2a^2}\eta^k = \left\{ \begin{array}{c} (k-1)!!\, a^k \\ 0 \end{array} \right\} \text{ for } k = \left\{ \begin{array}{c} \text{even} \\ \text{odd} \end{array} \right\}, \tag{3.879}$$

we find the explicit smeared potential

$$V^{\rm int}_{a^2}(x_0) = \sum_{k=4,6,\dots}^{\infty} \frac{(k-1)!!}{k!} V^{(k)}(x_0) a^k(x_0). \tag{3.880}$$

3.26 Perturbative Approach to Scattering Amplitude

In Eq. (2.747) we have derived a path integral representation for the scattering amplitude. It involves calculating a path integral of the general form

$$\int d^3y_a \int d^3z_a \int \mathcal{D}^3y \int \mathcal{D}^3z \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \frac{M}{2}\left(\dot{\mathbf{y}}^2 - \dot{\mathbf{z}}^2\right)\right] F[\mathbf{y}(t) - \mathbf{z}(0)], \tag{3.881}$$

where the paths $\mathbf{y}(t)$ and $\mathbf{z}(t)$ vanish at the final time $t = t_b$ whereas the initial positions are integrated out. In lowest approximation, we may neglect the fluctuations in $\mathbf{y}(t)$ and $\mathbf{z}(0)$ and obtain the eikonal approximation (2.750). In order to calculate higher-order corrections to path integrals of the form (3.881) we find the generating functional of all correlation functions of $\mathbf{y}(t) - \mathbf{z}(0)$.

3.26.1 Generating Functional

For the sake of generality we calculate the harmonic path integral over $\mathbf{y}$:

$$Z[\mathbf{j}_\mathbf{y}] \equiv \int d^3y_a \int \mathcal{D}^3y \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \left[\frac{M}{2}\left(\dot{\mathbf{y}}^2 - \omega^2\mathbf{y}^2\right) - \mathbf{j}_\mathbf{y}\mathbf{y}\right]\right\}. \tag{3.882}$$

This differs from the amplitude calculated in (3.168) only by an extra Fresnel integral over the initial point and a trivial extension to three dimensions. This yields

$$\begin{aligned} Z[\mathbf{j}_\mathbf{y}] &= \int d^3y_a (\mathbf{y}_b t_b|\mathbf{y}_a t_a)_\omega^{\mathbf{j}_\mathbf{y}} \\ &= \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \frac{1}{\sin\omega(t_b - t_a)}\left[\mathbf{y}_b\left(\sin\left[\omega(t-t_a)\right] + \sin\left[\omega(t_b - t)\right]\right)\mathbf{j}_\mathbf{y}\right]\right\} \\ &\times \exp\left\{-\frac{i}{\hbar^2}\frac{\hbar}{M}\int_{t_a}^{t_b} dt \int_{t_a}^{t} dt'\, \mathbf{j}_\mathbf{y}(t)\bar{G}_{\omega^2}(t,t')\mathbf{j}_\mathbf{y}(t')\right\}, \end{aligned} \tag{3.883}$$

where $\bar{G}_{\omega^2}(t,t')$ is obtained from the Green function (3.36) with Dirichlet boundary conditions by adding the result of the quadratic completion in the variable $\mathbf{y}_b - \mathbf{y}_a$ preceding the evaluation of the integral over d^3y_a:

$$\bar{G}_{\omega^2}(t,t') = \frac{1}{\omega\sin\omega(t_b - t_a)}\sin\omega(t_b - t_>)\left[\sin\omega(t_< - t_a) + \sin\omega(t_b - t_<)\right]. \tag{3.884}$$

We need the special case $\omega = 0$ where

$$\bar{G}_{\omega^2}(t,t') = t_b - t_>. \tag{3.885}$$

In contrast to $G_{\omega^2}(t,t')$ of (3.36), this Green function vanishes only at the final time. This reflects the fact that the path integral (3.881) is evaluated for paths $\mathbf{y}(t)$ which vanish at the final time $t = t_b$.

A similar generating functional for $\mathbf{z}(t)$ leads to the same result with opposite sign in the exponent. Since the variable $\mathbf{z}(t)$ appears only with time argument zero in (3.881), the relevant generating functional is

$$\begin{aligned} Z[\mathbf{j}] &\equiv \int d^3y_a \int d^3z_a \int \mathcal{D}^3y \int \mathcal{D}^3z \\ &\times \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \left\{\frac{M}{2}\left[\dot{\mathbf{y}}^2 - \dot{\mathbf{z}}^2 - \omega^2\left(\mathbf{y}^2 - \mathbf{z}^2\right) - \mathbf{j}\,\mathbf{y}_\mathbf{z}\right]\right\}\right), \end{aligned} \tag{3.886}$$

with $\mathbf{y}_b = \mathbf{z}_b = 0$, where we have introduced the subtracted variable

$$\mathbf{y}_\mathbf{z}(t) \equiv \mathbf{y}(t) - \mathbf{z}(0), \tag{3.887}$$

for brevity. From the above calculations we can immediately write down the result

$$Z[\mathbf{j}] = \frac{1}{D_\omega} \exp\left\{-\frac{i}{\hbar^2}\frac{\hbar}{2M}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\; \mathbf{j}(t)\bar{G}'_{\omega^2}(t,t')\mathbf{j}(t')\right\}, \tag{3.888}$$

where D_ω is the functional determinant associated with the Green function (3.884) which is obtained by integrating (3.884) over $t \in (t_b, t_a)$ and over ω^2:

$$D_\omega = \frac{1}{\cos^2[\omega(t_b - t_a)]} \exp\left[\int_0^{t_b - t_a} \frac{dt}{t}\,(\cos\omega t - 1)\right], \tag{3.889}$$

and $\bar{G}'_{\omega^2}(t,t')$ is the subtracted Green function (3.884):

$$\bar{G}'_{\omega^2}(t,t') \equiv \bar{G}_{\omega^2}(t,t') - \bar{G}_{\omega^2}(0,0). \tag{3.890}$$

For $\omega = 0$ where $D_\omega = 1$, this is simply

$$\bar{G}'_0(t,t') \equiv -t_>, \tag{3.891}$$

where $t_>$ denotes the larger of the times t and t'. It is important to realize that thanks to the subtraction in the Green function (3.885) caused by the $\mathbf{z}(0)$-fluctuations, the limits $t_a \to -\infty$ and $t_b \to \infty$ can be taken in (3.888) without any problems.

3.26.2 Application to Scattering Amplitude

We can now apply this result to the path integral (2.747). With the abbreviation (3.887) we write it as

$$\begin{aligned} f_{\mathbf{p}_b\mathbf{p}_a} &= \frac{p}{2\pi i\hbar}\int d^2b\, e^{-i\mathbf{qb}/\hbar} \\ &\times \int \mathcal{D}^3 y_{\mathbf{z}} \exp\left\{\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, \frac{M}{2}\,\mathbf{y}_{\mathbf{z}}[\bar{G}'_0(t,t')]^{-1}\mathbf{y}_{\mathbf{z}}\right\}\left[e^{i\chi_{\mathbf{b},\mathbf{p}}[\mathbf{y}_{\mathbf{z}}]} - 1\right], \end{aligned} \tag{3.892}$$

where $[\bar{G}'_0(t,t')]^{-1}$ is the functional inverse of the subtracted Green function (3.891), and $\chi_{\mathbf{b},\mathbf{p}}[\mathbf{y}_{\mathbf{z}}]$ the integral over the interaction potential $V(\mathbf{x})$:

$$\chi_{\mathbf{b},\mathbf{p}}[\mathbf{y}_{\mathbf{z}}] \equiv -\frac{1}{\hbar}\int_{-\infty}^{\infty} dt\, V\left(\mathbf{b} + \frac{\mathbf{p}}{M}t + \mathbf{y}_{\mathbf{z}}(t)\right). \tag{3.893}$$

3.26.3 First Correction to Eikonal Approximation

The first correction to the eikonal approximation (2.750) is obtained by expanding (3.893) to first order in $\mathbf{y}_{\mathbf{z}}(t)$. This yields

$$\chi_{\mathbf{b},\mathbf{p}}[\mathbf{y}] = \chi^{\rm ei}_{\mathbf{b},\mathbf{p}} - \frac{1}{\hbar}\int_{-\infty}^{\infty} dt\, \boldsymbol{\nabla} V\left(\mathbf{b} + \frac{\mathbf{p}}{M}t\right)\mathbf{y}_{\mathbf{z}}(t). \tag{3.894}$$

The additional terms can be considered as an interaction

$$-\frac{1}{\hbar}\int_{-\infty}^{\infty} dt\, \mathbf{y}_{\mathbf{z}}(t)\,\mathbf{j}(t), \tag{3.895}$$

with the current

$$\mathbf{j}(t) \;=\; \boldsymbol{\nabla} V\left(\mathbf{b} + \frac{\mathbf{p}}{M}t\right). \tag{3.896}$$

Using the generating functional (3.888), this is seen to yield an additional scattering phase

$$\Delta_1\chi^{\rm ei}_{\mathbf{b},\mathbf{p}} = \frac{1}{2M\hbar}\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \,\boldsymbol{\nabla} V\left(\mathbf{b}+\frac{\mathbf{p}}{M}t_1\right)\boldsymbol{\nabla} V\left(\mathbf{b}+\frac{\mathbf{p}}{M}t_2\right) t_>. \tag{3.897}$$

To evaluate this we shall always change, as in (2.752), the time variables $t_{1,2}$ to length variables $z_{1,2} \equiv p_{1,2}t/M$ along the direction of $\mathbf{p}$.

For spherically symmetric potentials $V(r)$ with $r \equiv |\mathbf{x}| = \sqrt{b^2+z^2}$, we may express the derivatives parallel and orthogonal to the incoming particle momentum $\mathbf{p}$ as follows:

$$\boldsymbol{\nabla}_{\parallel} V = z\, V'/r, \quad \boldsymbol{\nabla}_{\perp} V = \mathbf{b}\, V'/r. \tag{3.898}$$

Then (3.897) reduces to

$$\Delta_1\chi^{\rm ei}_{\mathbf{b},\mathbf{p}} = \frac{M^2}{2\hbar p^3}\int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2 \frac{V'(r_1)}{r_1}\frac{V'(r_2)}{r_2}\left(b^2+z_1z_2\right) z_1. \tag{3.899}$$

The part of the integrand before the bracket is obviously symmetric under $z \to -z$ and under the exchange $z_1 \leftrightarrow z_2$. For this reason we can rewrite

$$\Delta_1\chi^{\rm ei}_{\mathbf{b},\mathbf{p}} = \frac{M^2}{\hbar p^3}\int_{-\infty}^{\infty} dz_1\, z_1 \frac{V'(r_1)}{r_1}\int_{-\infty}^{\infty} dz_2 \frac{V'(r_2)}{r_2}\left(b^2-z_2^2\right). \tag{3.900}$$

Now we use the relations (3.898) in the opposite direction as

$$zV'/r = \partial_z V, \quad bV'/r = \partial_b V, \tag{3.901}$$

and performing a partial integration in z_1 to obtain[21]

$$\Delta_1\chi^{\rm ei}_{\mathbf{b},\mathbf{p}} = -\frac{M^2}{\hbar p^3}\left(1+b\partial_b\right)\int_{-\infty}^{\infty} dz\, V^2\left(\sqrt{b^2+z^2}\right). \tag{3.902}$$

Compared to the leading eikonal phase (2.753), this is suppressed by a factor $V(0)M/p^2$.

Note that for the Coulomb potential where $V^2(\sqrt{b^2+z^2}) \propto 1/(b^2+z^2)$, the integral is proportional to $1/b$ which is annihilated by the factor $1+b\partial_b$. Thus there is no first correction to the eikonal approximation (1.506).

3.26.4 Rayleigh-Schrödinger Expansion of Scattering Amplitude

In Section 1.16 we have introduced the scattering amplitude as the limiting matrix element [see (1.516)]

$$\langle \mathbf{p}_b|\hat{S}|\mathbf{p}_a\rangle \;\equiv\; \lim_{t_b-t_a\to\infty} e^{i(E_b-E_a)t_b/\hbar}(\mathbf{p}_b 0|\mathbf{p}_a t_a)e^{-iE_at_a/\hbar}. \tag{3.903}$$

A perturbation expansion for these quantities can be found via a Fourier transformation of the expansion (3.477). We only have to set the oscillator frequency of the harmonic part of the action equal to zero, since the particles in a scattering process are free far away from the scattering center. Since scattering takes usually place in three dimensions, all formulas will be written down in such a space.

[21] This agrees with results from Schrödinger theory by S.J. Wallace, Ann. Phys. *78*, 190 (1973); S. Sarkar, Phys. Rev. D *21*, 3437 (1980). It differs from R. Rosenfelder's result (see Footnote 38 on p. 193) who derives a prefactor $p\cos(\theta/2)$ instead of the incoming momentum p.

We shall thus consider the perturbation expansion of the amplitude

$$(\mathbf{p}_b 0|\mathbf{p}_a t_a) = \int d^3x_b d^3x_a e^{-i\mathbf{p}_b\mathbf{x}_b}(\mathbf{x}_b 0|\mathbf{x}_a t_a)e^{i\mathbf{p}_a\mathbf{x}_a}, \tag{3.904}$$

where $(\mathbf{x}_b 0|\mathbf{x}_a t_a)$ is expanded as in (3.477). The immediate result looks as in the expansion (3.500), if we replace the external oscillator wave functions $\psi_n(x_b)$ and $\psi_a(x_b)$ by free-particle plane waves $e^{-i\mathbf{p}_b\mathbf{x}_b}$ and $e^{i\mathbf{p}_a\mathbf{x}_a}$:

$$\begin{aligned}(\mathbf{p}_b 0|\mathbf{p}_a t_a) &= (\mathbf{p}_b 0|\mathbf{p}_a t_a)_0 \\ &+\frac{i}{\hbar}\langle\mathbf{p}_b|\mathcal{A}_{\rm int}|\mathbf{p}_a\rangle_0 - \frac{1}{2!\hbar^2}\langle\mathbf{p}_b|\mathcal{A}_{\rm int}^2|\mathbf{p}_a\rangle_0 - \frac{i}{3!\hbar^3}\langle\mathbf{p}_b|\mathcal{A}_{\rm int}^3|\mathbf{p}_a\rangle_0 + \dots\ .\end{aligned} \tag{3.905}$$

Here

$$(\mathbf{p}_b 0|\mathbf{p}_a t_a)_0 = (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}_b - \mathbf{p}_a)e^{i\mathbf{p}_b^2 t_a/2M\hbar} \tag{3.906}$$

is the free-particle time evolution amplitude in momentum space [recall (2.73)] and the matrix elements are defined by

$$\langle\mathbf{p}_b|\dots|\mathbf{p}_a\rangle_0 \equiv \int d^3x_b d^3x_a e^{-i\mathbf{p}_b\mathbf{x}_b}\left(\int\mathcal{D}^3x\dots e^{i\mathcal{A}_0/\hbar}\right)e^{i\mathbf{p}_a\mathbf{x}_a}. \tag{3.907}$$

In contrast to (3.500) we have not divided out the free-particle amplitude (3.906) in this definition since it is too singular. Let us calculate the successive terms in the expansion (3.905). First

$$\begin{aligned}\langle\mathbf{p}_b|\mathcal{A}_{\rm int}|\mathbf{p}_a\rangle_0 \;\;=\;\; -\int_{t_a}^0 dt_1\int d^3x_b d^3x_a d^3x_1 e^{-i\mathbf{p}_b\mathbf{x}_b}(\mathbf{x}_b 0|\mathbf{x}_1 t_1)_0 \\ \times V(\mathbf{x}_1)(\mathbf{x}_1 t_1|\mathbf{x}_a t_a)_0 e^{i\mathbf{p}_a\mathbf{x}_a}.\end{aligned} \tag{3.908}$$

Since

$$\begin{aligned}\int d^3x_b e^{-i\mathbf{p}_b\mathbf{x}_b}(\mathbf{x}_b t_b|\mathbf{x}_1 t_1)_0 &= e^{-i\mathbf{p}_b\mathbf{x}_1}e^{-i\mathbf{p}_b^2(t_b-t_1)/2M\hbar}, \\ \int d^3x_a(\mathbf{x}_1 t_1|\mathbf{x}_a t_a)_0 e^{-i\mathbf{p}_b\mathbf{x}_b} &= e^{-i\mathbf{p}_a\mathbf{x}_1}e^{i\mathbf{p}_a^2(t_1-t_a)/2M\hbar},\end{aligned} \tag{3.909}$$

this becomes

$$\langle\mathbf{p}_b|\mathcal{A}_{\rm int}|\mathbf{p}_a\rangle_0 = -\int_{t_a}^0 dt_1 e^{i(\mathbf{p}_b^2-\mathbf{p}_a^2)t_1/2M\hbar}V_{\mathbf{p}_b\mathbf{p}_a}\, e^{i\mathbf{p}_a^2 t_a/2M\hbar}, \tag{3.910}$$

where

$$V_{\mathbf{p}_b\mathbf{p}_a} \equiv \langle\mathbf{p}_b|\hat{V}|\mathbf{p}_a\rangle = \int d^3x e^{i(\mathbf{p}_b-\mathbf{p}_a)\mathbf{x}/\hbar}V(\mathbf{x}) = \tilde{V}(\mathbf{p}_b - \mathbf{p}_a) \tag{3.911}$$

[recall (1.494)]. Inserting a damping factor $e^{\eta t_1}$ into the time integral, and replacing $\mathbf{p}^2/2M$ by the corresponding energy E, we obtain

$$\frac{i}{\hbar}\langle\mathbf{p}_b|\mathcal{A}_{\rm int}|\mathbf{p}_a\rangle_0 \;\;=\;\; -\frac{1}{E_b - E_a - i\eta}V_{\mathbf{p}_b\mathbf{p}_a}\, e^{iE_a t_a}. \tag{3.912}$$

Inserting this together with (3.906) into the expansion (3.905), we find for the scattering amplitude (3.903) the first-order approximation

$$\langle \mathbf{p}_b|\hat{S}|\mathbf{p}_a\rangle \equiv \lim_{t_b-t_a\to\infty} e^{i(E_b-E_a)t_b/\hbar}\left[(2\pi\hbar)^3\delta^{(3)}(\mathbf{p}_b-\mathbf{p}_a)-\frac{1}{E_b-E_a-i\eta}V_{\mathbf{p}_b\mathbf{p}_a}\right] \tag{3.913}$$

corresponding precisely to the first-order approximation of the operator expression (1.519), the Born approximation.

Continuing the evaluation of the expansion (3.905) we find that $V_{\mathbf{p}_b\mathbf{p}_a}$ in (3.913) is replaced by the T-matrix [recall (1.477)]

$$\begin{aligned} T_{\mathbf{p}_b\mathbf{p}_a} &= V_{\mathbf{p}_b\mathbf{p}_a} - \int\frac{d^3p_c}{(2\pi\hbar)^3}V_{\mathbf{p}_b\mathbf{p}_c}\frac{1}{E_c-E_a-i\eta}V_{\mathbf{p}_c\mathbf{p}_a} \qquad (3.914)\\ &+ \int\frac{d^3p_c}{(2\pi\hbar)^3}\int\frac{d^3p_d}{(2\pi\hbar)^3}V_{\mathbf{p}_b\mathbf{p}_c}\frac{1}{E_c-E_a-i\eta}V_{\mathbf{p}_c\mathbf{p}_d}\frac{1}{E_d-E_a-i\eta}V_{\mathbf{p}_d\mathbf{p}_a}+\dots\ . \end{aligned}$$

This amounts to an integral equation

$$T_{\mathbf{p}_b\mathbf{p}_a} = V_{\mathbf{p}_b\mathbf{p}_a} - \int\frac{d^3p_c}{(2\pi\hbar)^3}V_{\mathbf{p}_b\mathbf{p}_c}\frac{1}{E_c-E_a-i\eta}T_{\mathbf{p}_c\mathbf{p}_a}, \tag{3.915}$$

which is recognized as the Lippmann-Schwinger equation (1.525) for the T-matrix.

3.27 Functional Determinants from Green Functions

In Subsection 3.2.1 we have seen that there exists a simple method, due to Wronski, for constructing Green functions of the differential equation (3.27),

$$\mathcal{O}(t)G_{\omega^2}(t,t') \equiv [-\partial_t^2-\Omega^2(t)]G_{\omega^2}(t,t') = \delta(t-t'), \tag{3.916}$$

with Dirichlet boundary conditions. That method did not require any knowledge of the spectrum and the eigenstates of the differential operator $\mathcal{O}(t)$, except for the condition that zero-modes are absent. The question arises whether this method can be used to find also functional determinants.[22] The answer is positive, and we shall now demonstrate that Gelfand and Yaglom's initial-value problem (2.213), (2.214), (2.215) with the Wronski construction (2.225) for its solution represents the most concise formula for the functional determinant of the operator $\mathcal{O}(t)$. Starting point is the observation that a functional determinant of an operator $\mathcal{O}$ can be written as

$$\mathrm{Det}\,\mathcal{O} = e^{\mathrm{Tr}\,\log\mathcal{O}}, \tag{3.917}$$

and that a Green function of a harmonic oscillator with an arbitrary time-dependent frequency has the integral

$$\begin{aligned} \mathrm{Tr}\left\{\int_0^1 dg\,\Omega^2(t)[-\partial_t^2-g\Omega^2(t)]^{-1}\delta(t-t')\right\} &= -\mathrm{Tr}\left\{\log[-\partial_t^2-\Omega^2(t)]\delta(t-t')\right\}\\ &\quad+\mathrm{Tr}\left\{\log[-\partial_t^2]\delta(t-t')\right\}. \qquad (3.918) \end{aligned}$$

[22]See the reference in Footnote 6 on p. 247.

If we therefore introduce a strength parameter $g \in [0,1]$ and an auxiliary Green function $G_g(t,t')$ satisfying the differential equation

$$\mathcal{O}_g(t)G_g(t,t') \equiv [-\partial_t^2 - g\Omega^2(t)]G_g(t,t') = \delta(t-t'), \tag{3.919}$$

we can express the ratio of functional determinants $\text{Det}\,\mathcal{O}_1/\text{Det}\,\mathcal{O}_0$ as

$$\text{Det}\,(\mathcal{O}_0^{-1}\mathcal{O}_1) = e^{-\int_0^1 dg\,\text{Tr}\,[\Omega^2(t)G_g(t,t')]}. \tag{3.920}$$

Knowing of the existence of Gelfand-Yaglom's elegant method for calculating functional determinants in Section 2.4, we now try to relate the right-hand side in (3.920) to the solution of the Gelfand-Yaglom's equations (2.215), (2.213), and (2.214):

$$\mathcal{O}_g(t)D_g(t) = 0; \quad D_g(t_a) = 0, \quad \dot{D}_g(t_a) = 1. \tag{3.921}$$

By differentiating these equations with respect to the parameter g, we obtain for the g-derivative $D_g'(t) \equiv \partial_g D_g(t)$ the inhomogeneous initial-value problem

$$\mathcal{O}_g(t)D_g'(t) = \Omega^2(t)D_g(t); \quad D_g'(t_a) = 0, \; \dot{D}_g'(t_a) = 0. \tag{3.922}$$

The unique solution of equations (3.921) can be expressed as in Eq. (2.221) in terms of an arbitrary set of solutions $\eta_g(t)$ and $\xi_g(t)$ as follows

$$D_g(t) = \frac{\xi_g(t_a)\eta_g(t) - \xi_g(t)\eta_g(t_a)}{W_g} = \Delta_g(t,t_a), \tag{3.923}$$

where W_g is the constant Wronski determinant

$$W_g = \xi_g(t)\dot{\eta}_g(t) - \eta_g(t)\dot{\xi}_g(t). \tag{3.924}$$

We may also write

$$D_g(t_b) = \frac{\text{Det}\Lambda_g}{W_g} = \Delta_g(t_b,t_a), \tag{3.925}$$

where Λ_g is the constant 2×2 -matrix

$$\Lambda_g = \begin{pmatrix} \xi_g(t_a) & \eta_g(t_a) \\ \xi_g(t_b) & \eta_g(t_b) \end{pmatrix}. \tag{3.926}$$

With the help of the solution $\Delta_g(t,t')$ of the homogenous initial-value problem (3.921) we can easily construct a solution of the inhomogeneous initial-value problem (3.922) by superposition:

$$D_g'(t) = \int_{t_a}^{t} dt'\Omega^2(t')\Delta_g(t,t')\Delta_g(t',t_a). \tag{3.927}$$

Comparison with (3.59) shows that at the final point $t = t_b$

$$D_g'(t_b) = \Delta_g(t_b,t_a)\int_{t_a}^{t_b} dt'\,\Omega^2(t')G_g(t',t'). \tag{3.928}$$

Together with (3.925), this implies the following equation for the integral over the Green function which solves (3.916) with Dirichlet's boundary conditions:

$$\mathrm{Tr}\,[\Omega^2(t)G_g(t,t')] = -\partial_g \log\left(\frac{\det\Lambda_g}{W_g}\right) = -\partial_g \log D_g(t_b). \tag{3.929}$$

Inserting this into (3.918), we find for the ratio of functional determinants the simple formula

$$\mathrm{Det}\,(\mathcal{O}_0^{-1}\mathcal{O}_g) = C(t_b,t_a)D_g(t_b). \tag{3.930}$$

The constant of g-integration, which still depends in general on initial and final times, is fixed by applying (3.930) to the trivial case $g=0$, where $\mathcal{O}_0 = -\partial_t^2$ and the solution to the initial-value problem (3.921) is

$$D_0(t) = t - t_a. \tag{3.931}$$

At $g=0$, the left-hand side of (3.930) is unity, determining $C(t_b,t_a) = (t_b-t_a)^{-1}$ and the final result for $g=1$:

$$\mathrm{Det}\,(\mathcal{O}_0^{-1}\mathcal{O}_1) = \frac{\det\Lambda_1}{W_1}\bigg/\frac{\mathrm{Det}\Lambda_0}{W_0} = \frac{D_1(t_b)}{t_b-t_a}, \tag{3.932}$$

in agreement with the result of Section 2.7.

The same method permits us to find the Green function $G_{\omega^2}(\tau,\tau')$ governing quantum statistical harmonic fluctuations which satisfies the differential equation

$$\mathcal{O}_g(\tau)G_g^{\mathrm{p,a}}(\tau,\tau') \equiv [\partial_\tau^2 - g\Omega^2(\tau)]G_g^{\mathrm{p,a}}(\tau,\tau') = \delta^{\mathrm{p,a}}(\tau-\tau'), \tag{3.933}$$

with periodic and antiperiodic boundary conditions, frequency $\Omega(\tau)$, and δ-function. The imaginary-time analog of (3.918) for the ratio of functional determinants reads

$$\mathrm{Det}\,(\mathcal{O}_0^{-1}\mathcal{O}_1) = e^{-\int_0^1 dg\,\mathrm{Tr}\,[\Omega^2(\tau)G_g(\tau,\tau')]}. \tag{3.934}$$

The boundary conditions satisfied by the Green function $G_g^{\mathrm{p,a}}(\tau,\tau')$ are

$$\begin{aligned} G_g^{\mathrm{p,a}}(\tau_b,\tau') &= \pm G_g^{\mathrm{p,a}}(\tau_a,\tau'),\\ \dot G_g^{\mathrm{p,a}}(\tau_b,\tau') &= \pm \dot G_g^{\mathrm{p,a}}(\tau_a,\tau'). \end{aligned} \tag{3.935}$$

According to Eq. (3.166), the Green functions are given by

$$G_g^{\mathrm{p,a}}(\tau,\tau') = G_g(\tau,\tau') \mp \frac{[\Delta_g(\tau,\tau_a)\pm\Delta_g(\tau_b,\tau)][\Delta_g(\tau',\tau_a)\pm\Delta_g(\tau_b,\tau')]}{\bar\Delta_g^{\mathrm{p,a}}(\tau_a,\tau_b)\cdot\Delta_g(\tau_a,\tau_b)}, \tag{3.936}$$

where [compare (3.49)]

$$\Delta(\tau,\tau') = \frac{1}{W}\left[\xi(\tau)\eta(\tau') - \xi(\tau')\eta(\tau)\right], \tag{3.937}$$

with the Wronski determinant $W = \xi(\tau)\dot{\eta}(\tau) - \dot{\xi}(\tau)\eta(\tau)$, and [compare (3.165)]

$$\bar{\Delta}_g^{\rm p,a}(\tau_a, \tau_b) = 2 \pm \partial_\tau \Delta_g(\tau_a, \tau_b) \pm \partial_\tau \Delta_g(\tau_b, \tau_a). \tag{3.938}$$

The solution is unique provided that

$$\det \bar{\Lambda}_g^{\rm p,a} = W_g\, \bar{\Delta}_g^{\rm p,a}(\tau_a, \tau_b) \neq 0. \tag{3.939}$$

The right-hand side is well-defined unless the operator $\mathcal{O}_g(t)$ has a zero-mode with $\eta_g(t_b) = \pm\eta_g(t_a),\ \dot{\eta}_g(t_b) = \pm\dot{\eta}_g(t_a)$, which would make the determinant of the 2×2 -matrix $\bar{\Lambda}_g^{\rm p,a}$ vanish.

We are now in a position to rederive the functional determinant of the operator $\mathcal{O}(\tau) = \partial_\tau^2 - \Omega^2(\tau)$ with periodic or antiperiodic boundary conditions more elegantly than in Section 2.11. For this we formulate again a homogeneous initial-value problem, but with boundary conditions dual to Gelfand and Yaglom's in Eq. (3.921):

$$\mathcal{O}_g(\tau)\bar{D}_g(\tau) = 0; \quad \bar{D}_g(\tau_a) = 1, \quad \dot{\bar{D}}_g(\tau_a) = 0. \tag{3.940}$$

In terms of the previous arbitrary set $\eta_g(t)$ and $\xi_g(t)$ of solutions of the homogeneous differential equation, the unique solution of (3.940) reads

$$\bar{D}_g(\tau) = \frac{\xi_g(\tau)\dot{\eta}_g(\tau_a) - \dot{\xi}_g(\tau_a)\eta_g(\tau)}{W_g}. \tag{3.941}$$

This can be combined with the time derivative of (3.923) at $\tau = \tau_b$ to yield

$$\dot{D}_g(\tau_b) + \bar{D}_g(\tau_b) = \pm[2 - \bar{\Delta}_g^{\rm p,a}(\tau_a, \tau_b)]. \tag{3.942}$$

By differentiating Eqs. (3.940) with respect to g, we obtain the following inhomogeneous initial-value problem for $\bar{D}'_g(\tau) = \partial_g \bar{D}_g(\tau)$:

$$\mathcal{O}_g(\tau)\bar{D}'_g(\tau) = \Omega^2(\tau)\bar{D}'_g(\tau); \quad \bar{D}'_g(\tau_a) = 1,\ \dot{\bar{D}}'_g(\tau_a) = 0, \tag{3.943}$$

whose general solution reads by analogy with (3.927)

$$\bar{D}'_g(\tau) = -\int_{\tau_a}^{\tau} d\tau'\, \Omega^2(\tau')\Delta_g(\tau, \tau')\dot{\Delta}_g(\tau_a, \tau'), \tag{3.944}$$

where the dot on $\dot{\Delta}_g(\tau_a, \tau')$ acts on the first imaginary-time argument. With the help of identities (3.942) and (3.943), the combination $\dot{D}'(\tau) + \bar{D}'_g(\tau)$ at $\tau = \tau_b$ can now be expressed in terms of the periodic and antiperiodic Green functions (3.166), by analogy with (3.928),

$$\dot{D}'_g(\tau_b) + \bar{D}'_g(\tau_b) = \pm\bar{\Delta}_g^{\rm p,a}(\tau_a, \tau_b)\int_{\tau_a}^{\tau_b} d\tau\, \Omega^2(\tau)G_g^{\rm p,a}(\tau, \tau). \tag{3.945}$$

Together with (3.942), this gives for the temporal integral on the right-hand side of (3.920) the simple expression analogous to (3.929)

$$\begin{aligned} \mathrm{Tr}\,[\Omega^2(\tau)G_g^{\mathrm{p,a}}(\tau,\tau')] &= -\partial_g \log\left(\frac{\det\bar\Lambda_g^{\mathrm{p,a}}}{Wg}\right) \\ &= -\partial_g \log\left[2\mp\dot D_g(\tau_b)\mp\bar D_g(\tau_b)\right], \end{aligned} \tag{3.946}$$

so that we obtain the ratio of functional determinants with periodic and antiperiodic boundary conditions

$$\mathrm{Det}\,(\tilde{\mathcal O}^{-1}\mathcal O_g) = C(t_b,t_a)\left[2\mp\dot D_g(\tau_b)\mp\bar D_g(\tau_b)\right], \tag{3.947}$$

where $\tilde{\mathcal O} = \mathcal O_0 - \omega^2 = \partial_\tau^2 - \omega^2$. The constant of integration $C(t_b,t_a)$ is fixed in the way described after Eq. (3.918). We go to $g=1$ and set $\Omega^2(\tau)\equiv\omega^2$. For the operator $\mathcal O_1^\omega \equiv -\partial_\tau^2 - \omega^2$, we can easily solve the Gelfand-Yaglom initial-value problem (3.921) as well as the dual one (3.940) by

$$D_1^\omega(\tau) = \frac{1}{\omega}\sin\omega(\tau-\tau_a),\quad \bar D_1^\omega(\tau) = \cos\omega(\tau-\tau_a), \tag{3.948}$$

so that (3.947) determines $C(t_b,t_a)$ by

$$1 = C(t_b,t_a)\begin{cases} 4\sin^2[\omega(\tau_b-\tau_a)/2] & \text{periodic case,} \\ 4\cos^2[\omega(\tau_b-\tau_a)/2] & \text{antiperiodic case.}\end{cases} \tag{3.949}$$

Hence we find the final results for periodic boundary conditions

$$\mathrm{Det}\,(\tilde{\mathcal O}^{-1}\mathcal O_1) = \frac{\det\bar\Lambda_1^{\mathrm p}}{W_1}\Big/\frac{\mathrm{Det}\bar\Lambda_1^{\omega\,\mathrm p}}{W_1^\omega} = \frac{2-\dot D_1(\tau_b)-\bar D_1(\tau_b)}{4\sin^2[\omega(\tau_b-\tau_a)/2]}, \tag{3.950}$$

and for antiperiodic boundary conditions

$$\mathrm{Det}\,(\tilde{\mathcal O}^{-1}\mathcal O_1) = \frac{\det\bar\Lambda_1^{\mathrm a}}{W_1}\Big/\frac{\mathrm{Det}\bar\Lambda_1^{\omega\,\mathrm a}}{W_1^\omega} = \frac{2+\dot D_1(\tau_b)+\bar D_1(\tau_b)}{4\cos^2[\omega(\tau_b-\tau_a)/2]}. \tag{3.951}$$

The intermediate expressions in (3.932), (3.950), and (3.951) show that the ratios of functional determinants are ordinary determinants of two arbitrary independent solutions ξ and η of the homogeneous differential equation $\mathcal O_1(t)y(t)=0$ or $\mathcal O_1(\tau)y(\tau)=0$. As such, the results are manifestly invariant under arbitrary linear transformations of these functions $(\xi,\eta)\to(\xi',\eta')$.

It is useful to express the above formulas for the ratio of functional determinants (3.932), (3.950), and (3.951) in yet another form. We rewrite the two independent solutions of the homogenous differential equation $[-\partial_t^2-\Omega^2(t)]y(t)=0$ as follows

$$\xi(t) = q(t)\cos\phi(t),\quad \eta(t) = q(t)\sin\phi(t). \tag{3.952}$$

The two functions $q(t)$ and $\phi(t)$ parametrizing $\xi(t)$ and $\eta(t)$ satisfy the constraint

$$\dot{\phi}(t)q^2(t) = W, \tag{3.953}$$

where W is the constant Wronski determinant. The function $q(t)$ is a soliton of the Ermankov-Pinney equation[23]

$$\ddot{q} + \Omega^2(t)q - W^2 q^{-3} = 0. \tag{3.954}$$

For Dirichlet boundary conditions we insert (3.952) into (3.932), and obtain the ratio of fluctuation determinants in the form

$$\text{Det}\,(\mathcal{O}_0^{-1}\mathcal{O}_1) = \frac{1}{W}\frac{q(t_a)q(t_b)\sin[\phi(t_b) - \phi(t_a)]}{t_b - t_a}. \tag{3.955}$$

For periodic or antiperiodic boundary conditions with a corresponding frequency $\Omega(t)$, the functions $q(t)$ and $\phi(t)$ in Eq. (3.952) have the same periodicity. The initial value $\phi(t_a)$ may always be assumed to vanish, since otherwise $\xi(t)$ and $\eta(t)$ could be combined linearly to that effect. Substituting (3.952) into (3.950) and (3.951), the function $q(t)$ drops out, and we obtain the ratios of functional determinants for periodic boundary conditions

$$\text{Det}\,(\tilde{\mathcal{O}}^{-1}\mathcal{O}_1) = 4\sin^2\frac{\phi(t_b)}{2}\Big/ 4\sin^2\frac{\omega(t_b - t_a)}{2}, \tag{3.956}$$

and for antiperiodic boundary conditions

$$\text{Det}\,(\tilde{\mathcal{O}}^{-1}\mathcal{O}_1) = 4\cos^2\frac{\phi(t_b)}{2}\Big/ 4\cos^2\frac{\omega(t_b - t_a)}{2}. \tag{3.957}$$

For a harmonic oscillator with $\Omega(t) \equiv \omega$, Eq. (3.954) is solved by

$$q(t) \equiv \sqrt{\frac{W}{\omega}}, \tag{3.958}$$

and Eq. (3.953) yields

$$\phi(t) = \omega(t - t_a). \tag{3.959}$$

Inserted into (3.955), (3.956), and (3.957) we reproduce the known results:

$$\text{Det}\,(\mathcal{O}_0^{-1}\mathcal{O}_1) = \frac{\sin\omega(t_b - t_a)}{\omega(t_b - t_a)}, \qquad \text{Det}\,(\tilde{\mathcal{O}}^{-1}\mathcal{O}_1) = 1.$$

[23]For more details see J. Rezende, J. Math. Phys. *25*, 3264 (1984).

Appendix 3A Matrix Elements for General Potential

The matrix elements $\langle n|\hat{V}|m\rangle$ can be calculated for an arbitrary potential $\hat{V} = V(\hat{x})$ as follows: We represent $V(\hat{x})$ by a Fourier integral as a superposition of exponentials

$$V(\hat{x}) = \int_{-i\infty}^{i\infty} \frac{dk}{2\pi i} V(k) \exp(k\hat{x}), \tag{3A.1}$$

and express $\exp(k\hat{x})$ in terms of creation and annihilation operators as $\exp(k\hat{x}) = \exp[k(\hat{a}+\hat{a}^\dagger)/\sqrt{2}]$, set $k \equiv \sqrt{2}\epsilon$, and write down the obvious equation

$$\langle n|e^{\epsilon\sqrt{2}\hat{x}}|m\rangle = \frac{1}{\sqrt{n!m!}} \frac{\partial^n}{\partial\alpha^n} \frac{\partial^m}{\partial\beta^m} \langle 0|e^{\alpha\hat{a}} e^{\epsilon(\hat{a}+\hat{a}^\dagger)} e^{\beta\hat{a}^\dagger}|0\rangle \bigg|_{\alpha=\beta=0}. \tag{3A.2}$$

We now make use of the Baker-Campbell-Hausdorff Formula (2A.1) with (2A.6), and rewrite

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]+\frac{1}{12}([\hat{A},[\hat{A},\hat{B}]]+[\hat{B},[\hat{B},\hat{A}]])+\dots}. \tag{3A.3}$$

Identifying $\hat{A}$ and $\hat{B}$ with $\hat{a}$ and $\hat{a}^\dagger$, the property $[\hat{a},\hat{a}^\dagger] = 1$ makes this relation very simple:

$$e^{\epsilon(\hat{a}+\hat{a}^\dagger)} = e^{\epsilon\hat{a}} e^{\epsilon\hat{a}^\dagger} e^{-\epsilon^2/2}, \tag{3A.4}$$

and the matrix elements (3A.2) become

$$\langle 0|e^{\alpha\hat{a}} e^{\epsilon(\hat{a}+\hat{a}^\dagger)} e^{\beta\hat{a}^\dagger}|0\rangle = \langle 0|e^{(\alpha+\epsilon)\hat{a}} e^{(\beta+\epsilon)\hat{a}^\dagger}|0\rangle e^{-\epsilon^2/2}. \tag{3A.5}$$

The bra and ket states on the right-hand side are now eigenstates of the annihilation operator $\hat{a}$ with eigenvalues $\alpha+\epsilon$ and $\beta+\epsilon$, respectively. Such states are known as *coherent states*.[24] Using once more (3A.3), we obtain

$$\langle 0|e^{(\alpha+\epsilon)\hat{a}} e^{(\beta+\epsilon)\hat{a}^\dagger}|0\rangle = e^{(\epsilon+\alpha)(\epsilon+\beta)}, \tag{3A.6}$$

and (3A.2) becomes simply

$$\langle n|e^{\epsilon\sqrt{2}\hat{x}}|m\rangle = \frac{1}{\sqrt{n!m!}} \frac{\partial^n}{\partial\alpha^n} \frac{\partial^m}{\partial\beta^m} e^{(\alpha+\epsilon)(\beta+\epsilon)} e^{-\epsilon^2/2} \bigg|_{\alpha=\beta=0}. \tag{3A.7}$$

We now calculate the derivatives

$$\frac{\partial^n}{\partial\alpha^n} \frac{\partial^m}{\partial\beta^m} e^{(\epsilon+\alpha)(\epsilon+\beta)} \bigg|_{\alpha=\beta=0} = \frac{\partial^n}{\partial\alpha^n} (\epsilon+\alpha)^m e^{\epsilon(\epsilon+\alpha)} \bigg|_{\alpha=0}. \tag{3A.8}$$

Using the chain rule of differentiation for products $f(x) = g(x)\,h(x)$:

$$f^{(n)}(x) = \sum_{l=0}^{n} \binom{n}{l} g^{(l)}(x) h^{(n-l)}(x), \tag{3A.9}$$

the right-hand side becomes

$$\begin{aligned} \frac{\partial^n}{\partial\alpha^n} (\epsilon+\alpha)^m e^{\epsilon(\epsilon+\alpha)} \bigg|_{\alpha=0} &= \sum_{l=0}^{n} \binom{n}{l} \frac{\partial^l}{\partial\alpha^l} (\epsilon+\alpha)^m \frac{\partial^{n-l}}{\partial\alpha^{n-l}} e^{\epsilon(\epsilon+\alpha)} \bigg|_{\alpha=0} \\ &= \sum_{l=0}^{n} \binom{n}{l} m(m-1)\cdots(m-l+1)\epsilon^{n+m-2l} e^{\epsilon^2}. \end{aligned} \tag{3A.10}$$

[24] The use of coherent states was advanced by R.J. Glauber, Phys. Rev. **131**, 2766 (1963).

Hence we find

$$\langle n|e^{\epsilon\sqrt{2}\hat{x}}|m\rangle = \frac{1}{\sqrt{n!m!}}\sum_{l=0}^{n}\binom{n}{l}\binom{m}{l}l!\epsilon^{n+m-2l}e^{\epsilon^2/2}. \tag{3A.11}$$

From this we obtain the matrix elements of single powers $\hat{x}^p$ by forming, with the help of (3A.9) and $(\partial^q/\partial\epsilon^q)e^{\epsilon^2/2}|_{\epsilon=0} = q!!$, the derivatives

$$\left.\frac{\partial^p}{\partial\epsilon^p}\epsilon^{n+m-2l}e^{\epsilon^2/2}\right|_{\epsilon=0} = \binom{p}{n+m-2l}[2l-(n+m-p)]!! = \frac{p!}{2^{l-(n+m-p)/2}[l-p-(n+m-p)/2]!}. \tag{3A.12}$$

The result is

$$\langle n|\hat{x}^p|m\rangle = \frac{1}{\sqrt{n!m!}}\sum_{l=(n+m-p)/2}^{\min(n,m)}\binom{n}{l}\binom{m}{l}l!\,\frac{p!}{2^{l+p-(n+m)/2}[l-(n+m-p)/2]!}. \tag{3A.13}$$

For the special case of a pure fourth-order interaction, this becomes

$$\begin{aligned}
\langle n|\hat{x}^4|n-4\rangle &= \tfrac{1}{4}\sqrt{n-3}\sqrt{n-2}\sqrt{n-1}\sqrt{n},\\
\langle n|\hat{x}^4|n-2\rangle &= \tfrac{1}{4}(4n-2)\sqrt{n-1}\sqrt{n},\\
\langle n|\hat{x}^4|n\rangle &= \tfrac{1}{4}(6n^2+6n+3),\\
\langle n|\hat{x}^4|n+2\rangle &= \tfrac{1}{4}(4n+6)\sqrt{n+1}\sqrt{n+2},\\
\langle n|\hat{x}^4|n+4\rangle &= \tfrac{1}{4}\sqrt{n+1}\sqrt{n+2}\sqrt{n+3}\sqrt{n+4}.
\end{aligned} \tag{3A.14}$$

For a general potential (3A.1) we find

$$\langle n|V(\hat{x})|m\rangle = \frac{1}{\sqrt{n!m!}}\sum_{l=0}^{n}\binom{n}{l}\binom{m}{l}l!\frac{1}{2^{l-(n+m)/2}}\int_{-i\infty}^{i\infty}\frac{dk}{2\pi i}V(k)k^{n+m-2l}e^{k^2/4}. \tag{3A.15}$$

Appendix 3B Energy Shifts for $gx^4/4$-Interaction

For the specific polynomial interaction $V(x) = gx^4/4$, the shift of the energy $E^{(n)}$ to any desired order is calculated most simply as follows. Consider the expectations of powers $\hat{x}^4(z_1)\hat{x}^4(z_2)\cdots\hat{x}^4(z_n)$ of the operator $\hat{x}(z) = (\hat{a}^\dagger z + \hat{a}z^{-1})$ between the excited oscillator states $\langle n|$ and $|n\rangle$. Here $\hat{a}$ and $\hat{a}^\dagger$ are the usual creation and annihilation operators of the harmonic oscillator, and $|n\rangle = (a^\dagger)^n|0\rangle/\sqrt{n!}$. To evaluate these expectations, we make repeated use of the commutation rules $[\hat{a},\hat{a}^\dagger] = 1$ and of the ground state property $\hat{a}|0\rangle = 0$. For $n = 0$ this gives

$$\begin{aligned}
&\langle x^4(z)\rangle_\omega = 3,\\
&\langle x^4(z_1)x^4(z_2)\rangle_\omega = 72z_1^{-2}z_2^2 + 24z_1^{-4}z_2^4 + 9,\\
&\langle x^4(z_1)x^4(z_2)x^4(z_3)\rangle_\omega = 27\cdot 8z_1^{-2}z_2^2 + 63\cdot 32z_1^{-2}z_2^{-2}z_3^4\\
&\qquad + 351\cdot 8z_1^{-2}z_3^2 + 9\cdot 8z_1^{-4}z_2^4 + 63\cdot 32z_1^{-4}z_2^2z_3^2 + 369\cdot 8z_1^{-4}z_3^4\\
&\qquad + 27\cdot 8z_2^{-2}z_3^2 + 9\cdot 8z_2^{-4}z_3^4 + 27.
\end{aligned} \tag{3B.1}$$

The cumulants are

$$\begin{aligned}
&\langle x^4(z_1)x^4(z_2)\rangle_{\omega,\mathrm{c}} = 72z_1^{-2}z_2^2 + 24z_1^{-4}z_2^4,\\
&\langle x^4(z_1)x^4(z_2)x^4(z_3)\rangle_{\omega,\mathrm{c}} = 288(7z_1^{-2}z_2^{-2}z_3^4 + 9z_1^{-2}z_3^2 + 7z_1^{-4}z_2^2z_3^2 + 10z_1^{-4}z_3^4).
\end{aligned} \tag{3B.2}$$

The powers of z show by how many steps the intermediate states have been excited. They determine the energy denominators in the formulas (3.518) and (3.519). Apart from a factor $(g/4)^n$ and a factor $1/(2\omega)^{2n}$ which carries the correct length scale of $x(z)$, the energy shifts $\Delta E = \Delta_1 E_0 + \Delta_2 E_0 + \Delta_3 E_0$ are thus found to be given by

$$\begin{aligned}
\Delta_1 E_0 &= 3, \\
\Delta_2 E_0 &= -\left(72 \cdot \frac{1}{2} + 24 \cdot \frac{1}{4}\right), \qquad (3B.3)\\
\Delta_3 E_0 &= 288\left(7 \cdot \frac{1}{2} \cdot \frac{1}{4} + 9 \cdot \frac{1}{2} \cdot \frac{1}{2} + 7 \cdot \frac{1}{4} \cdot \frac{1}{2} + 10 \cdot \frac{1}{4} \cdot \frac{1}{4}\right) = 333 \cdot 4.
\end{aligned}$$

Between excited states, the calculation is somewhat more tedious and yields

$$\langle x^4(z)\rangle_\omega = 6n^2 + 6n + 3, \qquad (3B.4)$$

$$\begin{aligned}
\langle x^4(z_1)x^4(z_2)\rangle_{\omega,\mathrm{c}} &= (16n^4 + 96n^3 + 212n^2 + 204n + 72)z_1^{-2}z_2^2 \\
&+ (n^4 + 10n^3 + 35n^2 + 50n + 24)z_1^{-4}z_2^4 \\
&+ (n^4 - 6n^3 + 11n^2 - 6n)z_1^4 z_2^{-4} \\
&+ (16n^4 - 32n^3 + 20n^2 - 4n)z_1^2 z_2^{-2}, \qquad (3B.5)
\end{aligned}$$

$$\begin{aligned}
\langle x^4(z_1)x^4(z_2)x^4(z_3)\rangle_{\omega,\mathrm{c}} &= [(16n^6 + 240n^5 + 1444n^4 + 4440n^3 + 7324n^2 + 6120n + 2016) \\
&\qquad\qquad \times (z_1^{-2}z_2^{-2}z_3^4 + z_1^{-4}z_2^2z_3^2) \\
&+ (384n^5 + 2880n^4 + 8544n^3 + 12528n^2 + 9072n + 2592)z_1^{-2}z_3^2 \\
&+ (48n^5 + 600n^4 + 2880n^3 + 6600n^2 + 7152n + 2880)z_1^{-4}z_3^4 \\
&+ (16n^6 - 144n^5 + 484n^4 - 744n^3 + 508n^2 - 120n)z_1^4 z_2^{-2}z_3^{-2} \\
&+ (-48n^5 + 360n^4 - 960n^3 + 1080n^2 - 432n)z_1^4 z_3^{-4} \\
&+ (16n^6 + 48n^5 + 4n^4 - 72n^3 - 20n^2 + 24n)z_1^2 z_2^{-4}z_3^2 \\
&+ (-384n^5 + 960n^4 - 864n^3 + 336n^2 - 48n)z_1^2 z_3^{-2} \\
&+ (16n^6 - 144n^5 + 484n^4 - 744n^3 + 508n^2 - 120n)z_1^2 z_2^2 z_3^{-4} \\
&+ (16n^6 + 48n^5 + 4n^4 - 72n^3 - 20n^2 + 24n)z_1^{-2}z_2^4 z_3^{-2}]. \qquad (3B.6)
\end{aligned}$$

From these we obtain the reduced energy shifts:

$$\Delta_1 E_0 = 6n^2 + 6n + 3, \qquad (3B.7)$$

$$\begin{aligned}
\Delta_2 E_0 &= -(16n^4 + 96n^3 + 212n^2 + 204n + 72) \cdot \tfrac{1}{2} \\
&\quad -(n^4 + 10n^3 + 35n^2 + 50n + 24) \cdot \tfrac{1}{4} \\
&\quad -(n^4 - 6n^3 + 11n^2 - 6n) \cdot \tfrac{-1}{4} \\
&\quad -(16n^4 - 32n^3 + 20n^2 - 4n) \cdot \tfrac{-1}{2} \\
&= 2 \cdot (34n^3 + 51n^2 + 59n + 21), \qquad (3B.8)
\end{aligned}$$

$$\begin{aligned}
\Delta_3 E_0 &= [(16n^6 + 240n^5 + 1444n^4 + 4440n^3 + 7324n^2 + 6120n + 2016) \cdot (\tfrac{1}{2} \cdot \tfrac{1}{4} + \tfrac{1}{4} \cdot \tfrac{1}{2}) \\
&\quad +(384n^5 + 2880n^4 + 8544n^3 + 12528n^2 + 9072n + 2592) \cdot \tfrac{1}{2} \cdot \tfrac{1}{2} \\
&\quad +(48n^5 + 600n^4 + 2880n^3 + 6600n^2 + 7152n + 2880) \cdot \tfrac{1}{4} \cdot \tfrac{1}{4} \\
&\quad +(16n^6 - 144n^5 + 484n^4 - 744n^3 + 508n^2 - 120n) \cdot \tfrac{1}{4} \cdot \tfrac{1}{2} \\
&\quad +(-48n^5 + 360n^4 - 960n^3 + 1080n^2 - 432n) \cdot \tfrac{1}{4} \cdot \tfrac{1}{4} \\
&\quad +(16n^6 + 48n^5 + 4n^4 - 72n^3 - 20n^2 + 24n) \cdot \tfrac{1}{2} \cdot \tfrac{1}{4} \\
&\quad +(-384n^5 + 960n^4 - 864n^3 + 336n^2 - 48n) \cdot \tfrac{1}{2} \cdot \tfrac{1}{2} \\
&\quad +(16n^6 - 144n^5 + 484n^4 - 744n^3 + 508n^2 - 120n) \cdot \tfrac{1}{2} \cdot \tfrac{1}{4} \\
&\quad +(16n^6 + 48n^5 + 4n^4 - 72n^3 - 20n^2 + 24n) \cdot \tfrac{1}{2} \cdot \tfrac{-1}{2}] \\
&= 4 \cdot 3 \cdot (125n^4 + 250n^3 + 472n^2 + 347n + 111). \qquad (3B.9)
\end{aligned}$$

Appendix 3C Recursion Relations for Perturbation Coefficients of Anharmonic Oscillator

Bender and Wu[25] were the first to solve to high orders recursion relations for the perturbation coefficients of the ground state energy of an anharmonic oscillator with a potential $x^2/2 + gx^4/4$. Their relations are similar to Eqs. (3.537), (3.538), and (3.539), but not the same. Extending their method, we derive here a recursion relation for the perturbation coefficients of all energy levels of the anharmonic oscillator in any number of dimensions D, where the radial potential is $l(l+D-2)/2r^2 + r^2/2 + (g/2)(a_4r^4 + a_6r^6 + \ldots + a_{2q}x^{2q})$, where the first term is the centrifugal barrier of angular momentum l in D dimensions. We shall do this in several steps.

3C.1 One-Dimensional Interaction x^4

In natural physical units with $\hbar = 1, \omega = 1, M = 1$, the Schrödinger equation to be solved reads

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + gx^4\right)\psi^{(n)}(x) = E^{(n)}\psi^{(n)}(x). \tag{3C.1}$$

At $g = 0$, this is solved by the harmonic oscillator wave functions

$$\psi^{(n)}(x, g = 0) = N^n e^{-x^2/2} H_n(x), \tag{3C.2}$$

with proper normalization constant N^n, where $H_n(x)$ are the Hermite polynomial of nth degree

$$H_n(x) = \sum_{p=0}^{n} h_n^p x^p. \tag{3C.3}$$

Generalizing this to the anharmonic case, we solve the Schrödinger equation (3C.1) with the power series ansatz

$$\psi^{(n)}(x) = e^{-x^2/2}\sum_{k=0}^{\infty}(-g)^k\,\Phi_k^{(n)}(x), \tag{3C.4}$$

$$E^{(n)} = \sum_{k=0}^{\infty} g^k E_k^{(n)}. \tag{3C.5}$$

To make room for derivative symbols, the superscript of $\Phi_k^{(n)}(x)$ is now dropped. Inserting (3C.4) and (3C.5) into (3C.1) and equating the coefficients of equal powers of g, we obtain the equations

$$x\Phi_k'(x) - n\Phi_k(x) = \frac{1}{2}\Phi_k''(x) - x^4\Phi_{k-1}(x) + \sum_{k'=1}^{k}(-1)^{k'} E_{k'}^{(n)}\Phi_{k-k'}(x), \tag{3C.6}$$

where we have inserted the unperturbed energy

$$E_0^{(n)} = n + 1/2, \tag{3C.7}$$

and defined $\Phi_k(x) \equiv 0$ for $k < 0$. The functions $\Phi_k(x)$ are anharmonic versions of the Hermite polynomials. They turn out to be polynomials of $(4k+n)$th degree:

$$\Phi_k(x) = \sum_{p=0}^{4k+n} A_k^p x^p. \tag{3C.8}$$

[25] C.M. Bender and T.T. Wu, Phys. Rev. *184*, 1231 (1969); Phys. Rev. D *7*, 1620 (1973).

In a more explicit notation, the expansion coefficients A_k^p would of course carry the dropped superscript of $\Phi_k^{(n)}$. All higher coefficients vanish:

$$A_k^p \equiv 0 \quad \text{for} \quad p \geq 4k+n+1. \tag{3C.9}$$

From the harmonic wave functions (3C.2),

$$\Phi_0(x) = N^n H_n(x) = N^n \sum_{p=0}^{n} h_n^p x^p, \tag{3C.10}$$

we see that the recursion starts with

$$A_0^p = h_n^p N^n. \tag{3C.11}$$

For levels with an even principal quantum number n, the functions $\Phi_k(x)$ are symmetric. It is convenient to choose the normalization $\psi^{(n)}(0) = 1$, such that $N^n = 1/h_n^0$ and

$$A_k^0 = \delta_{0k}. \tag{3C.12}$$

For odd values of n, the wave functions $\Phi_k(x)$ are antisymmetric. Here we choose the normalization $\psi^{(n)\prime}(0) = 3$, so that $N^n = 3/h_n^1$ and

$$A_k^1 = 3\delta_{0k}. \tag{3C.13}$$

Defining

$$A_k^p \equiv 0 \quad \text{for} \quad p < 0 \quad \text{or} \quad k < 0, \tag{3C.14}$$

we find from (3C.6), by comparing coefficients of x^p,

$$(p-n)A_k^p = \frac{1}{2}(p+2)(p+1)A_k^{p+2} + A_{k-1}^{p-4} + \sum_{k'=1}^{k}(-1)^{k'} E_{k'}^{(n)} A_{k-k'}^p. \tag{3C.15}$$

The last term on the right-hand side arises after exchanging the order of summation as follows:

$$\sum_{k'=1}^{k}(-1)^{k'} E_{k'}^{(n)} \sum_{p=0}^{4(k-k')+n} A_{k-k'}^p x^p = \sum_{p=0}^{4k+n} x^p \sum_{k'=1}^{k}(-1)^{k'} E_{k'}^{(n)} A_{k-k'}^p. \tag{3C.16}$$

For even n, Eq. (3C.15) with $p = 0$ and $k > 0$ yields [using (3C.14) and (3C.12)] the desired expansion coefficients of the energies

$$E_k^{(n)} = -(-1)^k A_k^2. \tag{3C.17}$$

For odd n, we take Eq. (3C.15) with $p = 1$ and odd $k > 0$ and find [using (3C.13) and (3C.14)] the expansion coefficients of the energies:

$$E_k^{(n)} = -(-1)^k A_k^3. \tag{3C.18}$$

For even n, the recursion relations (3C.15) obviously relate only coefficients carrying even indices with each other. It is therefore useful to set

$$n = 2n', \quad p = 2p', \quad A_k^{2p'} = C_k^{p'}, \tag{3C.19}$$

leading to

$$2(p'-n')C_k^{p'} = (2p'+1)(p'+1)C_k^{p'+1} + C_{k-1}^{p'-2} - \sum_{k'=1}^{k} C_{k'}^1 C_{k-k'}^{p'}. \tag{3C.20}$$

For odd n, the substitution

$$n = 2n' + 1 \ , \quad p = 2p' + 1 \ , \ A_k^{2p'+1} = C_k^{p'} \ , \tag{3C.21}$$

leads to

$$2(p' - n')C_k^{p'} = (2p' + 3)(p' + 1)C_k^{p'+1} + C_{k-1}^{p'-2} - \sum_{k'=1}^{k} C_{k'}^1 C_{k-k'}^{p'}. \tag{3C.22}$$

The rewritten recursion relations (3C.20) and (3C.22) are the same for even and odd n, except for the prefactor of the coefficient $C_k^{p'+1}$. The common initial values are

$$C_0^{p'} = \begin{cases} h_n^{2p'}/h_n^0 & \text{for} \quad 0 \leq p' \leq n', \\ 0 & \qquad \text{otherwise.} \end{cases} \tag{3C.23}$$

The energy expansion coefficients are given in either case by

$$E_k^{(n)} = -(-1)^k C_k^1. \tag{3C.24}$$

The solution of the recursion relations proceeds in three steps as follows. Suppose we have calculated for some value of k all coefficients $C_{k-1}^{p'}$ for an upper index in the range $1 \leq p' \leq 2(k-1) + n'$.

In a first step, we find $C_k^{p'}$ for $1 \leq p' \leq 2k + n'$ by solving Eq. (3C.20) or (3C.22), starting with $p' = 2k + n'$ and lowering p' down to $p' = n' + 1$. Note that the knowledge of the coefficients C_k^1 (which determine the yet unknown energies and are contained in the last term of the recursion relations) is not required for $p' > n'$, since they are accompanied by factors $C_0^{p'}$ which vanish due to (3C.23).

Next we use the recursion relation with $p' = n'$ to find equations for the coefficients C_k^1 contained in the last term. The result is, for even k,

$$C_k^1 = \left[(2n' + 1)(n' + 1)C_k^{n'+1} + C_{k-1}^{n'-2} - \sum_{k'=1}^{k-1} C_{k'}^1 C_{k-k'}^{n'} \right] \frac{1}{C_0^{n'}} \ . \tag{3C.25}$$

For odd k, the factor $(2n' + 1)$ is replaced by $(2n' + 3)$. These equations contain once more the coefficients $C_k^{n'}$.

Finally, we take the recursion relations for $p' < n'$, and relate the coefficients $C_k^{n'-1}, \ldots, C_k^1$ to $C_k^{n'}$. Combining the results we determine from Eq. (3C.24) all expansion coefficients $E_k^{(n)}$.

The relations can easily be extended to interactions which are an arbitrary linear combination

$$V(x) = \sum_{n=2}^{\infty} a_{2n} \epsilon^n x^{2n}. \tag{3C.26}$$

A short Mathematica program solving the relations can be downloaded from the internet.[26]

The expansion coefficients have the remarkable property of growing, for large order k, like

$$E_k^{(n)} \longrightarrow -\frac{1}{\pi} \sqrt{\frac{6}{\pi}} \frac{12}{n!} (-3)^k \Gamma(k + n + 1/2). \tag{3C.27}$$

This will be shown in Eq. (17.323). Such a factorial growth implies the perturbation expansion to have a zero radius of convergence. The reason for this will be explained in Section 17.10. At the expansion point $g = 0$, the energies possess an essential singularity. In order to extract meaningful numbers from a Taylor series expansion around such a singularity, it will be necessary to find a convergent resummation method. This will be provided by the variational perturbation theory to be developed in Section 5.14.

[26]See `http://www.physik.fu-berlin/~kleinert/b3/programs`.

3C.2 General One-Dimensional Interaction

Consider now an arbirary interaction which is expandable in a power series

$$v(x) = \sum_{k=1}^{\infty} g^k v_{k+2} x^{k+2}. \tag{3C.28}$$

Note that the coupling constant corresponds now to the square root of the previous one, the lowest interaction terms being $gv_3x^3 + g^2v_4x^4 + \dots$. The powers of g count the number of loops of the associated Feynman diagrams. Then Eqs. (3C.6) and (3C.15) become

$$x\Phi_k'(x) - n\Phi_k(x) = \frac{1}{2}\Phi_k''(x) - \sum_{k'=1}^{k}(-1)^{k'} v_{k'+2} x^{k'+2}\Phi_{k-k'} + \sum_{k'=1}^{k}(-1)^{k'} E_{k'}^{(n)}\Phi_{k-k'}(x), \tag{3C.29}$$

and

$$(p-n)A_k^p = \frac{1}{2}(p+2)(p+1)A_k^{p+2} - \sum_{k'=1}^{k}(-1)^{k'} v_{k'+2} A_{k-k'}^{p-j-2} + \sum_{k'=1}^{k}(-1)^{k'} E_{k'}^{(n)} A_{k-k'}^{p}. \tag{3C.30}$$

The expansion coefficients of the energies are, as before, given by (3C.17) and (3C.18) for even and odd n, respectively, but the recursion relation (3C.30) has to be solved now in full.

3C.3 Cumulative Treatment of Interactions x^4 and x^3

There exists a slightly different recursive treatment which we shall illustrate for the simplest mixed interaction potential

$$V(x) = \frac{M}{2}\omega^2 x^2 + gv_3x^3 + g^2v_4x^4\,. \tag{3C.31}$$

Instead of the ansatz (3C.4) we shall now factorize the wave function of the ground state as follows:

$$\psi^{(n)}(x) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{M\omega}{2\hbar}x^2 + \phi^{(n)}(x)\right], \tag{3C.32}$$

i.e., we allow for powers series expansion in the exponent:

$$\phi^{(n)}(x) = \sum_{k=1}^{\infty} g^k\, \phi_k^{(n)}(x)\,. \tag{3C.33}$$

We shall find that this expansion contains fewer terms than in the Bender-Wu expansion of the correction factor in Eq. (3C.4). For completeness, we keep here physical dimensions with explicit constants $\hbar, \omega, M$.

Inserting (3C.32) into the Schrödinger equation

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + \left(\frac{M}{2}\omega^2x^2 + gv_3x^3 + g^2v_4x^4\right) - E^{(n)}\right]\psi^{(n)}(x) = 0, \tag{3C.34}$$

we obtain, after dropping everywhere the superscript (n), the differential equation for $\phi^{(n)}(x)$:

$$-\frac{\hbar^2}{2M}\phi''(x) + \hbar\omega\, x\, \phi'(x) - \frac{\hbar^2}{2M}\left[\phi'(x)\right]^2 + gv_3x^3 + g^2v_4x^4 = n\hbar\omega + \epsilon, \tag{3C.35}$$

where ϵ denotes the correction to the harmonic energy

$$E = \hbar\omega\left(n + \frac{1}{2}\right) + \epsilon\,. \tag{3C.36}$$

We shall calculate ϵ as a power series in g:

$$\epsilon = \sum_{k=1}^{\infty} g^k \epsilon_k . \tag{3C.37}$$

From now on we shall consuder only the ground state with $n = 0$. Inserting expansion (3C.33) into (3C.35), and comparing coefficients, we obtain the infinite set of differential equations for $\phi_k(x)$:

$$-\frac{\hbar^2}{2M}\phi_k''(x) + \hbar\omega\, x\, \phi_k'(x) - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1} \phi_{k-l}'(x)\, \phi_l'(x) + \delta_{k,1} v_3 x^3 + \delta_{k,2} v_4 x^4 = \epsilon_k . \tag{3C.38}$$

Assuming that $\phi_k(x)$ is a polynomial, we can show by induction that its degree cannot be greater than $k+2$, i.e.,

$$\phi_k(x) = \sum_{m=1}^{\infty} c_m^{(k)}\, x^m , \qquad \text{with } c_m^{(k)} \equiv 0 \quad \text{for } m > k+2 , \tag{3C.39}$$

The lowest terms $c_0^{(k)}$ have been omitted since they will be determined at the end the normalization of the wave function $\psi(x)$. Inserting (3C.39) into (3C.38) for $k = 1$, we find

$$c_1^{(1)} = -\frac{v_3}{M\omega^2}, \quad c_2^{(1)} = 0, \qquad c_3^{(1)} = -\frac{v_3}{3\hbar\omega}, \qquad \epsilon_1 = 0 . \tag{3C.40}$$

For $k = 2$, we obtain

$$c_1^{(2)} = 0, \;\; c_2^{(2)} = \frac{7v_3^2}{8M^2\omega^4} - \frac{3v_4}{4M\omega^2}, \;\; c_3^{(2)} = 0, \;\; c_4^{(2)} = \frac{v_3^2}{8M\hbar\omega^3} - \frac{v_4}{4\hbar\omega}, \tag{3C.41}$$

$$\epsilon_2 = -\frac{11 v_3^2 \hbar^2}{8M^3\omega^4} + \frac{3v_4\hbar^2}{4M^2\omega^2} . \tag{3C.42}$$

For the higher-order terms we must solve the recursion relations

$$c_m^{(k)} = \frac{(m+2)(m+1)\hbar}{2mM\omega}\, c_{m+2}^{(k)} + \frac{\hbar}{2mM\omega}\sum_{l=1}^{k-1}\sum_{n=1}^{m+1} n(m+2-n)\, c_n^{(l)}\, c_{m+2-n}^{(k-l)}, \tag{3C.43}$$

$$\epsilon_k = -\frac{\hbar^2}{M}\, c_2^{(k)} - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1} c_1^{(l)}\, c_1^{(k-l)} . \tag{3C.44}$$

Evaluating this for $k = 3$ yields

$$\begin{aligned} c_1^{(3)} &= -\frac{5v_3^3\hbar}{M^4\omega^7} + \frac{6v_3v_4\hbar}{M^3\omega^5}, \;\; c_2^{(3)} = 0, \;\; c_3^{(3)} = -\frac{13v_3^3}{12M^3\omega^6} + \frac{3v_3v_4}{2M^2\omega^4}, \\ & c_4^{(3)} = 0, \;\; c_5^{(3)} = -\frac{v_3^3}{10M^2\hbar\omega^5} + \frac{v_3v_4}{5M\hbar\omega^3}, \;\; \epsilon_3 = 0, \end{aligned} \tag{3C.45}$$

and for $k = 4$:

$$\begin{aligned} c_1^{(4)} &= 0, \;\; c_2^{(4)} = \frac{305v_3^4\hbar}{32M^5\omega^9} - \frac{123v_3^2v_4\hbar}{8M^4\omega^7} + \frac{21v_4^2\hbar}{8M^3\omega^5}, \;\; c_3^{(4)} = 0, \;\; c_4^{(4)} = \frac{99v_3^4}{64M^4\omega^8} - \frac{47v_3^2v_4}{16M\omega^6} + \frac{11v_4^2}{16M^2\omega^4}, \\ c_5^{(4)} &= 0, \;\; c_6^{(4)} = \frac{5v_3^4}{48M^3\hbar\omega^7} - \frac{v_3^2v_4}{4M^2\hbar\omega^5} + \frac{v_4^2}{12M\hbar\omega^3}, \end{aligned} \tag{3C.46}$$

$$\epsilon_4 = -\frac{465v_3^4\hbar^3}{32M^6\omega^9} + \frac{171v_3^2v_4\hbar^3}{8M^5\omega^7} - \frac{21v_4^2\hbar^3}{8M^4\omega^5} . \tag{3C.47}$$

The general form of the coefficients is, now in natural units with $\hbar = 1$, $M = 1$,:

$$c_m^{(k)} = \sum_{\lambda=0}^{\lfloor k/2 \rfloor} \frac{v_3^{k-2\lambda} v_4^{\lambda}}{\omega^{5k/2-m/2-2\lambda}} c_{m,\lambda}^{(k)}, \quad \text{with } c_{m,\lambda}^{(k)} \equiv 0 \text{ for } m > k+2, \text{ or } \lambda > \left\lfloor \frac{k}{2} \right\rfloor, \tag{3C.48}$$

$$\epsilon_k = \sum_{\lambda=0}^{\lfloor k/2 \rfloor} \frac{v_3^{k-2\lambda} v_4^{\lambda}}{\omega^{5k/2-1-2\lambda}} \epsilon_{k,\lambda}. \tag{3C.49}$$

This leads to the recursion relations

$$c_{m,\lambda}^{(k)} = \frac{(m+2)(m+1)}{2m} c_{m+2,\lambda}^{(k)} + \frac{1}{2m} \sum_{l=1}^{k-1} \sum_{n=1}^{m+1} \sum_{\lambda'=0}^{\lambda} n(m+2-n) c_{n,\lambda-\lambda'}^{(l)} c_{m+2-n,\lambda'}^{(k-l)}, \tag{3C.50}$$

with $c_{m,\lambda}^{(k)} \equiv 0$ for $m > k+2$ or $\lambda > \lfloor k/2 \rfloor$. The starting values follow by comparing (3C.40) and (3C.41) with (3C.48):

$$c_{1,0}^{(1)} = -1, \quad c_{2,0}^{(1)} = 0, \quad c_{3,0}^{(1)} = -\frac{1}{3}, \tag{3C.51}$$

$$\begin{aligned} &c_{1,0}^{(2)} = 0, \quad c_{1,1}^{(2)} = 0, \quad c_{2,0}^{(2)} = \frac{7}{8}, \quad c_{2,1}^{(2)} = -\frac{3}{4}, \\ &c_{3,0}^{(2)} = 0, \quad c_{3,1}^{(2)} = 0, \quad c_{4,0}^{(2)} = \frac{1}{8}, \quad c_{4,1}^{(2)} = -\frac{1}{4}. \end{aligned} \tag{3C.52}$$

The expansion coefficients $\epsilon_{k,\lambda}$ for the energy corrections ϵ_k are obtained by inserting (3C.49) and (3C.48) into (3C.44) and going to natural units:

$$\epsilon_{k,\lambda} = -c_{2,\lambda}^{(k)} - \frac{1}{2} \sum_{l=1}^{k-1} \sum_{\lambda'=0}^{\lambda} c_{1,\lambda-\lambda'}^{(l)} c_{1,\lambda'}^{(k-l)}. \tag{3C.53}$$

Table 3.1 shows the nonzero even energy corrections ϵ_k up to the tenth order.

3C.4 Ground-State Energy with External Current

In the presence of a constant external current j, the time-independent Schrödinger reads

$$-\frac{\hbar^2}{2M} \psi''(x) + \left(\frac{M}{2} \omega^2 x^2 + g v_3 x^3 + g^2 v_4 x^4 - jx \right) \psi(x) = E \psi(x). \tag{3C.54}$$

For zero coupling constant $g = 0$, we may simply introduce the new variables x' and E':

$$x' = x - \frac{j}{M\omega^2} \quad \text{and} \quad E' = E + \frac{j^2}{2M\omega^2}, \tag{3C.55}$$

and the system becomes a harmonic oscillator in x' with energy $E' = \hbar\omega/2$. Thus we make the ansatz for the wave function

$$\psi(x) \propto e^{\phi(x)}, \quad \text{with} \quad \phi(x) = \frac{j}{\hbar\omega} x - \frac{M\omega}{2\hbar} x^2 + \sum_{k=1}^{\infty} g^k \phi_k(x), \tag{3C.56}$$

and for the energy

$$E(j) = \frac{\hbar\omega}{2} - \frac{j^2}{2M\omega^2} + \sum_{k=1}^{\infty} g^k \epsilon_k. \tag{3C.57}$$

k	ϵ_k
2	$\dfrac{-11v_3^2+6v_4\omega^2}{8\omega^4}$
4	$-\dfrac{465v_3^4-684v_3^2v_4\omega^2+84v_4^2\omega^4}{32\omega^9}$
6	$\dfrac{-39709v_3^6+91014v_3^4v_4\omega^2-47308v_3^2v_4^2\omega^4+2664v_4^3\omega^6}{128\omega^{14}}$
8	$-3(6416935v_3^8-19945048v_3^6v_4\omega^2+18373480v_3^4v_4^2\omega^4$ $+4962400v_3^2v_4^3\omega^6 164720v_4^4\omega^8)/(2048\omega^{19})$
10	$(-2944491879v_3^{10}+11565716526v_3^8v_4\omega^2-15341262168v_3^6v_4^2\omega^4$ $+7905514480v_3^4v_4^3\omega^6-1320414512v_3^2v_4^4\omega^8+29335392v_4^5\omega^{10})/(8192\omega^{24})$

Table 3.1 Expansion coefficients for the ground-state energy of the anharmonic oscillator (3C.31) up to the 10th order.

The equations (3C.38) become now

$$-\frac{\hbar^2}{2M}\phi_k''(x)-\frac{\hbar^2}{2M}\sum_{l=1}^{k-1}\phi_{k-l}'(x)\phi_l'(x)+\left(\hbar\omega x-\frac{j\hbar}{M\omega}\right)\phi_k'(x)+\delta_{k,1}v_3x^3+\delta_{k,2}v_4x^4=\epsilon_k. \tag{3C.58}$$

The results are now for $k=1$

$$c_1^{(1)}=-\frac{v_3}{M\omega^2}-\frac{j^2v_3}{M^2\hbar\omega^5},\ c_2^{(1)}=-\frac{jv_3}{2M\hbar\omega^3},\ c_3^{(1)}=-\frac{v_3}{3\hbar\omega},\ \epsilon_1=\frac{3\hbar jv_3}{2M\omega^3}+\frac{j^3v_3}{M^3\omega^6}, \tag{3C.59}$$

and for $k=2$:

$$\begin{aligned}
c_1^{(2)} &= \frac{17jv_3^2}{4M^3\omega^6}+\frac{4j^3v_3^2}{M^4\hbar\omega^9}-\frac{5jv_4}{2M^2\omega^4}-\frac{j^3v_4}{M^3\hbar\omega^7},\\
c_2^{(2)} &= \frac{7v_3^2}{8M^2\omega^4}+\frac{3j^2v_3^2}{2M^3\hbar\omega^7}-\frac{3v_4}{4M\omega^2}-\frac{j^2v_4}{2M^2\hbar\omega^5},\\
c_3^{(2)} &= \frac{jv_3^2}{2M^2\hbar\omega^5}-\frac{jv_4}{3M\hbar\omega^3},\quad c_4^{(2)}=\frac{v_3^2}{8M\hbar\omega^3}-\frac{v_4}{4\hbar\omega},\\
\epsilon_2 &= -\frac{11\hbar^2v_3^2}{8M^3\omega^4}-\frac{27\hbar j^2v_3^2}{4M^4\omega^7}-\frac{9j^4v_3^2}{2M^5\omega^{10}}+\frac{3\hbar^2v_4}{4M^2\omega^2}+\frac{3\hbar j^2v_4}{M^3\omega^5}+\frac{j^4v_4}{M^4\omega^8}.
\end{aligned} \tag{3C.60}$$

The recursive equations (3C.43) and (3C.44) become

$$\begin{aligned}
c_m^{(k)} &= \frac{(m+2)(m+1)\hbar}{2mM\omega}c_{m+2}^{(k)}+\frac{\hbar}{2mM\omega}\sum_{l=1}^{k-1}\sum_{n=1}^{m+1}n(m+2-n)c_n^{(l)}c_{m+2-n}^{(k-l)}\\
&\quad+\frac{j(m+1)}{Mm\omega^2}c_{m+1}^{(k)},
\end{aligned} \tag{3C.61}$$

$$\epsilon_k = -\frac{j\hbar}{M\omega}c_1^{(k)} - \frac{\hbar^2}{M}c_2^{(k)} - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1} c_1^{(l)}c_1^{(k-l)}. \tag{3C.62}$$

Table 3.2 shows the energy corrections ϵ_k in the presence of an external current up to the sixth order using natural units, $\hbar = 1$, $M = 1$.

k	ϵ_k
1	$\dfrac{v_3 j(2j^2+3\omega^3)}{2\omega^6}$
2	$\dfrac{2v_4\omega^2(4j^4+12j^2\omega^3+3\omega^6)-v_3^2(36j^4+54j^2\omega^3+11\omega^6)}{8\omega^{10}}$
3	$\dfrac{v_3 j[3v_3^2(36j^4+63j^2\omega^3+22\omega^6)-2v_4\omega^2(24j^4+66j^2\omega^3+31\omega^6)]}{4\omega^{14}}$
4	$[36v_3^2v_4\omega^2(112j^6+324j^4\omega^3+212j^2\omega^6+19\omega^9)$ $-4v_4^2\omega^4(64j^6+264j^4\omega^3+248j^2\omega^6+21\omega^9)$ $-3v_3^4(2016j^6+4158j^4\omega^3+2112j^2\omega^6+155\omega^9)]/(32\omega^{10})$
5	$v_3 j[27v_3^4(1728j^6+4158j^4\omega^3+2816j^2\omega^6+465\omega^9)$ $+4v_4^2\omega^4(1536j^6+6408j^4\omega^3+7072j^2\omega^6+1683\omega^9)$ $-12v_3^2v_4\omega^2(3456j^6+10908j^4\omega^3+9176j^2\omega^6+1817\omega^9)]/(32\omega^{22})$
6	$[8v_4^3\omega^6(1536j^8+8544j^6\omega^3+14144j^4\omega^6+6732j^2\omega^9+333\omega^{12})$ $-4v_3^2v_4^2\omega^4(103680j^8+454032j^6\omega^3+584928j^4\omega^6+221706j^2\omega^9+11827\omega^{12})$ $+6v_3^4v_4\omega^2(285120j^8+991224j^6\omega^3+1024224j^4\omega^6+323544j^2\omega^9+15169\omega^{12})$ $-v_3^6(1539648j^8+4266108j^6\omega^3+3649536j^4\omega^6+979290j^2\omega^9+39709\omega^{12})]/(128\omega^{26})$

Table 3.2 Expansion coefficients for the ground-state energy of the anharmonic oscillator (3C.31) in the presence of an external current up to the 6th order.

3C.5 Recursion Relation for Effective Potential

It is possible to derive a recursion relation directly for the zero-temperature effective potential (5.259). To this we observe that according to Eq. (3.774), the fluctuating part of the effective potential is given by the Euclidean path integral

$$e^{-\beta V_{\rm eff}^{\rm fl}(X)} = \int \mathcal{D}\delta x \exp\left(-\frac{1}{\hbar}\left\{\mathcal{A}[X+\delta x]-\mathcal{A}[X]-\mathcal{A}_X[X]\delta x - V_{{\rm eff}\,X}^{\rm fl}(X)\delta x\right\}\right). \tag{3C.63}$$

This can be rewritten as [recall (3.771)]

$$e^{-\beta[V_{\rm eff}(X)-V(X)]} = \oint \mathcal{D}\delta x \, \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \right.$$
$$\left. \times \left[\frac{M}{2}\delta\dot{x}^2(\tau)+V(X+\delta x)-V(X)-V_{\rm eff}'(X)\delta x\right]\right\}. \tag{3C.64}$$

Going back to the integration variable $x = X + \delta x$, and taking all terms depending only on X to the left-hand side, this becomes

$$e^{-\beta[V_{\rm eff}(X)-V'_{\rm eff}(X)X]} = \oint \mathcal{D}x \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}^2(\tau) + V(x) - V'_{\rm eff}(X)x\right]\right\}. \tag{3C.65}$$

In the limit of zero temperature, the right-hand side is equal to $e^{-\beta E^{(0)}(X)}$, where $E^{(0)}(X)$ is the ground state of the Schrödinger equation associated with the path integral. Hence we obtain

$$-\frac{\hbar^2}{2M}\psi''(x) + [V(x) - V'_{\rm eff}(X)x]\psi(x) = [V_{\rm eff}(X) - V'_{\rm eff}(X)X]\psi(x). \tag{3C.66}$$

For the mixed interaction of the previous subsection, this reads

$$\begin{aligned}-\frac{\hbar^2}{2M}\psi''(x) + \left[\frac{M}{2}\omega^2x^2 + gv_3x^3 + g^2v_4x^4 - V'_{\rm eff}(X)x\right]\psi(x)&\\ = [V_{\rm eff}(X) - V'_{\rm eff}(X)X]\,\psi(x),&\end{aligned} \tag{3C.67}$$

and may be solved recursively. We expand the effective potential in powers of is expanded in the coupling constant g:

$$V_{\rm eff}(X) = \sum_{k=0}^{\infty} g^k V_k(X)\,, \tag{3C.68}$$

and assume $V_k(X)$ to be a polynomial in X:

$$V_k(X) = \sum_{m=0}^{k+2} C_m^{(k)} X^m\,. \tag{3C.69}$$

Comparison with Eq. (3C.54) shows that we may set $j = V'_{\rm eff}(X)$ and calculate $V_{\rm eff}(X) - V'_{\rm eff}(X)X$ by analogy to the energy in (3C.57). Inserting the ansatz (3C.68), (3C.69) into (3C.67) we find all equations for $V_k(X)$ by comparing coefficients of g^k and X^m. It turns out that for even or odd k, also $V_k(X)$ is even or odd in X, respectively. Table 3.3 shows the first six orders of the effective potential, which have been obtained in this way.

The equations for $V_k(X)$ are obtained as follows. We insert into (3C.67) the ansatz for the wave function $\psi(x) \propto e^{\phi(x)}$ with

$$\phi(x) = \frac{M\omega X}{\hbar}x - \frac{M\omega}{2\hbar}x^2 + \sum_{k=1}^{\infty} g^k\phi_k(x), \tag{3C.70}$$

and expand

$$V_{\rm eff}(X) = \frac{\hbar\omega}{2} + \frac{M}{2}\omega^2X^2 + \sum_{k=1}^{\infty} g^k V_k(X), \tag{3C.71}$$

to obtain the set of equations

$$\begin{aligned}-\frac{\hbar^2}{2M}\phi_k''(x) - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1}\phi'_{k-l}(x)\phi'_l(x) + \hbar\omega(x-X)\phi'_k(x) - xV'_k(X) + \delta_{k,1}v_3x^3 + \delta_{k,2}v_4x^4&\\ = V_k(X) - V'_k(X)X.&\end{aligned} \tag{3C.72}$$

From these we find for $k = 1$:

$$c_1^{(1)} = \frac{v_3}{2M\omega^2} + \frac{2v_3X^2}{\hbar\omega},\ c_2^{(1)} = -\frac{v_3X}{2\hbar\omega},\ c_3^{(1)} = -\frac{v_3}{3\hbar\omega},\ V_1(X) = \frac{3v_3\hbar}{2M\omega} + v_3X^3, \tag{3C.73}$$

k	$V_k(X)$
0	$\dfrac{\omega}{2}+\dfrac{\omega^2}{2}X^2$
1	$v_3X^3+\dfrac{3v_3}{2\omega}X$
2	$v_4X^4-\dfrac{v_3^2(1+9\omega X^2)+v_4\omega^2(3+12\omega X^2)}{4\omega^4}$
3	$\dfrac{v_3X[3v_3^2(4+9\omega X^2)-2v_4\omega^2(13+18\omega X^2)]}{4\omega^6}$
4	$-[4v_4^2\omega^4(21+104\omega X^2+72\omega^2X^4)-12v_3^2v_4\omega^2(13+152\omega X^2+108\omega^2X^4)$ $+v_3^4(51+864\omega X^2+810\omega^2X^4)]/(32\omega^9)$
5	$3v_3X[9v_3^4(51+256\omega X^2+126\omega^2X^4)+4v_4^2\omega^4(209+544\omega X^2+216\omega^2X^4)$ $-4v_3^2v_4\omega^2(341+1296\omega X^2+540\omega^2X^4)]/(32\omega^{11})$
6	$[24v_4^3\omega^6(111+836\omega X^2+1088\omega^2X^4+288\omega^3X^6)$ $-36v_3^2v_4^2\omega^4(365+5654\omega X^2+8448\omega^2X^4+2160\omega^3X^6)$ $+6v_3^4v_4\omega^2(2129+46008\omega X^2+85248\omega^2X^4+22680\omega^3X^6)$ $-v_3^6(3331+90882\omega X^2+207360\omega^2X^4+61236\omega^3X^6)]/(128\omega^{14})$

Table 3.3 Effective potential of the anharmonic oscillator (3C.31) up to the 6th order, expanded in the coupling constant g (in natural units with $\hbar=1$ and $M=1$). The lowest terms agree, of course, with the two-loop result (3.770).

and for $k=2$:

$$\begin{aligned} c_1^{(2)} &= -\frac{13v_3^2X}{4M^2\omega^4}-\frac{2v_3^2X^3}{M\hbar\omega^3}+\frac{7v_4X}{2M\omega^2}+\frac{3v_4X^3}{\hbar\omega},\quad c_2^{(2)}=\frac{v_3^2}{8M^2\omega^4}-\frac{3v_4}{4M\omega^2}-\frac{v_4X^2}{2\hbar\omega},\\ c_3^{(2)} &= \frac{v_3^2X}{2M\hbar\omega^3}-\frac{v_4X}{3\hbar\omega}c_4^{(2)}=\frac{v_3^2}{8M\hbar\omega^3}-\frac{v_4}{4\hbar\omega}, \end{aligned} \tag{3C.74}$$

$$V_2(X) = -\frac{\hbar^2v_3^2}{4M^3\omega^4}-\frac{9\hbar v_3^2X^2}{4M^2\omega^3}+\frac{3\hbar^2v_4}{4M^2\omega^2}+\frac{3\hbar v_4X^2}{M\omega}+v_4X^4. \tag{3C.75}$$

For $k\geq 3$, we must solve recursively

$$\begin{aligned} c_m^{(k)} &= \frac{(m+2)(m+1)\hbar}{2mM\omega}c_{m+2}^{(k)}+\frac{\hbar}{2mM\omega}\sum_{l=1}^{k-1}\sum_{n=1}^{m+1}n(m+2-n)c_n^{(l)}c_{m+2-n}^{(k-l)}\\ &\quad+\frac{X(m+1)}{m}c_{m+1}^{(k)}\ \text{for } m\geq 2 \text{ and with } c_m^{(k)}\equiv 0 \text{ for } m>k+2, \end{aligned} \tag{3C.76}$$

$$c_1^{(k)} = \frac{3\hbar}{M\omega}c_3^{(k)}+2Xc_2^{(k)}+\frac{\hbar}{M\omega}\sum_{l=1}^{k-1}\left(c_2^{(k-l)}c_1^{(l)}+c_1^{(k-l)}c_2^{(l)}\right)+\frac{1}{\hbar\omega}V_k'(X), \tag{3C.77}$$

$$V_k(X) = -\frac{\hbar^2}{M}c_2^{(k)} - \frac{3\hbar^2}{M}Xc_3^{(k)} - 2\hbar\omega X^2 c_2^{(k)} - \frac{\hbar^2}{M}X\sum_{l=1}^{k-1}\left(c_2^{(k-l)}c_1^{(l)} + c_1^{(k-l)}c_2^{(l)}\right)$$
$$-\frac{\hbar^2}{2M}\sum_{l=1}^{k-1}c_1^{(l)}c_1^{(k-l)}. \tag{3C.78}$$

The results are listed in Table 3.3.

3C.6 Interaction r^4 in D-Dimensional Radial Oscillator

It is easy to generalize these relations further to find the perturbation expansions for the eigenvalues of the radial Schrödinger equation of an anharmonic oscillator in D dimensions

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{2}\frac{D-1}{r}\frac{d}{dr} + \frac{l(l+D-2)}{2r^2} + \frac{1}{2}r^2 + \frac{g}{4}r^4\right]R_n(r) = E^{(n)}R_n(r). \tag{3C.79}$$

The case $g = 0$ will be solved in Section 9.2, with the energy eigenvalues

$$E^{(n)} = 2n' + l + D/2 = n + D/2, \qquad n = 0, 1, 2, 3, \dots \quad , l = 0, 1, 2, 3, \dots . \tag{3C.80}$$

For a fixed principal quantum number $n = 2n_r + l$, the angular momentum runs through $l = 0, 2, \dots, n$ for even, and $l = 1, 3, \dots, n$ for odd n. There are $(n+1)(n+2)/2$ degenerate levels. Removing a factor r^l from $R_n(r)$, and defining $R_n(r) = r^l w_n(r)$, the Schrödinger equation becomes

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{2}\frac{2l+D-1}{r}\frac{d}{dr} + \frac{1}{2}r^2 + \frac{g}{4}r^4\right)w_n(r) = E^{(n)}w_n(r). \tag{3C.81}$$

The second term modifies the differential equation (3C.6) to

$$r\Phi_k'(r) - 2n'\Phi_k(r) = \frac{1}{2}\Phi_k''(r) + \frac{(2l+D-1)}{2r}\Phi_k'(r) + r^4\Phi_{k-1}(r) + \sum_{k'=1}^{k}(-1)^{k'}E_{k'}^{(n)}\Phi_{k-k'}(r). \tag{3C.82}$$

The extra terms change the recursion relation (3C.15) into

$$(p-2n')A_k^p = \frac{1}{2}[(p+2)(p+1) + (p+2)(2l+D-1)]A_k^{p+2} + A_{k-1}^{p-4} + \sum_{k'=1}^{k}(-1)^{k'}E_{k'}^{(n)}A_{k-k'}^p. \tag{3C.83}$$

For even $n = 2n' + l$ with $l = 0, 2, 4, \dots, n$, we normalize the wave functions by setting

$$C_k^0 = (2l + D)\delta_{0k}, \tag{3C.84}$$

rather than (3C.12), and obtain

$$2(p'-n')C_k^{p'} = [(2p'+1)(p'+1) + (p'+1)(l+D/2-1/2)]C_k^{p'+1} + C_{k-1}^{p'-2} - \sum_{k'=1}^{k}C_{k'}^1 C_{k-k'}^{p'}, \tag{3C.85}$$

instead of (3C.20).

For odd $n = 2n' + l$ with $l = 1, 3, 5, \dots, n$, the equations analogous to (3C.13) and (3C.22) are

$$C_k^1 = 3(2l + D)\delta_{0k} \tag{3C.86}$$

and

$$2(p'-n')C_k^{p'} = [(2p'+3)(p'+1) + (p'+3/2)(l+D/2-1/2)]C_k^{p'+1} + C_{k-1}^{p'-2} - \sum_{k'=1}^{k}C_{k'}^1 C_{k-k'}^{p'}. \tag{3C.87}$$

In either case, the expansion coefficients of the energy are given by

$$E_k^{(n)} = -\frac{(-1)^k}{2}\frac{2l+D+1}{2l+D}C_k^1. \tag{3C.88}$$

3C.7 Interaction r^{2q} in D Dimensions

A further extension of the recursion relation applies to interactions $gx^{2q}/4$. Then Eqs. (3C.20) and (3C.22) are changed in the second terms on the right-hand side which become $C_k^{p'-q}$. In a first step, these equations are now solved for $C_k^{p'}$ for $1 \leq p \leq qk+n$, starting with $p' = qk + n'$ and lowering p' down to $p' = n' + 1$. As before, the knowledge of the coefficients C_k^1 (which determine the yet unknown energies and are contained in the last term of the recursion relations) is not required for $p' > n'$. The second and third steps are completely analogous to the case $q = 2$.

The same generalization applies to the D-dimensional case.

3C.8 Polynomial Interaction in D Dimensions

If the Schrödinger equation has the general form

$$\Big[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{2}\frac{D-1}{r}\frac{d}{dr} + \frac{l(l+D-2)}{2r^2} + \frac{1}{2}r^2 \\ + \frac{g}{4}(a_4 r^4 + a_6 r^6 + \ldots + a_{2q}x^{2q})\Big] R_n(r) = E^{(n)} R_n(r), \tag{3C.89}$$

we simply have to replace in the recursion relations (3C.85) and (3C.87) the second term on the right-hand side as follows

$$C_{k-1}^{p'-2} \to a_4 C_{k-1}^{p'-2} + a_6 C_{k-1}^{p'-3} + \ldots + a_{2q} C_{k-1}^{p'-q}, \tag{3C.90}$$

and perform otherwise the same steps as for the potential $gr^{2q}/4$ alone.

Appendix 3D Feynman Integrals for $T \neq 0$

The calculation of the Feynman integrals (3.550) can be done straightforwardly with the help of the symbolic program Mathematica. The first integral in Eqs. (3.550) is trivial. The second and forth integrals are simple, since one overall integration over, say, τ_3 yields merely a factor $\hbar\beta$, due to translational invariance of the integrand along the τ-axis. The triple integrals can then be split as

$$\begin{aligned}
&\int_0^{\hbar\beta}\int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2 d\tau_3\ f(|\tau_1-\tau_2|,|\tau_2-\tau_3|,|\tau_3-\tau_1|) \\
&= \hbar\beta \int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2\ f(|\tau_1-\tau_2|,|\tau_2|,|\tau_1|) \\
&= \hbar\beta \left(\int_0^{\hbar\beta} d\tau_2 \int_0^{\tau_2} d\tau_1 f(\tau_2-\tau_1,\tau_2,\tau_1) + \int_0^{\hbar\beta} d\tau_2 \int_{\tau_2}^{\hbar\beta} d\tau_1 f(\tau_1-\tau_2,\tau_2,\tau_1)\right),
\end{aligned} \tag{3D.1}$$

to ensure that the arguments of the Green function have the same sign in each term. The lines represent the thermal correlation function

$$G^{(2)}(\tau,\tau') = \frac{\hbar}{2M\omega}\frac{\cosh\omega[|\tau-\tau'| - \hbar\beta/2]}{\sinh(\omega\hbar\beta/2)}. \tag{3D.2}$$

With the dimensionless variable $x \equiv \omega\hbar\beta$, the result for the quantities α_V^{2L} defined in (3.550) in the Feynman diagrams with L lines and V vertices is

$$a^2 = \frac{1}{2}\coth\frac{x}{2}, \tag{3D.3}$$

$$\alpha_2^4 = \frac{1}{8}\frac{1}{\sinh^2\frac{x}{2}}\left(x + \sinh x\right), \tag{3D.4}$$

$$\alpha_3^6 = \frac{1}{64}\frac{1}{\sinh^3\frac{x}{2}}\left(-3\ \cosh\frac{x}{2} + 2\,x^2\cosh\frac{x}{2} + 3\ \cosh\frac{3x}{2} + 6\,x\sinh\frac{x}{2}\right), \tag{3D.5}$$

$$\alpha_2^8 = \frac{1}{256}\frac{1}{\sinh^4\frac{x}{2}}\left(6\,x + 8\ \sinh x + \sinh 2x\right), \tag{3D.6}$$

$$\alpha_3^{10} = \frac{1}{4096}\frac{1}{\sinh^5\frac{x}{2}}\left(-40\ \cosh\frac{x}{2} + 24\,x^2\ \cosh\frac{x}{2} + 35\ \cosh\frac{3x}{2}\right.$$
$$\left. + 5\ \cosh\frac{5x}{2} + 72\,x\sinh\frac{x}{2} + 12\,x\sinh\frac{3x}{2}\right), \tag{3D.7}$$

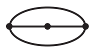
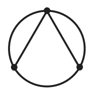
$$\alpha_3^{12} = \frac{1}{16384}\frac{1}{\sinh^6\frac{x}{2}}\left(-48 + 32\,x^2 - 3\ \cosh x + 8\,x^2\ \cosh x\right.$$
$$\left. + 48\ \cosh 2\,x + 3\ \cosh 3\,x + 108\,x\sinh x\right), \tag{3D.8}$$

$$\alpha_2^6 = \frac{1}{24}\frac{1}{\sinh^2\frac{x}{2}}\left(5 + 24\cosh x\right), \tag{3D.9}$$

$$\alpha_3^8 = \frac{1}{72}\frac{1}{\sinh^3\frac{x}{2}}\left(3\,x\cosh\frac{x}{2} + 9\ \sinh\frac{x}{2} + \sinh\frac{3x}{2}\right), \tag{3D.10}$$

$$\alpha_{3'}^{10} = \frac{1}{2304}\frac{1}{\sinh^4\frac{x}{2}}\left(30\,x + 104\sinh x + 5\sinh 2x\right). \tag{3D.11}$$

For completeness, we have also listed the integrals α_2^6, α_3^8, and $\alpha_{3'}^{10}$, corresponding to the three diagrams

 ,  ,  , (3D.12)

respectively, which occur in perturbation expansions with a cubic interaction potential x^3. These will appear in a modified version in Chapter 5.

In the low-temperature limit where $x = \omega\hbar\beta \to \infty$, the x-dependent factors α_V^{2L} in Eqs. (3D.3)–(3D.11) converge towards the constants

$$1/2,\quad 1/4,\quad 3/16,\quad 1/32,\quad 5/(8\cdot 2^5),\quad 3/(8\cdot 2^6),\quad 1/12,\quad 1/18,\ 5/(9\cdot 2^5), \tag{3D.13}$$

respectively. From these numbers we deduce the relations (3.553) and, in addition,

$$a_2^6 \to \frac{2}{3}a^6,\quad a_3^8 \to \frac{8}{9}a^8,\quad a_{3'}^{10} \to \frac{5}{9}a^{10}. \tag{3D.14}$$

In the high-temperature limit $x \to 0$, the Feynman integrals $\hbar\beta(1/\omega)^{V-1}a_V^{2L}$ with L lines and V vertices diverge like $\beta^V(1/\beta)^L$. The first V factors are due to the V-integrals over τ, the second are the consequence of the product of $n/2$ factors a^2. Thus, a_V^{2L} behaves for $x \to 0$ like

$$a_V^{2L} \propto \left(\frac{\hbar}{M\omega}\right)^L x^{V-1-L}. \tag{3D.15}$$

Indeed, the x-dependent factors α_V^{2L} in (3D.3)–(3D.11) grow like

$$\begin{aligned}
\alpha^2 &\approx 1/x + x/12 + \dots,\\
\alpha_2^4 &\approx 1/x + x^3/720,\\
\alpha_3^6 &\approx 1/x + x^5/30240 + \dots,\\
\alpha_2^8 &\approx 1/x^3 + x/120 - x^3/3780 + x^5/80640 + \dots,\\
\alpha_3^{10} &\approx 1/x^3 + x/240 - x^3/15120 + x^7/6652800 + \dots,
\end{aligned}$$

$$\begin{aligned}
\alpha_3^{12} &\approx 1/x^4 + 1/240 + x^2/15120 - x^6/4989600 + 701\, x^8/34871316480 + \dots, \\
\alpha_2^{6} &\approx 1/x^2 + x^2/240 - x^4/6048 + \dots, \\
\alpha_3^{8} &\approx 1/x^2 + x^2/720 - x^6/518400 + \dots, \\
\alpha_{3'}^{10} &\approx 1/x^3 + x/360 - x^5/1209600 + 629\, x^9/261534873600 + \dots\ .
\end{aligned} \tag{3D.16}$$

For the temperature behavior of these Feynman integrals see Fig. 3.16. We have plotted the reduced Feynman integrals $\hat{a}_V^{2L}(x)$ in which the low-temperature behaviors (3.553) and (3D.14) have been divided out of a_V^{2L}.

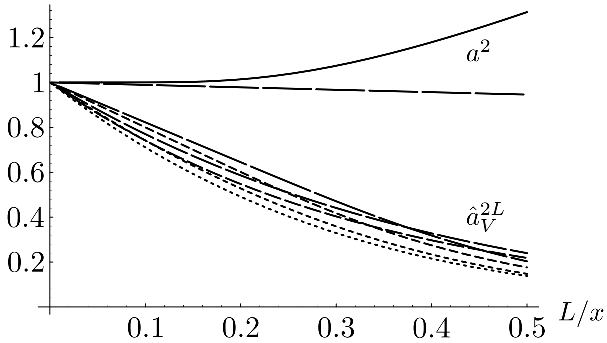


Figure 3.16 Plot of reduced Feynman integrals $\hat{a}_V^{2L}(x)$ as a function of $L/x = Lk_BT/\hbar\omega$. The integrals (3D.4)–(3D.11) are indicated by decreasing dash-lengths.

The integrals (3D.4) and (3D.5) for a_2^4 and a_3^6 can be obtained from the integral (3D.3) for a^2 by the operation

$$\frac{\hbar^n}{n!M^n}\left(-\frac{\partial}{\partial\omega^2}\right)^n = \frac{\hbar^n}{n!M^n}\left(-\frac{1}{2\omega}\frac{\partial}{\partial\omega}\right)^n, \tag{3D.17}$$

with $n=1$ and $n=2$, respectively. This follows immediately from the fact that the Green function

$$G_\omega^{(2)}(\tau,\tau') = \frac{1}{\hbar M\beta}\sum_{m=-\infty}^{\infty} e^{-i\omega_m(\tau-\tau')}\frac{\hbar}{\omega_m^2+\omega^2}, \tag{3D.18}$$

with ω^2 shifted to $\omega^2+\delta\omega^2$ can be expanded into a geometric series

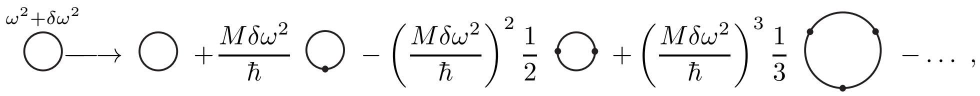
$$\begin{aligned}
pace{-}1.9cm G^{(2)}_{\sqrt{\omega^2+\delta\omega^2}}(\tau,\tau') = \frac{1}{\hbar M\beta}\sum_{m=-\infty}^{\infty} e^{-i\omega_m(\tau-\tau')}\Bigg[\frac{\hbar}{\omega_m^2+\omega^2} - \frac{\delta\omega^2}{\hbar}\frac{\hbar^2}{(\omega_m^2+\omega^2)^2} \\
pace1.0cm + \left(\frac{\delta\omega^2}{\hbar}\right)^2\frac{\hbar^3}{(\omega_m^2+\omega^2)^3} + \dots\Bigg],
\end{aligned} \tag{3D.19}$$

which corresponds to a series of convoluted τ-integrals

$$\begin{aligned}
G^{(2)}_{\sqrt{\omega^2+\delta\omega^2}}(\tau,\tau') &= G_\omega^{(2)}(\tau,\tau') - \frac{M\delta\omega^2}{\hbar}\int_0^{\hbar\beta} d\tau_1 G_\omega^{(2)}(\tau,\tau_1)G_\omega^{(2)}(\tau_1,\tau') \\
&+ \left(\frac{M\delta\omega^2}{\hbar}\right)^2\int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau_1 d\tau_2 G_\omega^{(2)}(\tau,\tau_1)G_\omega^{(2)}(\tau_1,\tau_2)G_\omega^{(2)}(\tau_2,\tau') + \dots\ .
\end{aligned} \tag{3D.20}$$

In the diagrammatic representation, the derivatives (3D.17) insert n points into a line. In quantum field theory, this operation is called a *mass insertion*. Similarly, the Feynman integral (3D.7) is obtained from (3D.6) via a differentiation (3D.17) with $n=1$ [see the corresponding diagrams in (3.550)]. A factor 4 must be removed, since the differentiation inserts a point into each of the four lines which are indistinguishable. Note that from these rules, we obtain directly the relations 1, 2, and 4 of (3.553).

Note that the same type of expansion allows us to derive the three integrals from the one-loop diagram (3.549). After inserting (3D.20) into (3.549) and re-expanding the logarithm we find the series of Feynman integrals



from which the integrals (3D.3)–(3D.5) can be extracted. As an example, consider the Feynman integral

 $= \hbar\beta \frac{1}{\omega}\, a_2^4.$

It is obtained from the second-order Taylor expansion term of the tracelog as follows:

$$-\frac{1}{2}\hbar\beta\frac{1}{\omega}a_1^4 = \frac{\hbar^2}{2!M^2}\left(\frac{\partial}{\partial\omega^2}\right)^2[-2\beta V_\omega]. \tag{3D.21}$$

A straightforward calculation, on the other hand, yields once more a_2^4 of Eq. (3D.5).

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See in particular Eqs. (51)–(61).
Its efficient graphical evaluation is given in
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