Beyond Effective Potential via Variational Perturbation Theory

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Chapter 1

Introduction

In the vast majority of cases, information about a physical system can only be obtained by means of approximation methods. This is due to the fact that the equations which describe physical phenomena normally cannot be solved analytically. Therefore, over the course of the history of physics, many different approximation techniques have been developed in order to treat non-analytically solvable systems. These methods can be roughly classified into two different categories: numerical methods, which exploit the possibility to rapidly execute calculations on a computer, and analytical approximation methods, where certain assumptions are made in order to simplify the original problem. Numerical methods have proven to be an enormously powerful and successful tool to describe even the most complicated physical scenarios, and computational physics has become an independent branch of physics itself [1]. Nevertheless, the accuracy of numerical methods is not always superior to that of analytical ones, and usually more insight into physical principles is obtained by means of analytical approximation approaches.

Perturbation theory is one of the most well-known analytical approximation methods. It can be applied when a system is exactly solvable for a particular value of a coupling constant (normally, for vanishing coupling). One then seeks to expand the physical quantity in which one is interested into a power series of the coupling constant. However, the convergence of a perturbation expansion is not at all a trivial issue. Indeed, it turns out that most perturbation series are divergent, i.e. their convergence radius vanishes. This divergence of perturbation series may, nevertheless, not necessarily be a handicap for practical calculations. Namely, for asymptotic series, the results which are obtained for small coupling constants in low orders seem to converge to the exact result so that the divergence of such a series only becomes noticeable when the expansion is driven to higher orders. However, when a system can only be described correctly in the strong-coupling limit, i.e. for large coupling constants, the original weak-coupling series will be completely inadequate to describe the system. In either case, in order for the description of a system to be closed and complete, it must be possible that the exact result can be approached to any desired accuracy, at least in principle. Therefore, it is necessary to find means for treating divergent perturbation se-

ries. For this purpose, different resummation techniques have been developed. Often, these methods are based on introducing an artificial parameter, which is later revoked from the equations by setting it to some special value or by performing some limit.

In recent years, based on a variational approach due to Feynman and Kleinert [2], a systematic and uniformly convergent *variational perturbation expansion* has been developed, which has become known as variational perturbation theory (VPT) [3–7]. VPT permits the turning of divergent weak-coupling into convergent strong-coupling expansions and has been applied successfully in different fields of physics, such as quantum mechanics, quantum statistics, field theory, condensed matter physics, theory of critical phenomena, etc. In order to examine the quality of VPT, in Refs. [8,9] its accuracy has been tested extensively for the ground-state energy of the system

$$V(x) = \frac{M}{2}\omega^2 x^2 + g x^4 \,. \tag{1.1}$$

In the strong-coupling limit, Eq. (1.1) effectively becomes a purely quartic potential. Apart from a generalization to D dimensions, one might suppose that a cubic potential would be the next easiest test system. However, for real A, the potential $V(x) = Ax^3$ is not quantum-mechanically stable. Interestingly, if the parameter A is chosen to be imaginary,

$$V(x) = ix^3 \,, \tag{1.2}$$

the spectrum of the Hamiltonian associated with (1.2) turns out to be real and positive. This remarkable property of the hence non-Hermitian Hamilton can be attributed to the fact that it obeys to a different symmetry: it is invariant under the combined application of the parity and time-reversal operation [10–14].

It is one purpose of this work to examine how VPT can be applied in the case of the imaginary cubic potential (1.2). In a first approach, the weak-coupling series of the ground-state energy for the anharmonic oscillator

$$V(x) = \frac{M}{2}\omega^2 x^2 + igx^3 \tag{1.3}$$

is resummed via VPT. In the strong-coupling limit, the potential (1.3) reduces to (1.2). It turns out that the VPT-result approaches the corresponding numerical value for the ground-state energy of (1.2), but the convergence is much slower than in the case of the quartic potential. However, the combination of VPT with another variational technique of field theory, namely the effective potential, permits the improvement of the rate of convergence of the result. In a refined approach, we thus treat the effective potential with VPT.

In Chapter 2, the effective action is introduced as the functional Legendre transform of the free energy with respect to an external current. The effective potential is obtained in the special case of the current being constant. Subsequently, the standard method for calculating the effective action or the effective potential, the background method [15,16], is presented. In

the background method, the effective potential is obtained from all one-particle irreducible vacuum Feynman diagrams. Chapter 2 ends with a diagrammatical calculation of the weak-coupling perturbation series for the ground-state energy of an anharmonic oscillator with both, cubic and quartic anharmonicity:

$$V(x) = \frac{M}{2}\omega^2 x^2 + gAx^3 + g^2 Bx^4 \; . \tag{1.4}$$

In Chapter 3, it is demonstrated how the weak-coupling perturbation series for (1.4) can be obtained more efficiently by deriving an algebraic recursion relation for the expansion coefficients using the method developed by C.M. Bender and T.T. Wu [17,18]. In the diagrammatical approach, only Feynman diagrams with a special topology, i.e. the connected vacuum diagrams, contribute to the ground-state energy. The Bender-Wu method thus yields a recursion relation for the sum of connected Feynman diagrams. In Section 3.4, we develop a recursion for the effective potential along similar lines. Since the effective potential is obtained from a subset of the connected Feynman diagrams, namely the one-particle irreducible diagrams, this amounts to a recursion relation for the sum of one-particle irreducible Feynman diagrams.

The method of VPT is introduced in Chapter 4. First, its application to the potential (1.1) is examined by resumming the corresponding perturbation series and proceeding to the strong-coupling limit. Then, in Section 4.5.1, it is shown that in the case of the oscillator with cubic anharmonicity (1.3), an analogous approach leads to results whose convergence is less satisfactory. In Section 4.5.2, it is demonstrated how the convergence can be improved by applying VPT not to the weak-coupling series of the ground-state energy, but to the effective potential.

The anharmonic oscillator (1.1) is generalized to D spatial dimensions in Chapter 5. In particular, the cases $D = 2,\ 3,\ 10$ are examined. The convergence of the result is found to improve with increasing dimension. In Section 5.2, the calculation of the effective potential by applying the background method is performed for an arbitrary rotationally symmetric potential in D dimensions up to two loops.

Finally, in the outlook, further problems to which the methods developed in this work could be extended are examined.

Chapter 2

Effective Action

In addition to the operator formalism of quantum mechanics and quantum statistics, there exists another, equivalent formalism in which operators are avoided by using infinite products of integrals, called *path integrals*. This formalism may lead to a more transparent understanding of quantum phenomena than the operator formalism [4,19,20]. In this chapter, the effective action will be introduced using the path integral formalism. While in classical mechanics all information on the dynamics of a system can be extracted from its action, in quantum statistics, the effective action permits the deriving of the statistical properties of a system.

2.1 Wick Rotation

For time-independent Hamiltonians $\hat{H}$, the time displacement operator is given by

$$\hat{U}(t_b, t_a) = e^{-i\hat{H}(t_b - t_a)/\hbar} \,. \tag{2.1}$$

Its matrix elements in the localized basis states are

$$(x_b\, t_b | x_a\, t_a) := \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle \,, \qquad t_b > t_a \,. \tag{2.2}$$

In the path integral formalism, the matrix elements of the time displacement operator can be obtained by calculating the sum over all paths in configuration space with a phase factor that contains the form of the action $\mathcal{A}[x]$ [4, Sec. 2.1]:

$$(x_b\, t_b | x_a\, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \, \exp\left\{ \frac{i}{\hbar}\, \mathcal{A}[x] \right\} \,. \tag{2.3}$$

For a point particle of mass M moving in a one-dimensional potential $V(x)$, the action is given in the form

$$\mathcal{A}[x] := \int_{t_a}^{t_b} dt \left[\frac{M}{2} \dot{x}^2(t) - V(x(t)) \right] \,. \tag{2.4}$$

Quantum statistical systems in the state of thermal equilibrium and in contact with a reservoir of temperature T are described by the density operator

$$\hat{\rho}(\beta) := \frac{1}{Z}\, e^{-\beta \hat{H}} \,, \tag{2.5}$$

where Z denotes a normalization factor,

$$Z = \mathrm{Tr}\, \left(e^{-\beta \hat{H}} \right) \,, \tag{2.6}$$

and $\beta := 1/k_B T$ is proportional to the inverse temperature. Z is called the *partition function*. It allows the determination of the bulk thermodynamic quantities for the system in question. In the local particle basis $|x\rangle$, the partition function reads

$$Z = \int_{-\infty}^{\infty} dx\, \langle x | e^{-\beta \hat{H}} | x \rangle \,. \tag{2.7}$$

Now, it is an important observation that the matrix elements of the time displacement operator $(x_b\, t_b | x_a\, t_a)$ can be linked to those of the density operator (2.5) according to the substitution

$$t_b - t_a \to -i\hbar\beta \,. \tag{2.8}$$

Setting

$$t_a = 0, \quad t_b = -i\hbar\beta \tag{2.9}$$

and performing a so-called Wick rotation [21], i.e. substituting

$$t = -i\tau \,, \tag{2.10}$$

one obtains formally identical descriptions of quantum mechanics and quantum statistics:

$$\begin{aligned} \rho(x_b, x_a; \beta) &:= \frac{1}{Z} \langle x_b | e^{-\beta \hat{H}} | x_a \rangle = \frac{1}{Z}\, (x_b\, \hbar\beta | x_a\, 0) \\ &= \frac{1}{Z} \int_{x(0)=x_a}^{x(-i\hbar\beta)=x_b} \mathcal{D}x\, \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[\frac{M}{2} \dot{x}^2(-i\tau) + V(x(-i\tau)) \right] \right\} \,. \end{aligned} \tag{2.11}$$

Here, the dot denotes the derivative with respect to the imaginary time τ, and the identity

$$\frac{d}{dt} = \frac{d\tau}{dt} \frac{d}{d\tau} = i \frac{d}{d\tau} \tag{2.12}$$

has been used. Here and in the following, the imaginary time τ always denotes a quantity within the interval $[0,\, \hbar\beta]$. Introducing a new function $\tilde{x}(\tau) = x(-i\tau)$ and renaming $\tilde{x}$ to x yields

$$(x_b\, \hbar\beta | x_a\, 0) = \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}x\, \exp\left\{ -\frac{1}{\hbar}\, \mathcal{A}[x] \right\} \,, \tag{2.13}$$

with the imaginary-time action

$$\mathcal{A}[x] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}^2(\tau) + V(x(\tau)) \right] . \tag{2.14}$$

Note that its integrand coincides with the classical Hamilton function. In the same way as the matrix elements of the density operator (2.13), the quantum-statistical partition function (2.6) in the form (2.7) can be expressed as a path integral:

$$Z = \int_{-\infty}^{\infty} dx' \int_{x(0)=x'}^{x(\hbar\beta)=x'} \mathcal{D}x \, \exp\left\{ -\frac{1}{\hbar}\,\mathcal{A}[x] \right\} =: \oint \mathcal{D}x \, \exp\left\{ -\frac{1}{\hbar}\,\mathcal{A}[x] \right\} . \tag{2.15}$$

Whereas in (2.13) the integration is performed with respect to all paths with Dirichlet boundary conditions, one has periodic boundary conditions in (2.15).

2.2 Definition of the Effective Action

In the presence of an external current $j(\tau)$, define

$$\mathcal{A}[x, j] := \mathcal{A}[x] - \int_0^{\hbar\beta} d\tau \; j(\tau)x(\tau) . \tag{2.16}$$

Consider the generating functional of all Green functions

$$Z[j] := \oint \mathcal{D}x \, \exp\left\{ -\frac{1}{\hbar}\,\mathcal{A}[x, j] \right\} , \tag{2.17}$$

where the integration runs over all periodic paths, $x(0) = x(\hbar\beta)$. Note that for a vanishing current, $j \equiv 0$, the generating functional (2.17) equals the partition function (2.15):

$$Z[j]\Big|_{j=0} \equiv Z . \tag{2.18}$$

Thus, the free energy $F := -k_B T \ln Z$ becomes a functional of the current $j(\tau)$:

$$F[j] = -\frac{1}{\beta} \ln Z[j] . \tag{2.19}$$

The expectation value of the path $x(\tau)$, i.e. the average

$$X(\tau) := X[j](\tau) := \langle x(\tau) \rangle [j] := \frac{1}{Z[j]} \oint \mathcal{D}x \, x(\tau) \, \exp\left\{ -\frac{1}{\hbar}\,\mathcal{A}[x, j] \right\} , \tag{2.20}$$

is proportional to the first functional derivative of the free energy

$$\frac{\delta F[j]}{\delta j(\tau)} = -\frac{1}{\hbar\beta} X(\tau) . \tag{2.21}$$

The last identity is obtained by replacing the path $x(\tau)$ in the integrand of the right-hand side of (2.20) with the first functional derivative with respect to the external current multiplied by the reduced Planck constant $\hbar$:

$$x(\tau) \to \hbar \, \frac{\delta}{\delta j(\tau)} \, . \tag{2.22}$$

Assume that the identity (2.21) can be inverted to yield the current $j(\tau)$ as a functional of the path average $X(\tau)$:

$$j(\tau) = j[X](\tau) \, . \tag{2.23}$$

Then, Eq. (2.21) serves as a motivation to define the functional Legendre transform of $F[j]$ with respect to the current $j(\tau)$. Due to dimensional considerations, a factor $\hbar\beta$ is included in the definition:

$$\Gamma[X] := \hbar\beta \, F[j[X]] + \int_0^{\hbar\beta} d\tau \, j[X](\tau) \, X(\tau) \, . \tag{2.24}$$

This quantity is called the *effective action*. Note that it has indeed the dimension of an action. The first functional derivative of the effective action leads to

$$\frac{\delta\Gamma[X]}{\delta X(\tau)} = \hbar\beta \int_0^{\hbar\beta} d\tau' \, \frac{\delta F[j[X]]}{\delta j[X](\tau')} \frac{\delta j[X](\tau')}{\delta X(\tau)} + \int_0^{\hbar\beta} d\tau' \, \frac{\delta j[X](\tau')}{\delta X(\tau)} X(\tau') + j[X](\tau) \, . \tag{2.25}$$

Thus, due to (2.21), one reobtains the external current:

$$\frac{\delta\Gamma[X]}{\delta X(\tau)} = j[X](\tau) \, . \tag{2.26}$$

The situation when the external current $j(\tau)$ vanishes is of particular interest. In this case, the path average $X[j](\tau)$ is denoted by

$$X_{\mathrm{e}}(\tau) := X[j \equiv 0](\tau) \, . \tag{2.27}$$

From (2.26), one reads off that the particular path average (2.27) has the property of extremizing the effective action:

$$\left. \frac{\delta\Gamma[X]}{\delta X(\tau)} \right|_{X(\tau)=X_{\mathrm{e}}(\tau)} \equiv 0 \, . \tag{2.28}$$

Furthermore, from (2.24), it follows that in the case of a vanishing current one has

$$F[0] = \frac{1}{\hbar\beta} \Gamma[X_{\mathrm{e}}] \, . \tag{2.29}$$

Thus, the free energy F can be obtained by extremizing the effective action.

The *effective potential*, which will be introduced in the following section, is closely related to the effective action. The calculation of the effective potential constitutes an approach that is less general than the concept of the effective action, since there the current $j(\tau)$ is assumed to be τ-independent. Nevertheless, the effective potential also permits the determination of the free energy.

2.3 Definition of the Effective Potential

The procedure in this section is similar to that of the previous one. In order to define the effective potential, it is assumed that the external current from the previous section $j(\tau)$ is now a τ-independent current j. It is then merely necessary to replace functionals of $j(\tau)$ by corresponding functions of j.

In the presence of an external current that is constant in the imaginary time τ, $j(\tau) \equiv j$, define

$$\mathcal{A}[x](j) := \mathcal{A}[x] - j \int_0^{\hbar\beta} d\tau\, x(\tau) = \mathcal{A}[x,j]\Big|_{j(\tau)=j} . \tag{2.30}$$

Consider the generating function

$$Z(j) := \oint \mathcal{D}x\, \exp\left\{-\frac{1}{\hbar}\,\mathcal{A}[x](j)\right\} = Z[j]\Big|_{j(\tau)=j} . \tag{2.31}$$

Again, for a vanishing current, $j = 0$, the partition function (2.15) is reobtained:

$$Z(j)\Big|_{j=0} \equiv Z . \tag{2.32}$$

And the free energy reads

$$F(j) = -\frac{1}{\beta} \ln Z(j) \tag{2.33}$$

The first derivative of $F(j)$ now yields

$$\frac{\partial F(j)}{\partial j} = -\frac{1}{\hbar\beta Z(j)} \oint \mathcal{D}x\, \exp\left\{-\frac{1}{\hbar}\,\mathcal{A}[x](j)\right\} \int_0^{\hbar\beta} d\tau\, x(\tau) =: -X . \tag{2.34}$$

As with the other definitions of this section, the quantity $X(\tau)$ defined by (2.20) becomes simply the quantity X defined by the last identity in the case of a constant current $j(\tau) \equiv j$. This is due to the fact that in the case of a τ-independent Lagrangian the path average (2.20) is also τ-independent. Furthermore, the τ-integral and the path integral in (2.34) are interchangeable, and the τ-integral thus merely gives a factor $\hbar\beta$.

Assume that (2.34) can be inverted to yield j as a function of X:

$$j = j(X) . \tag{2.35}$$

Again, (2.34) leads to the Legendre transform of $F(j)$:

$$V_{\text{eff}}(X) := F(j(X)) + j(X)X . \tag{2.36}$$

This quantity is called the effective potential. Indeed, as comparison with (2.24) shows, except for the factor $1/\hbar\beta$, it corresponds to the effective action evaluated at a constant average $X(\tau) \equiv X$:

$$V_{\text{eff}}(X) = \frac{1}{\hbar\beta}\Gamma[X]\Big|_{X(\tau)=X} . \tag{2.37}$$

Due to (2.34), the first derivative of the effective potential gives back the external current j:

$$\frac{\partial V_{\text{eff}}(X)}{\partial X} = \frac{\partial F(j(X))}{\partial j(X)} \frac{\partial j(X)}{\partial X} + \frac{\partial j(X)}{\partial X} X + j(X) = j(X) \,. \tag{2.38}$$

As above, the free energy F is obtained in the case of a vanishing current j. And therefore, according to (2.38), it can be determined by evaluating the effective potential at the average X_{e} that extremizes it.

$$F = V_{\text{eff}}(X_{\text{e}}) \,, \tag{2.39}$$

where X_{e} is determined by the condition

$$\left. \frac{\partial V_{\text{eff}}(X)}{\partial X} \right|_{X=X_{\text{e}}} = 0 \,. \tag{2.40}$$

Note that, since the free energy $F = E - TS$ equals the ground-state energy in the limit $T \to 0$, the latter can be determined from the effective potential:

$$E_0 = \lim_{T \to 0} V_{\text{eff}}(X_{\text{e}}) \,. \tag{2.41}$$

The effective potential has another remarkable property: it is convex for all values of the average X. The validity of this statement can be seen as follows. According to (2.38) the second derivative of the effective potential with respect to the average X reads

$$\frac{\partial^2 V_{\text{eff}}(X)}{\partial X^2} = \frac{\partial j(X)}{\partial X} = \left[\left. \frac{\partial X(j)}{\partial j} \right|_{j=j(X)} \right]^{-1} \,. \tag{2.42}$$

Due to (2.34), the last identity can be rewritten in the form

$$\frac{\partial^2 V_{\text{eff}}(X)}{\partial X^2} = - \left[\left. \frac{\partial^2 F(j)}{\partial j^2} \right|_{j=j(X)} \right]^{-1} \,. \tag{2.43}$$

Using the result (2.34) for the first derivative of $F(j)$ with respect to the constant current j and the definitions (2.30), (2.31), one obtains the second derivative

$$\begin{aligned} \frac{\partial^2 F(j)}{\partial j^2} \;=\; & \frac{1}{\hbar^2 \beta Z^2(j)} \left(\oint \mathcal{D}x \int_0^{\hbar\beta} d\tau \; x(\tau) \; \exp\left\{ -\frac{1}{\hbar} \mathcal{A}[x](j) \right\} \right)^2 \\ & - \frac{1}{\hbar^2 \beta Z(j)} \oint \mathcal{D}x \int_0^{\hbar\beta} d\tau_1 \; x(\tau_1) \int_0^{\hbar\beta} d\tau_2 \; x(\tau_2) \; \exp\left\{ -\frac{1}{\hbar} \mathcal{A}[x](j) \right\} \,. \end{aligned} \tag{2.44}$$

Using the definition of the expectation value in (2.20), where the current j is now constant, the last identity can be rewritten as

$$\frac{\partial^2 F(j)}{\partial j^2} = -\frac{1}{\hbar^2 \beta} \left\{ \left\langle \left[\int_0^{\hbar\beta} d\tau \; x(\tau) \right]^2 \right\rangle (j) \;-\; \left[\left\langle \int_0^{\hbar\beta} d\tau \; x(\tau) \right\rangle (j) \right]^2 \right\} \,. \tag{2.45}$$

And one obtains

$$\frac{\partial^2 F(j)}{\partial j^2} = -\frac{1}{\hbar^2 \beta} \left\langle \left[\int_0^{\hbar\beta} d\tau \; x(\tau) - \left\langle \int_0^{\hbar\beta} d\tau \; x(\tau) \right\rangle \right]^2 \right\rangle (j) \;\leq\; 0 \,. \tag{2.46}$$

Together with (2.43), this proves that the effective potential $V_{\text{eff}}(X)$ is convex for all values of the average X.

2.4 Example: Harmonic Oscillator

Consider, as an illustrative example, the harmonic oscillator with the imaginary-time action

$$\mathcal{A}_\omega[x] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\, \dot{x}^2(\tau) + \frac{M}{2}\omega^2 x^2(\tau) \right] \tag{2.47}$$

and its generating functional

$$Z_\omega[j] = \oint \mathcal{D}x \, \exp\left\{ -\frac{1}{\hbar}\, \mathcal{A}_\omega[x,j] \right\} . \tag{2.48}$$

Here, the quantity $\mathcal{A}_\omega[x,j]$ is defined as in (2.16). Inserting (2.47) into (2.48) permits the rewriting of the imaginary-time action in the integrand of the path integral:

$$Z_\omega[j] = \oint \mathcal{D}x \, \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau_1 \left[\int_0^{\hbar\beta} d\tau_2 \, \frac{1}{2}\, x(\tau_1) G_\omega^{-1}(\tau_1,\tau_2) x(\tau_2) - j(\tau_1) x(\tau_1) \right] \right\} , \tag{2.49}$$

with the integral kernel

$$G_\omega^{-1}(\tau_1,\tau_2) := \frac{\delta^2 \mathcal{A}_\omega[x]}{\delta x(\tau_1)\delta x(\tau_2)} = M \left(-\frac{d^2}{d\tau_1^2} + \omega^2 \right) \delta(\tau_1 - \tau_2) . \tag{2.50}$$

The validity of the identity (2.49) can be seen by integrating out the τ_2-integral and performing an integration by parts for the first term of the τ_1-integral. Note that the surface term vanishes since the path integration only runs over paths that are periodic in the imaginary time τ. Thus, one has:

$$x(0) = x(\hbar\beta) \qquad \text{and} \qquad \dot{x}(0) = \dot{x}(\hbar\beta) . \tag{2.51}$$

In Appendix A, the generating functional (2.49) is calculated, yielding

$$Z_\omega[j] = Z_w \, \exp\left[\frac{1}{2\hbar^2} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, G_\omega(\tau_1,\tau_2) j(\tau_1) j(\tau_2) \right] , \tag{2.52}$$

where the partition function Z_ω reads

$$Z_\omega = \frac{1}{2\sinh(\hbar\beta\omega/2)} . \tag{2.53}$$

Furthermore, the propagator $G_\omega(\tau_1,\tau_2)$ is defined as the inverse of the kernel $G_\omega^{-1}(\tau_1,\tau_2)$ by the identity

$$\int_0^{\hbar\beta} d\tau \, G_\omega^{-1}(\tau_1,\tau) G_\omega(\tau,\tau_2) \equiv \hbar \, \delta(\tau_1 - \tau_2) . \tag{2.54}$$

As shown in Appendix A, $G_\omega(\tau_1,\tau_2)$ can be expressed explicitly in the form

$$G_\omega(\tau_1,\tau_2) = \frac{\hbar}{2M\omega} \, \frac{\cosh(\omega|\tau_1 - \tau_2| - \hbar\beta\omega/2)}{\sinh(\hbar\beta\omega/2)} , \tag{2.55}$$

which in the limit $T \to 0$ simplifies to

$$\lim_{T\to 0} G_\omega(\tau_1, \tau_2) = \frac{\hbar}{2M\omega}\, e^{-\omega|\tau_1-\tau_2|} \,. \tag{2.56}$$

Note that the propagator (2.55) is symmetric in its two arguments

$$G_\omega(\tau_1, \tau_2) = G_\omega(\tau_2, \tau_1) \,. \tag{2.57}$$

Using the result (2.52), one obtains the free energy in presence of a τ-dependent external current (2.19) for the harmonic oscillator:

$$F_\omega[j] = -\frac{1}{\beta} \ln Z_\omega - \frac{1}{2\hbar^2\beta} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, G_\omega(\tau_1, \tau_2) j(\tau_1) j(\tau_2) \,. \tag{2.58}$$

Using this result together with the property (2.57) of the propagator, the identity (2.21) for the path average reduces to

$$X_\omega[j](\tau) = \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau'\, G_\omega(\tau, \tau') j(\tau') \,. \tag{2.59}$$

From the identities (2.54) and (2.59), one obtains the current $j(\tau)$ as a functional of the path average $X_\omega(\tau)$:

$$j[X_\omega](\tau) = \int_0^{\hbar\beta} d\tau'\, G_\omega^{-1}(\tau, \tau') X_\omega(\tau') \,. \tag{2.60}$$

The effective action (2.24) for the harmonic oscillator then follows from the results (2.58) and (2.60) by taking into account the identity (2.54):

$$\Gamma_\omega[X_\omega] = -\hbar \ln Z_\omega + \frac{1}{2} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, X_\omega(\tau_1) G_\omega^{-1}(\tau_1, \tau_2) X_\omega(\tau_2) \,. \tag{2.61}$$

Using the definition (2.50), the effective action can be rewritten in the form

$$\Gamma_\omega[X_\omega] = -\hbar \ln Z_\omega + \int_0^{\hbar\beta} d\tau \left[-\frac{M}{2} X_\omega(\tau) \frac{d^2}{d\tau^2} X_\omega(\tau) + \frac{M}{2} \omega^2 X_\omega^2(\tau) \right] \,. \tag{2.62}$$

Since according to the definition (2.20) the average $X_\omega(\tau)$ and its first derivative are periodic in the imaginary time τ, i.e.

$$X_\omega(0) = X_\omega(\hbar\beta) \qquad \text{and} \qquad \dot{X}_\omega(0) = \dot{X}_\omega(\hbar\beta) \,, \tag{2.63}$$

integration by parts of the first term of the integrand on the right-hand side of the identity (2.62) yields

$$\Gamma_\omega[X_\omega] = -\hbar \ln Z_\omega + \int_0^{\hbar\beta} d\tau \left[\frac{M}{2} \dot{X}_\omega^2(\tau) + \frac{M}{2} \omega^2 X_\omega^2(\tau) \right] \,. \tag{2.64}$$

Note that the extremal condition (2.28) for the path average $X_\omega(\tau)$ reduces to the classical equation of motion for the harmonic oscillator in imaginary time:

$$\left.\frac{\delta\Gamma_\omega[X_\omega]}{\delta X_\omega(\tau)}\right|_{X_\omega(\tau)=X_{\omega,\mathrm{e}}(\tau)} = \int_0^{\hbar\beta} d\tau' \left[M\dot{X}_\omega(\tau')\frac{d}{d\tau'}\delta(\tau-\tau') + M\omega^2 X_\omega(\tau')\delta(\tau-\tau')\right]\Bigg|_{X_\omega(\tau)=X_{\omega,\mathrm{e}}(\tau)}$$
$$= M\left[-\ddot{X}_{\omega,\mathrm{e}}(\tau) + \omega^2 X_{\omega,\mathrm{e}}(\tau)\right] = 0\,. \tag{2.65}$$

The minus sign in front of the second derivative of the extremizing path average $\ddot{X}_{\omega,\mathrm{e}}(\tau)$ reflects the fact that the equation of motion is considered in imaginary time. According to the result (2.37), evaluating the identity (2.64) for a τ-independent path-average, $X_\omega(\tau) \equiv X$, allows us to obtain the effective potential for the harmonic oscillator by taking into account (2.53):

$$V_{\mathrm{eff}}(X_\omega) = \frac{M}{2}\omega^2 X_\omega^2 + \frac{1}{\beta}\ln\left[2\sinh(\hbar\beta\omega/2)\right]\,. \tag{2.66}$$

Note that the effective potential (2.66) is the sum of the classical harmonic potential and the free energy of the harmonic oscillator. In the limit $T \to 0$, i.e. $\beta \to \infty$, the effective potential becomes

$$\lim_{T\to 0} V_{\mathrm{eff}}(X_\omega) = \frac{M}{2}\omega^2 X_\omega^2 + \frac{\hbar\omega}{2}\,. \tag{2.67}$$

This reflects the fact that the free energy in the zero temperature limit equals the ground-state energy.

The effective potential can also be obtained directly, without calculating the effective action, as demonstrated in Section 2.3. This procedure will be illustrated in the following by applying it to the harmonic oscillator. Due to (2.31) and the results (2.52), (2.53), (2.55), the harmonic oscillator's partition function in presence of a constant external current is given by

$$Z_\omega(j) = \frac{1}{2\sinh(\hbar\beta\omega/2)} \times \exp\left[\frac{j^2}{4M\hbar\omega\sinh(\hbar\beta\omega/2)}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\ \cosh(\omega|\tau_1-\tau_2| - \hbar\beta\omega/2)\right]\,. \tag{2.68}$$

Using the result (B.4), one obtains

$$Z_\omega(j) = \frac{1}{2\sinh(\hbar\beta\omega/2)}\exp\left(\frac{\beta}{2M\omega^2}\,j^2\right)\,. \tag{2.69}$$

This leads to the free energy

$$F_\omega(j) = \frac{1}{\beta}\ln[2\sinh(\hbar\beta\omega/2)] - \frac{j^2}{2M\omega^2}\,. \tag{2.70}$$

Its first derivative with respect to j yields the negative of the average X

$$X = \frac{j}{M\omega^2} \qquad \text{or equivalent} \qquad j = M\omega^2 X \; . \tag{2.71}$$

Thus, the effective potential (2.36) reads

$$V_{\text{eff}}(X) = \frac{1}{\beta} \ln[2 \sinh(\hbar\beta\omega/2)] + \frac{M}{2}\omega^2 X^2 \; . \tag{2.72}$$

Indeed, one has again found (2.66).

2.5 Example: Ordinary Integral

In the following, the structure of the effective action is further investigated by considering the example of an ordinary integral in the so-called saddle-point approximation, i.e. in the limit $\hbar \to 0$. The example of an ordinary integral corresponds to an application of the formalism introduced above in zero dimensions.

Let $\mathcal{A}(x)$ be an arbitrary function which is only required to be sufficiently smooth in order that the following definitions are valid. Then define

$$Z(j) := \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \exp\left[-\frac{1}{\hbar}\, \mathcal{A}(x,j)\right] \; , \tag{2.73}$$

where

$$\mathcal{A}(x,j) := \mathcal{A}(x) - \hbar\beta \, jx \; . \tag{2.74}$$

Here, the factor $\hbar\beta$ has been included in the definition, so that (2.16) becomes (2.74) when the former is evaluated for a constant current, $j(\tau) \equiv j$, and a constant position variable, $x(\tau) \equiv x$. The argument of the exponential function in (2.73) becomes extremal when x takes its classical value x_{cl}, which is defined by the condition

$$\left.\frac{\partial\, \mathcal{A}(x,j)}{\partial x}\right|_{x=x_{\text{cl}}} = 0 \; , \tag{2.75}$$

or equivalent

$$\left.\frac{\partial \mathcal{A}(x)}{\partial x}\right|_{x=x_{\text{cl}}} = \hbar\beta \; j \; . \tag{2.76}$$

Performing a Taylor expansion of $\mathcal{A}(x,j)$ around x_{cl} and applying (2.76) yields

$$\mathcal{A}(x,j) = \mathcal{A}(x_{\text{cl}},j) + \frac{1}{2}\, \mathcal{A}''(x_{\text{cl}})\delta x^2 + \frac{1}{6}\, \mathcal{A}'''(x_{\text{cl}})\delta x^3 + \frac{1}{24}\mathcal{A}^{(4)}(x_{\text{cl}})\delta x^4 + \mathcal{O}(\delta x^5) \; , \tag{2.77}$$

where $\delta x := x - x_{\text{cl}}$ denotes the deviation from x_{cl}.

The aim is now to expand $Z(j)$ until the first order in $\hbar$. For this purpose, it is useful to recall the following result [22, p. 337]:

$$\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, x^n \exp\left(-\frac{1}{2\hbar}\lambda x^2\right) = \frac{(n-1)!!\,\hbar^{n/2}}{\sqrt{\lambda^{n+1}}} \qquad [\lambda > 0]\,, \tag{2.78}$$

where n is an arbitrary even integer. For n being odd the integral vanishes. Inserting the expansion (2.77) into (2.73) and expanding the exponential function into a Taylor series yields

$$\begin{aligned} Z(j) &= \frac{1}{\sqrt{2\pi\hbar}} \exp\left[-\frac{1}{\hbar}\mathcal{A}(x_{\rm cl}, j)\right] \int_{-\infty}^{\infty} d\delta x\, \exp\left[-\frac{1}{2\hbar}\mathcal{A}''(x_{\rm cl})\delta x^2\right] \\ &\quad \times \left[1 - \frac{1}{6\hbar}\mathcal{A}'''(x_{\rm cl})\delta x^3 - \frac{1}{24\hbar}\mathcal{A}^{(4)}(x_{\rm cl})\delta x^4 + \frac{1}{72\hbar^2}\left(A'''(x_{\rm cl})\right)^2 \delta x^6 + \ldots\right]\,, \end{aligned} \tag{2.79}$$

where terms contributing to $Z(j)$ in an order higher than linear in $\hbar$ according to the result (2.78) have been omitted. Applying (2.78) then yields

$$Z(j) = \exp\left[-\frac{1}{\hbar}\mathcal{A}(x_{\rm cl}, j)\right]\left[\frac{1}{\sqrt{\mathcal{A}''(x_{\rm cl})}} - \frac{\hbar}{8}\frac{\mathcal{A}^{(4)}(x_{\rm cl})}{\sqrt{(\mathcal{A}''(x_{\rm cl}))^5}} + \frac{5\hbar}{24}\frac{(\mathcal{A}'''(x_{\rm cl}))^2}{\sqrt{(\mathcal{A}''(x_{\rm cl}))^7}} + \mathcal{O}(\hbar^2)\right]\,. \tag{2.80}$$

This expression can be converted, using the Taylor expansion

$$\ln(1-x) = -\left(x + \frac{x^2}{2} + \frac{x^3}{3} + \ldots + \frac{x^n}{n} + \ldots\right)\,, \tag{2.81}$$

into the form

$$Z(j) = \exp\left[-\frac{1}{\hbar}\mathcal{A}(x_{\rm cl}, j) - \frac{1}{2}\ln\mathcal{A}''(x_{\rm cl}) + \hbar\left\{\frac{5}{24}\frac{[\mathcal{A}'''(x_{\rm cl})]^2}{[\mathcal{A}''(x_{\rm cl})]^3} - \frac{1}{8}\frac{\mathcal{A}^{(4)}(x_{\rm cl})}{[\mathcal{A}''(x_{\rm cl})]^2}\right\} + \mathcal{O}(\hbar^2)\right]\,. \tag{2.82}$$

Defining

$$F(j) := -\frac{1}{\beta}\ln Z(j)\,, \tag{2.83}$$

one obtains

$$F(j) = \frac{1}{\hbar\beta}\mathcal{A}(x_{\rm cl}, j) + \frac{\hbar}{2\hbar\beta}\ln\mathcal{A}''(x_{\rm cl}) - \frac{\hbar^2}{\hbar\beta}\left\{\frac{5}{24}\frac{[\mathcal{A}'''(x_{\rm cl})]^2}{[\mathcal{A}''(x_{\rm cl})]^3} - \frac{1}{8}\frac{\mathcal{A}^{(4)}(x_{\rm cl})}{[\mathcal{A}''(x_{\rm cl})]^2}\right\} + \mathcal{O}\left(\hbar^3\right)\,. \tag{2.84}$$

In the saddle-point approximation, the reduced Planck constant $\hbar$ is considered a small quantity. Nevertheless, in order to include the zero-temperature limit, i.e. $\beta \to \infty$, in the calculation, a factor $\hbar\beta$ cannot be considered a small, but rather an arbitrary quantity. Moreover, a factor $1/\beta$ has to be rewritten as $\hbar/\hbar\beta$. The average X is now defined by

$$X := X(j) := \frac{1}{Z(j)}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, x \exp\left[-\frac{1}{\hbar}\mathcal{A}(x, j)\right]\,. \tag{2.85}$$

Consequently, its negative is given by the first derivative of $F(j)$ with respect to j

$$-X = \frac{\partial F(j)}{\partial j} \,. \tag{2.86}$$

From the identity (2.76), it follows that

$$\mathcal{A}''(x_{\rm cl}) = \hbar\beta \, \frac{\partial j}{\partial x_{\rm cl}} \tag{2.87}$$

or, correspondingly,

$$\frac{\partial x_{\rm cl}}{\partial j} = \frac{\hbar\beta}{\mathcal{A}''(x_{\rm cl})} \,. \tag{2.88}$$

Using the last identity and the results (2.84), (2.86), the average X takes the form

$$\begin{aligned} X &= x_{\rm cl} - \frac{\hbar}{2}\frac{\mathcal{A}'''(x_{\rm cl})}{[\mathcal{A}''(x_{\rm cl})]^2} \\ &\quad + \hbar^2 \left\{ \frac{2}{3}\frac{\mathcal{A}'''(x_{\rm cl})\mathcal{A}^{(4)}(x_{\rm cl})}{[\mathcal{A}''(x_{\rm cl})]^4} - \frac{5}{8}\frac{[\mathcal{A}'''(x_{\rm cl})]^3}{[\mathcal{A}''(x_{\rm cl})]^5} - \frac{1}{8}\frac{\mathcal{A}^{(5)}(x_{\rm cl})}{[\mathcal{A}''(x_{\rm cl})]^3} \right\} + \mathcal{O}(\hbar^3) \,. \end{aligned} \tag{2.89}$$

Inverting (2.89) leads to

$$\begin{aligned} x_{\rm cl} &= X + \frac{\hbar}{2}\frac{\mathcal{A}'''\left(X + \hbar\,\mathcal{A}'''(X)/2[\mathcal{A}''(X)]^2\right)}{\left\{\mathcal{A}''\left(X + \hbar\,\mathcal{A}'''(X)/2[\mathcal{A}''(X)]^2\right)\right\}^2} \\ &\quad + \hbar^2 \left\{ \frac{1}{8}\frac{\mathcal{A}^{(5)}(X)}{[\mathcal{A}''(X)]^3} - \frac{2}{3}\frac{\mathcal{A}'''(X)\mathcal{A}^{(4)}(X)}{[\mathcal{A}''(X)]^4} + \frac{5}{8}\frac{[\mathcal{A}'''(X)]^3}{[\mathcal{A}''(X)]^5} \right\} + \mathcal{O}(\hbar^3) \,. \end{aligned} \tag{2.90}$$

Performing a Taylor expansion in powers of $\hbar$,

$$\mathcal{A}''\left(X + \hbar\frac{\mathcal{A}'''(X)}{2[\mathcal{A}''(X)]^2}\right) = \mathcal{A}''(X) + \hbar\,\mathcal{A}'''(X)\frac{\mathcal{A}'''(X)}{2\left[\mathcal{A}''(X)\right]^2} + \mathcal{O}(\hbar^2) \,, \tag{2.91}$$

and using the expansion

$$\frac{1}{(1+x)^2} = 1 - 2x + 3x^2 - 4x^3 + \ldots + (n+1)(-x)^n + \ldots \tag{2.92}$$

leads to

$$x_{\rm cl} = X + \hbar X_1 + \hbar^2 X_2 + \mathcal{O}(\hbar^3) \,, \tag{2.93}$$

where the first-order correction reads

$$X_1 = \frac{1}{2}\frac{\mathcal{A}'''(X)}{[\mathcal{A}''(X)]^2} \,, \tag{2.94}$$

and the second-order correction is given by

$$X_2 = \frac{1}{8}\frac{\mathcal{A}^{(5)}(X)}{[\mathcal{A}''(X)]^3} - \frac{5}{12}\frac{\mathcal{A}'''(X)\mathcal{A}^{(4)}(X)}{[\mathcal{A}''(X)]^4} + \frac{1}{8}\frac{[\mathcal{A}'''(X)]^3}{[\mathcal{A}''(X)]^5} \,. \tag{2.95}$$

The Legendre transform of $F(j)$ with respect to j multiplied by a factor $\hbar\beta$ now reads

$$\Gamma(X) := \hbar\beta\,[F(j) + jX] \ . \tag{2.96}$$

It corresponds to the effective action defined in Section 2.2. Using the result (2.84), one obtains $\Gamma(X)$ by expanding $\mathcal{A}(x)$ around $x_{\rm cl}$ as given in (2.93):

$$\begin{aligned}\Gamma(X) \ &= \ \mathcal{A}(X) + \hbar\beta\, jX + \frac{\partial\mathcal{A}(X)}{\partial X}(\hbar X_1 + \hbar^2 X_2) - \hbar\beta\, j(X + \hbar X_1 + \hbar^2 X_2) \\ &\quad + \frac{\hbar}{2}\ln\mathcal{A}''(X + \hbar X_1) - \ \hbar^2\left\{\frac{5}{24}\frac{[\mathcal{A}'''(X)]^2}{[\mathcal{A}''(X)]^3} - \frac{1}{8}\frac{\mathcal{A}^{(4)}(X)}{[\mathcal{A}''(X)]^2}\right\} + \mathcal{O}(\hbar^3)\ . \end{aligned}\tag{2.97}$$

Using the identity (2.76) together with the result (2.94) then yields

$$\Gamma(X) = \mathcal{A}(X) + \frac{\hbar}{2}\ln\mathcal{A}''(X) + \hbar^2\left\{\frac{1}{8}\frac{\mathcal{A}^{(4)}(X)}{[\mathcal{A}''(X)]^2} - \frac{1}{12}\frac{[\mathcal{A}'''(X)]^2}{[\mathcal{A}''(X)]^3}\right\} + \mathcal{O}(\hbar^3)\ . \tag{2.98}$$

Thus, the second-order correction (2.95) to the average X does not contribute to $\Gamma(X)$ in (2.98). Furthermore, note that in the limit $\hbar \to 0$ the result (2.98) takes the form

$$\lim_{\hbar\to 0}\Gamma(X) = \mathcal{A}(X)\ . \tag{2.99}$$

2.6 Background Method: Ordinary Integral

In this section, an important method to efficiently determine the loop expansion for the effective action will be introduced. This so-called background method [4, Ch. 3] was originally introduced by B. De Witt in field theory of gravitation [15]. Later, the background method was further elaborated and established by R. Jackiw in relativistic quantum field theory [16]. It constitutes an important simplification for evaluating the saddle point approximation of functional integrals. Here, the background method will be illustrated first for the ordinary integral from the previous section. To this end, the following steps are performed. Consider the integral (2.73) without the artificial current j, i.e.

$$Z = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\exp\left[-\frac{1}{\hbar}\,\mathcal{A}(x)\right]\ , \tag{2.100}$$

and expand the function $\mathcal{A}(x)$ around some background X, which corresponds to the average introduced in (2.85). By introducing $\delta x := x - X$ as the deviation of the integration variable x from the background X, one obtains

$$\mathcal{A}(X + \delta x) = \mathcal{A}(X) + \mathcal{A}'(X)\delta x + \frac{1}{2}\,\mathcal{A}''(X)\delta x^2 + \mathcal{A}^{(\rm int)}(\delta x)\ , \tag{2.101}$$

with the interaction

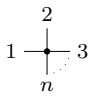
$$\mathcal{A}^{(\rm int)}(\delta x) = \frac{1}{6}\,\mathcal{A}'''(X)\delta x^3 + \frac{1}{24}\,\mathcal{A}^{(4)}(X)\delta x^4 + \ldots\ . \tag{2.102}$$

The respective terms in the expansion (2.101) have the following consequences for the effective action (2.96) [4, Ch. 3]: The zeroth order $\mathcal{A}(X)$ appears directly in the effective action as stated in (2.98). The first-order term $\mathcal{A}'(X)\delta x$ has to be neglected in the background method as it is implicitly taken into account when performing the Legendre transformation. The second-order term $\mathcal{A}''(X)\delta x^2/2$ leads to the expression $[\hbar \ln \mathcal{A}''(X)]/2$ as stated in (2.98). Furthermore, the remaining interactions (2.102) are characterized in terms of Feynman diagrams. To this end, the following Feynman rules are introduced:

- A line corresponds to the inverse of $\mathcal{A}''(X)$:

$$\text{—} \quad \equiv \quad \frac{\hbar}{\mathcal{A}''(X)} \,. \tag{2.103}$$

- An n-vertex with $n \geq 3$ stands for the nth derivative $\mathcal{A}^{(n)}(X)$:



$$\equiv \quad -\frac{1}{\hbar}\, \mathcal{A}^{(n)}(X) \,. \tag{2.104}$$

Thus, the effective action reads

$$\Gamma(X) = \mathcal{A}(X) + \frac{\hbar}{2} \ln \mathcal{A}''(X) + \Gamma^{(\mathrm{int})}(X) \,, \tag{2.105}$$

where $\Gamma^{(\mathrm{int})}(X)$ turns out to consist of all one-particle irreducible vacuum diagrams which are compatible with the Feynman rules (2.103), (2.104) [4, Ch. 3]. A diagram is referred to as a 'vacuum diagram' if it does not possess any lines that do not end in a vertex. It is called 'one-particle irreducible' if cutting an arbitrary line of the diagram does not lead to two unconnected diagrams. $\Gamma^{(\mathrm{int})}(X)$ can be expanded into the form

$$\Gamma^{(\mathrm{int})}(X) = -\hbar \sum_{l=2}^{\infty} \Gamma^{(l)}(X) \,, \tag{2.106}$$

where, in its diagrammatic representation, each order $\Gamma^{(l)}(X)$ consists of all one-particle irreducible vacuum diagrams with l loops. For such a diagram with N vertices, let n_i with $i = 1, 2, \ldots, N$ be the degree of the ith vertex. The number of loops for this diagram then reads

$$l = \frac{1}{2} \sum_{i=1}^{N} n_i - (N - 1) \,, \tag{2.107}$$

which can be proven by induction over the number of vertices N. On the other hand, as a consequence of the Feynman rules (2.103), (2.104), an arbitrary one-particle irreducible vacuum diagram contributes to $\Gamma^{(\mathrm{int})}(X)$ in the order $\hbar^m$, where

$$m = \frac{1}{2} \sum_{i=1}^{N} n_i - N \,. \tag{2.108}$$

Consequently, comparing (2.107) and (2.108) shows that diagrams with l loops lead to contributions to $\Gamma^{(l)}(X)$ which are of the order $\hbar^{l-1}$. So, according to (2.106), a diagram with l loops contributes to $\Gamma^{(\mathrm{int})}(X)$ in the order $\hbar^l$. The diagrams for $l = 2,\ 3$ and their respective weights are given by

$$\Gamma^{(2)}(X) \;=\; \frac{1}{8}$$  $$+\frac{1}{12}$$  , (2.109)

$$\Gamma^{(3)}(X) \;=\; \frac{1}{8}$$  $$+\frac{1}{12}$$  $$+\frac{1}{48}$$  $$+\frac{1}{16}$$ 

$$+\frac{1}{8}$$  $$+\frac{1}{8}$$  $$+\frac{1}{24}$$  $$+\frac{1}{16}$$  . (2.110)

Here, the weights of the diagrams follow from combinatorial considerations. For instance, the weights w_d of the diagrams with three- and four-vertices are given by [23]

$$w_d = \frac{1}{2!^{S+D}\, 3!^{T}\, 4!^{F}\, P}\,, \tag{2.111}$$

where S, D, T, F denote the number of self-, double, triple, fourfold connections, and P stands for the number of vertex permutations that leave the diagram unchanged. Consider, for example, the diagram  . This diagram possesses $D = 2$ double connections, and among the six possible vertex permutations two leave the topology of the diagram unchanged. Thus, one has $P = 2$. Therefore, the weight of this diagram reads

$$w_d\Big($$  $$\Big) = \frac{1}{2!^2 \cdot 2} = \frac{1}{8}\,. \tag{2.112}$$

Applying the Feynman rules (2.103), (2.104) to the results (2.109) and (2.110) leads to the analytical expression

$$\begin{aligned}\Gamma^{(\mathrm{int})}(X) \;=\; \hbar^2 \left[\frac{1}{8}\frac{\mathcal{A}^{(4)}(X)}{(\mathcal{A}''(X))^2} - \frac{1}{12}\frac{(\mathcal{A}'''(X))^2}{(\mathcal{A}''(X))^3}\right] + \hbar^3 \left[\frac{1}{8}\frac{\mathcal{A}^{(6)}(X)}{(\mathcal{A}''(X))^3} - \frac{1}{12}\frac{\mathcal{A}'''(X)\mathcal{A}^{(5)}(X)}{(\mathcal{A}''(X))^4}\right.\\ \left. - \frac{1}{12}\frac{(\mathcal{A}^{(4)}(X))^2}{(\mathcal{A}''(X))^4} + \frac{1}{4}\frac{(\mathcal{A}'''(X))^2\mathcal{A}^{(4)}(X)}{(\mathcal{A}''(X))^5} - \frac{5}{48}\frac{(\mathcal{A}'''(X))^4}{(\mathcal{A}''(X))^6}\right] + \mathcal{O}(\hbar^4)\,,\end{aligned} \tag{2.113}$$

where the $\hbar^2$-terms correspond to the previous result (2.98). All one-particle irreducible vacuum diagrams arising for 3- and 4-vertices follow from a recursive graphical construction method, which also determines their respective weights [23].

2.7 Background Method: Path Integral

In the following, the application of the background method will be examined for the partition function

$$Z = \oint \mathcal{D}x\ \exp\left\{-\frac{1}{\hbar}\,\mathcal{A}[x]\right\}\,. \tag{2.114}$$

Accordingly, a *functional* Taylor expansion of the action $\mathcal{A}[x]$ has to be performed around an arbitrarily chosen background $X(\tau)$:

$$\begin{aligned}\mathcal{A}[X+\delta x] &= \mathcal{A}[X] + \int_0^{\hbar\beta} d\tau_1 \, \frac{\delta \mathcal{A}[X]}{\delta X(\tau_1)} \, \delta x(\tau_1) \\ &+ \frac{1}{2} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, \frac{\delta^2 \mathcal{A}[X]}{\delta X(\tau_1) \delta X(\tau_2)} \, \delta x(\tau_1) \delta x(\tau_2) \\ &+ \frac{1}{6} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \, \frac{\delta^3 \mathcal{A}[X]}{\delta X(\tau_1) \delta X(\tau_2) \delta X(\tau_3)} \, \delta x(\tau_1) \delta x(\tau_2) \delta x(\tau_3) \\ &+ \frac{1}{24} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \int_0^{\hbar\beta} d\tau_4 \\ &\qquad \times \frac{\delta^4 \mathcal{A}[X]}{\delta X(\tau_1) \delta X(\tau_2) \delta X(\tau_3) \delta X(\tau_4)} \, \delta x(\tau_1) \delta x(\tau_2) \delta x(\tau_3) \delta x(\tau_4) + \dots \, . \end{aligned} \tag{2.115}$$

Again, $\delta x(\tau) := x(\tau) - X(\tau)$ denotes the deviation of the path $x(\tau)$ from the background $X(\tau)$. Similar to the procedure above, the first order term,

$$\int_0^{\hbar\beta} d\tau_1 \, \frac{\delta \mathcal{A}[X]}{\delta X(\tau_1)} \, \delta x(\tau_1) \, , \tag{2.116}$$

will be neglected, and terms being of higher than second order in δx define the interaction

$$\begin{aligned}\mathcal{A}^{(\mathrm{int})}[\delta x] &:= \frac{1}{6} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \, \frac{\delta^3 \mathcal{A}[X]}{\delta X(\tau_1) \delta X(\tau_2) \delta X(\tau_3)} \, \delta x(\tau_1) \delta x(\tau_2) \delta x(\tau_3) \\ &+ \frac{1}{24} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \int_0^{\hbar\beta} d\tau_4 \\ &\qquad \times \frac{\delta^4 \mathcal{A}[X]}{\delta X(\tau_1) \delta X(\tau_2) \delta X(\tau_3) \delta X(\tau_4)} \, \delta x(\tau_1) \delta x(\tau_2) \delta x(\tau_3) \delta x(\tau_4) + \dots \, . \end{aligned} \tag{2.117}$$

The integral kernel is defined as

$$G^{-1}(\tau_1, \tau_2) := \frac{\delta^2 \mathcal{A}[X]}{\delta X(\tau_1) \delta X(\tau_2)} \, , \tag{2.118}$$

and the partition function (2.114) can be written in the form

$$\begin{aligned} Z &= \exp\left\{ -\frac{1}{\hbar} \mathcal{A}[X] \right\} \\ &\times \oint \mathcal{D}\delta x \, \exp\left\{ -\frac{1}{2\hbar} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, G^{-1}(\tau_1, \tau_2) \delta x(\tau_1) \delta x(\tau_2) - \frac{1}{\hbar} \mathcal{A}^{(\mathrm{int})}[\delta x] \right\} \, . \end{aligned} \tag{2.119}$$

In order to determine the second-order contribution to the partition function, it is helpful to remember the result of the one-dimensional Gaußian integral

$$\int_{-\infty}^{\infty} dx \, \exp\left(-\frac{1}{2} A x^2 \right) = \sqrt{\frac{2\pi}{A}} \qquad [A > 0] \, . \tag{2.120}$$

In D dimensions, A can be taken as a matrix, and the Gaußian integral evaluates to

$$\int_{-\infty}^{\infty} d^D x \, \exp\left(-\frac{1}{2}\,\mathbf{x}^T A \mathbf{x}\right) = \frac{(2\pi)^{D/2}}{\sqrt{\det(A)}} \qquad [A = A^\dagger,\ \det(A) > 0]\,. \tag{2.121}$$

The path integral in (2.119) constitutes an infinite-dimensional integration. Therefore, one would expect that the second-order contribution to the partition function is the generalization of the result (2.121) to infinite dimension:

$$\oint \mathcal{D}\delta x \, \exp\left[-\frac{1}{2\hbar}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, G^{-1}(\tau_1,\tau_2)\delta x(\tau_1)\delta x(\tau_2)\right] = \frac{1}{\sqrt{\det(G^{-1})}}\,. \tag{2.122}$$

The determinant of the integral kernel is defined as the product of its eigenvalues λ_k, which are obtained by solving the eigenvalue problem

$$\int_0^{\hbar\beta} d\tau_2 \, G^{-1}(\tau_1,\tau_2)\, \delta x_k(\tau_2) = M\lambda_k \delta x_k(\tau_1)\,, \tag{2.123}$$

with $\delta x_k(\tau)$ being periodic in the imaginary time:

$$\delta x_k(0) = \delta x_k(\hbar\beta)\,. \tag{2.124}$$

Accordingly, the right-hand side of (2.122) can be rewritten in the form

$$\frac{1}{\sqrt{\det(G^{-1})}} = \exp\left(-\frac{1}{2}\,\mathrm{Tr}\ln G^{-1}\right)\,, \tag{2.125}$$

where the trace-log of the integral kernel $G^{-1}(\tau_1,\tau_2)$ is defined by

$$\mathrm{Tr}\ln G^{-1} := \sum_k \ln\lambda_k\,. \tag{2.126}$$

The preceding argument lacks, of course, mathematical rigor. In Appendix A, the partition function for the harmonic oscillator is calculated, and an analogous procedure could be applied to demonstrate that the result (2.122) – (2.126) is indeed valid. Since the application of the background method implies a vanishing external current j, one obtains from (2.24)

$$Z[X] = \exp\left\{-\frac{1}{\hbar}\Gamma[X]\right\}\,. \tag{2.127}$$

Thus, when neglecting the interactions, i.e. when setting $\mathcal{A}^{(\mathrm{int})}[\delta x] = 0$, from the last identity, (2.119), and (2.122) – (2.126), one obtains the first order approximation of the effective action:

$$\Gamma^{(0)}[X] + \Gamma^{(1)}[X] = \mathcal{A}[X] + \frac{\hbar}{2}\,\mathrm{Tr}\ln G^{-1}\,; \tag{2.128}$$

and the complete effective action is given by [4, Ch. 3]

$$\Gamma[X] = \mathcal{A}[X] + \frac{\hbar}{2}\,\mathrm{Tr}\ln G^{-1} + \Gamma^{(\mathrm{int})}[X]\,. \tag{2.129}$$

The zeroth-order term $\mathcal{A}[X]$ in (2.129) is referred to as 'tree-level'. As before, the remaining interactions $\Gamma^{(\mathrm{int})}[X]$ can be characterized in terms of Feynman diagrams. The respective Feynman rules are now:

- All outgoing lines of all vertices are numbered arbitrarily.

- A connection between the ith and the jth line corresponds to the propagator $G(\tau_i, \tau_j)$:

$$i \text{ —— } j \quad \equiv \quad G(\tau_i, \tau_j) \,, \tag{2.130}$$

  where the propagator $G(\tau_i, \tau_j)$ is defined by the identity

$$\int_0^{\hbar\beta} d\tau_i \, G^{-1}(\tau_h, \tau_i) G(\tau_i, \tau_j) \equiv \hbar \, \delta(\tau_h - \tau_j) \,. \tag{2.131}$$

- The resulting product of propagators is multiplied by functional derivatives of $\mathcal{A}[X]$ and then integrated. An n-vertex with $n \geq 3$ and the n outgoing lines $i,\ j,\ k,\ \ldots\ , m$ stands for the nth functional derivative of $A[X]$ with respect to $X(\tau_i),\ X(\tau_j),\ X(\tau_k),\ \ldots,\ X(\tau_m)$ and leads to the integration

$$\begin{array}{ccc} & j & \\ i & + & k \\ & m & \end{array} \quad \rightarrow \quad -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau_i \int_0^{\hbar\beta} d\tau_j \int_0^{\hbar\beta} d\tau_k \, \ldots \int_0^{\hbar\beta} d\tau_m \times \frac{\delta^n \mathcal{A}[X]}{\delta X(\tau_i)\, \delta X(\tau_j)\, \delta X(\tau_k) \, \ldots \, \delta X(\tau_m)} \,. \tag{2.132}$$

Again, $\Gamma^{(\mathrm{int})}[X]$ consists of all one-particle irreducible vacuum diagrams which are compatible with the Feynman rules (2.130) – (2.132). Furthermore, $\Gamma^{(\mathrm{int})}[X]$ can be obtained by a loop expansion,

$$\Gamma^{(\mathrm{int})}[X] = -\hbar \sum_{l=2}^{\infty} \Gamma^{(l)}[X] \,, \tag{2.133}$$

where each loop order l consists of all one-particle irreducible vacuum diagrams with l loops [4, Ch. 3]. Thus, the diagrams contributing to $\Gamma^{(\mathrm{int})}[X]$ with two and three loops are the same as in the case of an ordinary integral. Applying the Feynman rules (2.130) – (2.132) to the diagrams (2.109), (2.110) and taking into account (2.133) yields the analytical expression

for the interaction part of the effective action

$$
\begin{aligned}
\Gamma^{(\mathrm{int})}[X] \;=\; -\hbar \Big\{ & -\frac{1}{8\hbar}\int_{1234} G_{12}G_{34}\,\frac{\delta^4\mathcal{A}[X]}{\delta X_1\delta X_2\delta X_3\delta X_4} \\
& + \frac{1}{12\hbar^2}\int_{12\ldots6} G_{12}G_{34}G_{56}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_1\delta X_3\delta X_5}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_2\delta X_4\delta X_6} \\
& - \frac{1}{8\hbar}\int_{12\ldots6} G_{12}G_{34}G_{56}\,\frac{\delta^6\mathcal{A}[X]}{\delta X_1\delta X_2\delta X_3\delta X_4\delta X_5\delta X_6} \\
& + \frac{1}{12\hbar^2}\int_{12\ldots8} G_{12}G_{34}G_{56}G_{78}\,\frac{\delta^5\mathcal{A}[X]}{\delta X_1\delta X_3\delta X_5\delta X_7\delta X_8}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_2\delta X_4\delta X_6} \\
& + \frac{1}{48\hbar^2}\int_{12\ldots8} G_{12}G_{34}G_{56}G_{78}\,\frac{\delta^4\mathcal{A}[X]}{\delta X_1\delta X_3\delta X_5\delta X_7}\,\frac{\delta^4\mathcal{A}[X]}{\delta X_2\delta X_4\delta X_6\delta X_8} \\
& + \frac{1}{16\hbar^2}\int_{12\ldots8} G_{12}G_{34}G_{56}G_{78}\,\frac{\delta^4\mathcal{A}[X]}{\delta X_1\delta X_2\delta X_3\delta X_5}\,\frac{\delta^4\mathcal{A}[X]}{\delta X_4\delta X_6\delta X_7\delta X_8} \\
& - \frac{1}{8\hbar^3}\int_{12\ldots\bar{0}} G_{12}G_{34}G_{56}G_{78}G_{9\bar{0}}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_1\delta X_6\delta X_7}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_4\delta X_5\delta X_{\bar{0}}}\,\frac{\delta^4\mathcal{A}[X]}{\delta X_2\delta X_3\delta X_8\delta X_9} \\
& - \frac{1}{8\hbar^3}\int_{12\ldots\bar{0}} G_{12}G_{34}G_{56}G_{78}G_{9\bar{0}}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_1\delta X_7\delta X_9}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_4\delta X_8\delta X_{\bar{0}}}\,\frac{\delta^4\mathcal{A}[X]}{\delta X_2\delta X_3\delta X_5\delta X_6} \\
& + \frac{1}{24\hbar^4}\int_{12\ldots\bar{2}} G_{12}G_{34}G_{56}G_{78}G_{9\bar{0}}G_{\bar{1}\bar{2}}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_1\delta X_8\delta X_9}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_2\delta X_3\delta X_{\bar{1}}} \\
& \qquad\qquad \times \frac{\delta^3\mathcal{A}[X]}{\delta X_4\delta X_5\delta X_{\bar{0}}}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_6\delta X_7\delta X_{\bar{2}}} \\
& + \frac{1}{16\hbar^4}\int_{12\ldots\bar{2}} G_{12}G_{34}G_{56}G_{78}G_{9\bar{0}}G_{\bar{1}\bar{2}}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_1\delta X_8\delta X_9}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_2\delta X_3\delta X_{\bar{1}}} \\
& \qquad\qquad \times \frac{\delta^3\mathcal{A}[X]}{\delta X_4\delta X_5\delta X_{\bar{2}}}\,\frac{\delta^3\mathcal{A}[X]}{\delta X_6\delta X_7\delta X_{\bar{0}}} + \ldots \Big\}\,, \qquad (2.134)
\end{aligned}
$$

where the following abbreviations have been used:

$$
\int_{12\ldots n} := \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \ldots \int_0^{\hbar\beta} d\tau_n\,, \qquad (2.135)
$$

$G_{ij} := G(\tau_i,\tau_j)$, $X_i := X(\tau_i)$, and a digit with an overscore stands for the corresponding number plus ten, e.g. $\bar{2} = 12$.

At this point, it is not yet obvious that the loop expansion of the interaction part of the effective action corresponds to an expansion in powers of the reduced Planck constant $\hbar$. However, this is the case if the propagator $G(\tau_i,\tau_j)$ contains a factor $\hbar$. Note that this condition was valid for the harmonic propagator (2.55) and also for the propagator of the ordinary integral (2.103).

2.8 Calculation of the Effective Potential

In this section, it is demonstrated how the effective potential can be calculated for any given potential by applying the background method. To this end, due to (2.37), it is sufficient to evaluate the effective action (2.129), (2.134) for a constant background field $X(\tau) \equiv X$. For an arbitrary potential $V(x)$, the imaginary-time action $\mathcal{A}[X]$ is given by (2.14). Its first functional derivative reads

$$\frac{\delta \mathcal{A}[X]}{\delta X(\tau_1)} = -M\ddot{X}(\tau_1) + V'(x)\Big|_{x=X(\tau_1)} . \tag{2.136}$$

The second functional derivative, which according to definition (2.118) equals the integral kernel, is

$$G^{-1}(\tau_1, \tau_2) = \left[-M\frac{d^2}{d\tau_1^2} + V''(x)\Big|_{x=X(\tau_2)} \right] \delta(\tau_1 - \tau_2) . \tag{2.137}$$

For $n \geq 3$, the nth functional derivative of the imaginary-time action is given by

$$\frac{\delta^n \mathcal{A}[X]}{\delta X(\tau_1)\delta X(\tau_2)\dots\delta X(\tau_n)} = \delta(\tau_1 - \tau_2)\,\delta(\tau_2 - \tau_3)\dots\delta(\tau_{n-1} - \tau_n)\,V^{(n)}(x)\Big|_{x=X(\tau_n)} . \tag{2.138}$$

The propagator $G(\tau_1, \tau_2)$ is determined by the identity (2.131). However, since the aim of this section is only to calculate the effective potential rather than the effective action, it is sufficient to solve (2.131) for a constant background X. Together with (2.137), this leads to an ordinary differential equation of second order for the propagator in presence of a constant background $G_X(\tau, \tau_2)$:

$$\int_0^{\hbar\beta} d\tau \left[-M\frac{d^2}{d\tau_1^2} + V''(X) \right] \delta(\tau_1 - \tau) G_X(\tau, \tau_2) = \hbar\delta(\tau_1 - \tau_2) . \tag{2.139}$$

This equation can be reduced to the corresponding problem for the harmonic oscillator (2.50), (2.54) by introducing the frequency

$$\Omega := \sqrt{\frac{V''(X)}{M}} . \tag{2.140}$$

Thus, from the previous result (2.55), one obtains the propagator for an arbitrary potential and a constant background

$$G_\Omega(\tau_1, \tau_2) = \frac{\hbar}{2M\Omega} \frac{\cosh(\Omega|\tau_1 - \tau_2| - \hbar\beta\Omega/2)}{\sinh(\hbar\beta\Omega/2)} . \tag{2.141}$$

In the limit $T \to 0$, it simplifies to

$$\lim_{T\to 0} G_\Omega(\tau_1, \tau_2) = \frac{\hbar}{2M\Omega}\, e^{-\Omega|\tau_1 - \tau_2|} . \tag{2.142}$$

As in (2.133) for the interaction part of the effective action, the effective potential interactions will be expanded in the form

$$V_{\text{eff}}^{(\text{int})}(X) = -\hbar \sum_{l=2}^{\infty} V_{\text{eff}}^{(l)}(X) , \tag{2.143}$$

where, according to (2.37), each loop order $V_{\rm eff}^{(l)}(X)$ is obtained by evaluating the corresponding loop order of the effective action at a constant background X:

$$V_{\rm eff}^{(l)}(X) = \frac{1}{\hbar\beta}\Gamma^{(l)}[X]\Big|_{X(\tau)=X} . \tag{2.144}$$

In order to determine the interaction part of the effective potential for arbitrary temperatures until the third loop order, the integrals in (2.134) have to be evaluated for a constant background X and the propagator G_{ij} as specified in (2.140), (2.141). Taking into account (2.133), (2.143), and (2.144) and performing the integration over the delta functions stemming from (2.138) yields

$$\begin{aligned} V_{\rm eff}^{(\rm int)}(X) &= \frac{1}{\beta}\left\{\frac{V^{(4)}(X)}{8\hbar}\int_1 G_{11}^2 - \frac{[V^{(3)}(X)]^2}{12\hbar^2}\int_{12} G_{12}^3 + \frac{V^{(6)}(X)}{8\hbar}\int_1 G_{11}^3 \right. \\ &- \frac{V^{(3)}(X)V^{(5)}(X)}{12\hbar^2}\int_{12} G_{11}G_{12}^3 - \frac{[V^{(4)}(X)]^2}{48\hbar^2}\int_{12} G_{12}^4 - \frac{[V^{(4)}(X)]^2}{16\hbar^2}\int_{12} G_{11}G_{22}G_{12}^2 \\ &+ \frac{[V^{(3)}(X)]^2V^{(4)}(X)}{8\hbar^3}\int_{123}(G_{13}G_{12}^2G_{23}^2 + G_{12}G_{22}G_{23}G_{13}^2) \\ &\left. - \frac{[V^{(3)}(X)]^4}{\hbar^4}\int_{1234}\left(\frac{G_{12}G_{13}G_{14}G_{23}G_{24}G_{34}}{24} + \frac{G_{13}G_{24}G_{12}^2G_{34}^2}{16}\right) + \dots\right\} , \end{aligned} \tag{2.145}$$

where the same abbreviations have been used as in (2.134). This formula can also be derived by defining Feynman rules that are less general than (2.130) – (2.132), as they are only applicable in case of a constant background, and taking into account (2.143) and (2.144):

- The vertices of the diagram are numbered arbitrarily.
- A connection between the ith and the jth vertex stands for the propagator:

  $$\equiv \quad G_\Omega(\tau_i,\tau_j) , \tag{2.146}$$

  where $G_\Omega(\tau_i,\tau_j)$ for arbitrary temperatures is given by (2.140), (2.141) and in the zero-temperature limit by (2.140), (2.142).
- The resulting products of propagators is integrated. Let the ith vertex be of degree n, with $n \geq 3$; then it leads to the integration

  $$\rightarrow \quad -\frac{V^{(n)}(X)}{\hbar}\int_0^{\hbar\beta} d\tau_i . \tag{2.147}$$

In order to determine the interaction part of the effective potential for arbitrary temperatures until the second loop order, the first two integrals in (2.145) have to be evaluated with the propagator G_{ij} specified in (2.140), (2.141). Taking into account (2.143) yields the intermediate result

$$\begin{aligned} V_{\rm eff}^{(2)}(X) &= -\hbar\frac{V^{(4)}(X)}{8(2M\Omega)^2}\,\frac{1}{\tanh^2(\hbar\beta\Omega/2)} + \frac{[V^{(3)}(X)]^2}{12\beta(2M\Omega)^3}\frac{1}{\sinh^3(\hbar\beta\Omega/2)} \\ &\times \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, \cosh^3(\Omega|\tau_1-\tau_2| - \hbar\beta\Omega/2) . \end{aligned} \tag{2.148}$$

The remaining twofold integral is evaluated in Appendix B, yielding the result

$$V_{\rm eff}^{(2)}(X) = -\hbar \frac{V^{(4)}(X)}{8(2M\Omega)^2} \frac{1}{\tanh^2(\hbar\beta\Omega/2)} + \frac{\hbar}{6\Omega} \frac{[V^{(3)}(X)]^2}{(2M\Omega)^3} \left[\frac{1}{3} + \frac{1}{\sinh^2(\hbar\beta\Omega/2)}\right] . \quad (2.149)$$

In order to specify the total effective potential up to the second order in the reduced Planck constant $\hbar$, the tree-level and the trace-log term have to be included. For the harmonic oscillator (2.47), the interaction part of the effective action $\Gamma^{(\rm int)}[X]$ vanishes. Therefore, by comparing (2.14) and (2.64) with (2.129) and taking into account (2.53), one reads off the trace-log for the harmonic oscillator

$$\mathrm{Tr} \ln G_\omega^{-1} = -2 \ln Z_\omega = 2 \ln (2 \sinh \hbar\beta\omega/2) . \quad (2.150)$$

To obtain the trace-log for an arbitrary potential one merely has to replace the frequency ω by Ω. Thus, according to (2.37), (2.129), (2.143), and (2.149), the effective potential for an arbitrary potential reads

$$\begin{aligned} V_{\rm eff}(X) &= V(X) + \frac{\hbar}{\hbar\beta} \ln (2 \sinh \hbar\beta\Omega/2) + \hbar^2 \frac{V^{(4)}(X)}{8(2M\Omega)^2} \frac{1}{\tanh^2(\hbar\beta\Omega/2)} \\ &\quad - \frac{\hbar^2}{6\Omega} \frac{[V^{(3)}(X)]^2}{(2M\Omega)^3} \left[\frac{1}{3} + \frac{1}{\sinh^2(\hbar\beta\Omega/2)}\right] + \mathcal{O}(\hbar^3) . \end{aligned} \quad (2.151)$$

Note that in order to include the limit $T \to 0$, i.e. $\beta \to \infty$, in the calculation, terms including the product $\hbar\beta$ cannot be considered as merely depending on a term that is proportional to the reduced Planck constant $\hbar$, which goes to zero in this approximation. The product $\hbar\beta$ has rather to be considered an arbitrary quantity. Furthermore, a factor $1/\beta$ has to be extended to $\hbar/\hbar\beta$. In (2.151), only the tree-level is temperature-independent. In the zero-temperature limit, the effective potential (2.151) simplifies to

$$\lim_{T\to 0} V_{\rm eff}(X) = V(X) + \frac{\hbar\Omega}{2} + \hbar^2 \frac{V^{(4)}(X)}{8(2M\Omega)^2} - \frac{\hbar^2}{18\Omega} \frac{[V^{(3)}(X)]^2}{(2M\Omega)^3} + \mathcal{O}(\hbar^3) . \quad (2.152)$$

One can extend the last result to the third order by evaluating the Feynman diagrams (2.110) in the zero-temperature limit. Thus, the remaining eight multiple integrals in (2.145) have to be solved, where the propagator G_{ij} is specified by (2.142). Taking into account (2.143)

yields the intermediate result

$$\begin{aligned}
\lim_{T\to 0} V_{\rm eff}^{(3)}(X) &= -\frac{\hbar^2 V^{(6)}(X)}{8(2M\Omega)^3} + \frac{\hbar V^{(3)}(X)V^{(5)}(X)}{12(2M\Omega)^4\beta}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, \exp(-3\Omega|\tau_1-\tau_2|) \\
&+ \frac{\hbar[V^{(4)}(X)]^2}{(2M\Omega)^4\beta}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \left[\frac{1}{48}\exp(-4\Omega|\tau_1-\tau_2|) + \frac{1}{16}\exp(-2\Omega|\tau_1-\tau_2|)\right] \\
&- \frac{\hbar V^{(4)}(X)[V^{(3)}(X)]^2}{8(2M\Omega)^5\beta}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \\
&\qquad \times \Big[\exp(-2\Omega|\tau_1-\tau_2| - \Omega|\tau_1-\tau_3| - 2\Omega|\tau_2-\tau_3|) \\
&\qquad\quad + \exp(-\Omega|\tau_1-\tau_2| - 2\Omega|\tau_1-\tau_3| - \Omega|\tau_2-\tau_3|)\Big] \\
&+ \frac{\hbar[V^{(3)}(X)]^4}{(2M\Omega)^6\beta}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \int_0^{\hbar\beta} d\tau_4 \\
&\quad \times \Big[\frac{1}{24}\exp(-\Omega|\tau_1-\tau_2| - \Omega|\tau_1-\tau_3| - \Omega|\tau_1-\tau_4| - \Omega|\tau_2-\tau_3| - \Omega|\tau_2-\tau_4| - \Omega|\tau_3-\tau_4|) \\
&\qquad + \frac{1}{16}\exp(-\Omega|\tau_1-\tau_2| - 2\Omega|\tau_1-\tau_4| - 2\Omega|\tau_2-\tau_3| - \Omega|\tau_3-\tau_4|)\Big] . \qquad (2.153)
\end{aligned}$$

The remaining two-, three-, and fourfold integrals are calculated in Appendix B. Applying (B.15) and (B.27) – (B.30) to (2.153), one obtains

$$\begin{aligned}
\lim_{T\to 0} V_{\rm eff}^{(3)}(X) &= -\frac{\hbar^2 V^{(6)}(X)}{8(2M\Omega)^3} + \frac{\hbar^2 V^{(3)}(X)V^{(5)}(X)}{18\Omega(2M\Omega)^4} + \frac{7\hbar^2[V^{(4)}(X)]^2}{96\Omega(2M\Omega)^4} \\
&\quad - \frac{13\hbar^2 V^{(4)}(X)[V^{(3)}(X)]^2}{72\Omega^2(2M\Omega)^5} + \frac{17\hbar^2[V^{(3)}(X)]^4}{216\Omega^3(2M\Omega)^6} . \qquad (2.154)
\end{aligned}$$

Combining the last result with (2.152) and taking into account (2.143), one obtains the effective potential in the zero-temperature limit up to the third order in $\hbar$:

$$\begin{aligned}
\lim_{T\to 0} V_{\rm eff}(X) &= V(X) + \frac{\hbar\Omega}{2} + \hbar^2\frac{V^{(4)}(X)}{8(2M\Omega)^2} - \frac{\hbar^2}{18\Omega}\frac{[V^{(3)}(X)]^2}{(2M\Omega)^3} + \frac{\hbar^3}{8}\frac{V^{(6)}(X)}{(2M\Omega)^3} \\
&\quad - \frac{\hbar^3}{18\Omega}\frac{V^{(3)}(X)V^{(5)}(X)}{(2M\Omega)^4} - \frac{7\hbar^3}{96\Omega}\frac{[V^{(4)}(X)]^2}{(2M\Omega)^4} + \frac{13\hbar^3}{72\Omega^2}\frac{V^{(4)}(X)[V^{(3)}(X)]^2}{(2M\Omega)^5} \\
&\quad - \frac{17\hbar^3}{216\Omega^3}\frac{[V^{(3)}(X)]^4}{(2M\Omega)^6} + \mathcal{O}(\hbar^4) . \qquad (2.155)
\end{aligned}$$

2.9 Example: Anharmonic Oscillator

Consider an anharmonic oscillator with the potential

$$V(x) = \frac{M}{2}\omega^2 x^2 + gAx^3 + g^2 Bx^4 , \qquad (2.156)$$

where the parameter B is assumed to be positive, and g is the coupling constant. In this section, the effective potential for this oscillator will be calculated until the second loop order

for arbitrary temperatures and until the third loop order for $T = 0$ by applying the results from the previous section. To this end, one only needs to replace the derivatives of the arbitrary potential from the last section by their actual values for the anharmonic oscillator. The propagator $G_\Omega(\tau_1, \tau_2)$ of the anharmonic oscillator for arbitrary temperatures is given by (2.141), and in the zero-temperature limit by (2.142), where the frequency Ω reads

$$\Omega = \omega \sqrt{1 + \frac{6gAX}{M\omega^2} + \frac{12g^2BX^2}{M\omega^2}} \,. \tag{2.157}$$

Note that in order to ensure that Ω in (2.157) is real for all values of X, the condition

$$|A| \leq \sqrt{\frac{4M\omega^2 B}{3}} \tag{2.158}$$

must hold. Applying the result (2.151) to the anharmonic oscillator, one obtains its temperature dependent effective potential up to the second order in $\hbar$:

$$\begin{aligned} V_{\text{eff}}(X) \;=\; & \frac{M}{2}\omega^2 X^2 + gAX^3 + g^2BX^4 + \frac{\hbar}{\hbar\beta}\ln\left(2\sinh\hbar\beta\Omega/2\right) + \hbar^2\frac{3g^2B}{(2M\Omega)^2}\,\frac{1}{\tanh^2(\hbar\beta\Omega/2)} \\ & - \frac{\hbar^2}{6\Omega}\frac{(6gA + 24g^2BX)^2}{(2M\Omega)^3}\left[\frac{1}{3} + \frac{1}{\sinh^2(\hbar\beta\Omega/2)}\right] + \mathcal{O}(\hbar^3) \,. \end{aligned} \tag{2.159}$$

According to (2.39), one obtains the free energy by evaluating (2.159) for that particular average X that extremizes the effective potential. Since here the calculation is only up to the second order in the reduced Planck constant $\hbar$, the background X can be expanded in the form

$$X = X_0 + \hbar X_1 + \hbar^2 X_2 + \mathcal{O}(\hbar^3) \,. \tag{2.160}$$

Inserting this identity into the first derivative of (2.159), expanding it in powers of $\hbar$, and setting the resulting expression to zero leads to a system of three equations, each corresponding to the respective order in $\hbar$. This system of equations for the extremizing average X_{e} can be solved consecutively. First, one obtains

$$X_0^{(1)} = 0 \,, \qquad X_0^{(2)} = -\frac{3A + 9\sqrt{9A^2 - 16BM\omega^2}}{8gB} \,, \qquad X_0^{(3)} = \frac{-3A + 9\sqrt{9A^2 - 16BM\omega^2}}{8gB} \,. \tag{2.161}$$

Since the solution is required to be real for all allowed parameters A, B, only $X_0^{(1)} = 0$ is a valid solution. The solutions $X_0^{(2)}$ and $X_0^{(3)}$ are complex due to condition (2.158). Using this result, one further obtains

$$X_1 = -\frac{3gA}{2M^2\omega^3\tanh(\hbar\beta\omega/2)} \,. \tag{2.162}$$

Since X_0 vanishes, one reads off from (2.159) that X_2 does not contribute to the free energy in the second order of $\hbar$. This corresponds to the previous example of an ordinary integral in

Section 2.5, where the second-order correction of the average X did not affect the effective action in the order $\hbar^2$. Furthermore, the frequency Ω reduces to

$$\Omega = \omega + \mathcal{O}(\hbar) \,. \tag{2.163}$$

Inserting the solutions (2.161), (2.162) into (2.159) and expanding until the second order in $\hbar$ yields the free energy in this order:

$$\begin{aligned} F &= \frac{\hbar}{\hbar\beta} \ln\left(\sinh \hbar\beta\omega/2\right) \qquad (2.164)\\ &+ \hbar^2 \left\{ \left[\frac{3Bg^2}{4M^2\omega^2} - \frac{9A^2g^2}{8M^3\omega^4} \right] \frac{1}{\tanh^2\left(\hbar\beta\omega/2\right)} - \frac{3A^2g^2}{4M^3\omega^4} \left[\frac{1}{3} + \frac{1}{\sinh^2\left(\hbar\beta\omega/2\right)} \right] \right\} + \mathcal{O}(\hbar^3) \,. \end{aligned}$$

In the zero-temperature limit, the effective potential (2.159) simplifies to

$$\begin{aligned} \lim_{T\to 0} V_{\text{eff}}(X) &= \frac{M}{2}\omega^2 X^2 + gAX^3 + g^2BX^4 + \frac{\hbar\Omega}{2} + \hbar^2 \frac{3g^2B}{(2M\Omega)^2} \\ &- \frac{\hbar^2}{18\Omega} \frac{(6gA + 24g^2BX)^2}{(2M\Omega)^3} + \mathcal{O}(\hbar^3) \,. \end{aligned} \tag{2.165}$$

To obtain the ground-state energy, according to (2.41), one has to evaluate this expression for the particular average that extremizes the effective potential (2.165). To this end, the background X is expanded in the form (2.160). Inserting (2.160) into the first derivative of (2.165) with respect to average X, expanding this expression until the second order in $\hbar$, and determining the zeros for each order of $\hbar$ yields the result

$$X_0 = 0 \,, \tag{2.166}$$

$$X_1 = -\frac{3gA}{2M^2\omega^3} \,, \tag{2.167}$$

$$X_2 = -\frac{g^3A(33A^2 - 31BM\omega^2)}{2M^5\omega^8} \,. \tag{2.168}$$

Other possible solutions for X are ruled out, since they lead to a complex average X when the condition (2.158) is fulfilled. Note that (2.167) represents the $T \to 0$ limit of (2.162). Inserting (2.166) – (2.168) into (2.165) and expanding the resulting expression until the second order in $\hbar$ gives, according to (2.41), the ground-state energy of the anharmonic oscillator in this order:

$$E_0 = \hbar\frac{\omega}{2} + \hbar^2 \frac{g^2\left(-11A^2 + 6BM\omega^2\right)}{8M^3\omega^4} + \mathcal{O}(\hbar^3) \,. \tag{2.169}$$

Note that, as above, due to (2.165) and (2.166), the second-order correction X_2 does not contribute to the ground-state energy in this order. One can extend the previous calculation to the third order by using the result (2.155). Due to the fact that all of the anharmonic potential's derivatives of higher than fourth order vanish, the terms in (2.155) containing $V^{(5)}(X)$ or $V^{(6)}(X)$ do not contribute to this calculation. Thus, the effective potential for

the anharmonic oscillator in the zero-temperature limit up to the third order in $\hbar$ reads:

$$\begin{aligned}\lim_{T\to 0} V_{\rm eff}(X) &= \frac{M}{2}\omega^2 X^2 + gAX^3 + g^2BX^4 + \frac{\hbar\Omega}{2} + \hbar^2\frac{3g^2B}{(2M\Omega)^2} \\ &- \frac{\hbar^2}{18\Omega}\frac{(6gA+24g^2BX)^2}{(2M\Omega)^3} - \frac{7\hbar^3}{96\Omega}\frac{(24g^2B)^2}{(2M\Omega)^4} \\ &+ \frac{13\hbar^3}{72\Omega^2}\frac{24g^2B(6gA+24g^2BX)^2}{(2M\Omega)^5} - \frac{17\hbar^3}{216\Omega^3}\frac{(6gA+24g^2BX)^4}{(2M\Omega)^6} + \mathcal{O}(\hbar^4)\,.\end{aligned} \tag{2.170}$$

The ground-state energy of the anharmonic oscillator in the third order of $\hbar$ is then obtained in the same way as before. All calculations merely have to be extended by one order. From (2.170) it follows, when the zeroth order of the background vanishes, that it is sufficient to know the corrections to the background X up to the second order (2.166) – (2.168) to obtain the third-order correction for the oscillator's ground-state energy, as has been discussed above. Inserting (2.166) – (2.168) into (2.170) and expanding until the third order in $\hbar$ yields the result

$$\begin{aligned}E_0 &= \hbar\frac{\omega}{2} + \hbar^2\frac{g^2\left(-11A^2+6BM\omega^2\right)}{8M^3\omega^4} \\ &- \hbar^3\frac{g^4\left(465A^4-684A^2BM\omega^2+84B^2M^2\omega^4\right)}{32M^6\omega^9} + \mathcal{O}(\hbar^4)\,.\end{aligned} \tag{2.171}$$

In the next section, this three-loop result for the ground-state energy is verified by applying perturbation theory.

2.10 Perturbation Theory

In this section, the partition function for the anharmonic oscillator (2.156),

$$Z = \oint \mathcal{D}x\, \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \left[\frac{M}{2}\dot{x}^2(\tau) + \frac{M}{2}\omega^2 x^2(\tau) + gAx^3(\tau) + g^2Bx^4(\tau)\right]\right\}\,, \tag{2.172}$$

will be calculated perturbatively by an expansion in the coupling constant g. In a first step, separating harmonic and anharmonic contributions to Z and expanding the exponential function yields

$$\begin{aligned}Z &= \oint \mathcal{D}x\, \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \left[\frac{M}{2}\dot{x}^2(\tau) + \frac{M}{2}\omega^2 x^2(\tau)\right]\right\} \\ &\times\left\{1 - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau_1\, \left[gAx^3(\tau_1) + g^2Bx^4(\tau_1)\right]\right. \\ &\left. + \frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, \left[gAx^3(\tau_1) + g^2Bx^4(\tau_1)\right]\left[gAx^3(\tau_2) + g^2Bx^4(\tau_2)\right] + \ldots\right\}.\end{aligned} \tag{2.173}$$

Since all contributions to the path integral that are odd in the path $x(\tau)$ vanish, one obtains by using the result for the harmonic partition function (2.53) and introducing the notation

$$\langle\, \bullet\, \rangle_\omega = \frac{1}{Z_\omega}\oint \mathcal{D}x\, \bullet\, \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \left[\frac{M}{2}\dot{x}^2(\tau) + \frac{M}{2}\omega^2 x^2(\tau)\right]\right\} \tag{2.174}$$

the following expression for the partition function:

$$Z = Z_\omega \left[1 - \frac{g^2 B}{\hbar} \int_0^{\hbar\beta} d\tau_1 \, \langle x^4(\tau_1)\rangle_\omega + \frac{g^2 A^2}{2\hbar^2} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, \langle x^3(\tau_1) x^3(\tau_2)\rangle_\omega + \mathcal{O}(g^4)\right] . \tag{2.175}$$

Expectation values of products of an even number of paths can be transformed by applying Wick's rule [4, Sec. 3.9]:

- The expectation value of a product of two paths defines the corresponding propagator

$$G_\omega(\tau_1, \tau_2) := \langle x(\tau_1) x(\tau_2)\rangle_\omega . \tag{2.176}$$

- An expectation value of a product of n paths can be rewritten as a sum of $n-1$ products of propagators and expectation values of $n-2$ paths:

$$\begin{aligned} \langle x(\tau_1)x(\tau_2)x(\tau_3)\ldots x(\tau_n)\rangle_\omega &= G_\omega(\tau_1,\tau_2)\langle x(\tau_3)x(\tau_4)\ldots x(\tau_n)\rangle_\omega \\ &+ G_\omega(\tau_1,\tau_3)\langle x(\tau_2)x(\tau_4)\ldots x(\tau_n)\rangle_\omega + \ldots + G_\omega(\tau_1,\tau_n)\langle x(\tau_2)x(\tau_3)\ldots x(\tau_{n-1})\rangle_\omega . \end{aligned} \tag{2.177}$$

By applying Wick's rule (2.176), (2.177) one obtains

$$\langle x^4(\tau_1)\rangle_\omega = 3\, G_\omega^2(\tau_1,\tau_1) , \tag{2.178}$$

and

$$\langle x^3(\tau_1) x^3(\tau_2)\rangle_\omega = 9\, G_\omega(\tau_1,\tau_1) G_\omega(\tau_1,\tau_2) G_\omega(\tau_2,\tau_2) + 6\, G_\omega^3(\tau_1,\tau_2) . \tag{2.179}$$

Note that the propagator $G_\omega(\tau_1,\tau_2)$ defined by (2.174) and (2.176) is indeed identical with the propagator (2.55):

$$\begin{aligned} \langle x(\tau_1)x(\tau_2)\rangle_\omega &= \frac{\hbar^2}{Z_\omega}\frac{\delta^2}{\delta j(\tau_1) j(\tau_2)} \oint \mathcal{D}x \, \exp\left(-\frac{1}{\hbar}\left\{\mathcal{A}_\omega[x] + \int_0^{\hbar\beta} d\tau \, x(\tau) j(\tau)\right\}\right)\Bigg|_{j=0} \\ &\overset{(2.48),\,(2.52)}{=} \hbar^2 \frac{\delta^2}{\delta j(\tau_1) j(\tau_2)} \, \exp\left[\frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, G_\omega(\tau_1,\tau_2) j(\tau_1) j(\tau_2)\right]\Bigg|_{j=0} . \end{aligned} \tag{2.180}$$

Carrying out the functional derivatives and using (2.57) then yields the proposition.

Applying (2.178) and (2.179) to (2.175) yields

$$\begin{aligned} F &= -k_B T \ln Z = -k_B T \ln Z_\omega + k_B T \Bigg\{ \frac{3 g^2 B}{\hbar} \int_0^{\hbar\beta} d\tau_1 G_\omega^2(\tau_1,\tau_1) \\ &- \frac{g^2 A^2}{2\hbar^2} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, \left[9\, G_\omega(\tau_1,\tau_1) G_\omega(\tau_1,\tau_2) G_\omega(\tau_2,\tau_2) + 6\, G_\omega^3(\tau_1,\tau_2)\right] + \mathcal{O}(g^4)\Bigg\} , \end{aligned} \tag{2.181}$$

where the Taylor expansion (2.81) has been used. The free energy can be expressed in terms of Feynman diagrams. To this end, the following Feynman-rules are introduced:

- The vertices of the diagram are numbered arbitrarily.
- A connection between the ith and the jth vertex stands for the propagator $G_\omega(\tau_i, \tau_j)$

$$\equiv \; G_\omega(\tau_i, \tau_j)\,, \tag{2.182}$$

  where $G_\omega(\tau_i, \tau_j)$ for arbitrary temperatures is given by (2.55) and in the zero temperature limit by (2.56).

- The resulting product of propagators is integrated.
  A three-vertex leads to an integration

$$\rightarrow \; -\frac{6gA}{\hbar}\int_0^{\hbar\beta} d\tau_i\,. \tag{2.183}$$

  And a four-vertex leads to an integration

$$\rightarrow \; -\frac{24g^2B}{\hbar}\int_0^{\hbar\beta} d\tau_i\,. \tag{2.184}$$

Applying these Feynman rules to (2.181), one obtains the diagrammatic representation of the free energy in this order

$$F \;=\; -k_BT\ln Z_\omega - k_BT\Bigg\{\frac{1}{8}$$

$$+\frac{1}{8}$$

$$+\frac{1}{12}$$

$$+\mathcal{O}(g^4)\Bigg\}\,. \tag{2.185}$$

In Ref. [23], it is shown that the free energy can be obtained by a diagrammatic loop expansion, where each loop order l consists of all connected vacuum diagrams with l loops. This is in contrast to the interaction part of the effective action $\Gamma^{(\mathrm{int})}[X]$, which only consists of all one-particle irreducible vacuum diagrams (compare with Section 2.6). The diagrams contributing to the next loop order are given in Ref. [23] and lead to the following expression for the free energy

$$F \;=\; -k_BT\ln Z_\omega - k_BT\Bigg\{\frac{1}{8}$$

$$+\frac{1}{8}$$

$$+\frac{1}{12}$$

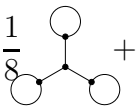
$$+\frac{1}{24}$$

$$+\frac{1}{16}$$

$$+\frac{1}{8}$$

$$+\frac{1}{16}$$

$$+\frac{1}{48}$$

$$+\frac{1}{8}$$

$$+\frac{1}{8}$$

$$+\frac{1}{12}$$

$$+\frac{1}{8}$$

$$+\frac{1}{16}$$

$$+\frac{1}{48}$$

$$+\frac{1}{16}$$

$$+\mathcal{O}(g^6)\Bigg\}\,. \tag{2.186}$$

The right-hand side of equation (2.181) with the propagator $G_\omega(\tau_1, \tau_2)$ being specified in (2.55) can be evaluated by using the results (B.4) and (B.7). In doing so, one obtains the free energy up to the second order in the coupling constant g

$$\begin{aligned} F \;&=\; -k_BT\ln Z_\omega \\ &+ g^2\left\{\left[\frac{3B\hbar^2}{(2M\omega)^2} - \frac{9A^2\hbar^2}{\omega(2M\omega)^3}\right]\frac{1}{\tanh^2(\hbar\beta\omega/2)} - \frac{6A^2\hbar^2}{\omega(2M\omega)^3}\left[\frac{1}{3} + \frac{1}{\sinh^2(\hbar\beta\omega/2)}\right]\right\} + \mathcal{O}(g^4)\,. \end{aligned} \tag{2.187}$$

To obtain the free energy in the zero-temperature limit, i.e. the ground-state energy, up to the fourth order in the coupling constant g, one can evaluate the Feynman diagrams (2.186) specified by the Feynman rules (2.182) – (2.184). In this limit, the trace-log term $-k_B T \ln Z_\omega$ becomes the ground-state energy of the harmonic oscillator $\hbar\omega/2$. Using the results (B.27) – (B.36), one obtains

$$E_0 = \frac{\hbar\omega}{2} + g^2 \frac{\hbar^2(6BM\omega^2 - 11A^2)}{8M^3\omega^4} - g^4 \frac{\hbar^3(465A^4 - 684A^2BM\omega^2 + 84B^2M^2\omega^4)}{32M^6\omega^9} + \mathcal{O}(g^6) \,. \tag{2.188}$$

Note that the ground-state energy is even in the coupling constant g. This is due to the fact that changing the sign of the coupling constant would only result in an oscillator potential that is mirrored by the ordinate-axis, and this would only affect the resulting wave functions but not the energy levels.

Chapter 3

Recursion Relations

3.1 Motivation

In this chapter, methods will be introduced which allow the obtaining of the sum of Feynman diagrams without explicitly evaluating the single diagrams. In Section 3.2, an expansion for the ground-state energy of the anharmonic oscillator (3.4) in terms of the coupling constant g will be obtained by applying the Bender-Wu recursion method. This method was developed by C.M. Bender and T.T. Wu to approximatively solve the time-independent Schrödinger equation in 1969/1973 [17,18]. Later on, its application was extended to the time-dependent Schrödinger equation [24] and to the Fokker-Planck equation [25]. While in principle two approaches, a perturbational expansion or a cumulant expansion, are possible, in this work the latter will be pursued. In the perturbational expansion, which is e.g. found in [4, App. 3E], the oscillator's ground-state wave function is expanded in the form

$$\psi(x) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{M\omega}{2\hbar}x^2\right)\left[1+\phi(x)\right] \ , \tag{3.1}$$

whereas in the cumulant expansion one chooses an ansatz of the form

$$\psi(x) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{M\omega}{2\hbar}x^2+\phi(x)\right] \ . \tag{3.2}$$

The correction to the wave function $\phi(x)$ is not to be understood as being identical for the two approaches. The correction $\phi(x)$ will be expanded in powers of the coupling constant g:

$$\phi(x) = \sum_{k=1}^{\infty} g^k \, \phi_k(x) \ . \tag{3.3}$$

Each expansion can be derived from the other. However, the cumulant expansion offers the advantage that fewer coefficients arise in the Taylor expansion of the $\phi_k(x)$, which is performed in a second step. In the following sections, the Bender-Wu recursion will be applied to an anharmonic oscillator with or without external current. In Section 3.4, we will extend it to a recursion for the effective potential $V_{\text{eff}}(X)$.

3.2 Ground-State Energy without External Current

For the potential

$$V(x) = \frac{M}{2}\omega^2 x^2 + gAx^3 + g^2 Bx^4 \,, \tag{3.4}$$

the time-independent Schrödinger equation reads

$$-\frac{\hbar^2}{2M}\,\psi''(x) + \left(\frac{M}{2}\omega^2 x^2 + gAx^3 + g^2 Bx^4\right)\psi(x) = E\,\psi(x)\,. \tag{3.5}$$

Inserting the ansatz (3.2) into the Schrödinger equation (3.5) yields an ordinary differential equation for the correction $\phi(x)$:

$$-\frac{\hbar^2}{2M}\phi''(x) + \hbar\omega\, x\, \phi'(x) - \frac{\hbar^2}{2M}\left[\phi'(x)\right]^2 + gAx^3 + g^2 Bx^4 = \epsilon\,, \tag{3.6}$$

where ϵ denotes the correction to the ground-state energy

$$E = \frac{\hbar\omega}{2} + \epsilon\,. \tag{3.7}$$

Expanding the ground-state energy of the oscillator in powers of the coupling constant g,

$$E = \frac{\hbar\omega}{2} + \sum_{k=1}^{\infty} g^k\,\epsilon_k\,, \tag{3.8}$$

inserting the expansion (3.3) into (3.6), and performing a coefficients comparison, one obtains a differential equation for the $\phi_k(x)$:

$$-\frac{\hbar^2}{2M}\phi_k''(x) + \hbar\omega\, x\, \phi_k'(x) - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1}\phi_{k-l}'(x)\,\phi_l'(x) + \delta_{k,1}Ax^3 + \delta_{k,2}Bx^4 = \epsilon_k\,. \tag{3.9}$$

Assuming that $\phi_k(x)$ is a polynomial, one can show by induction that its degree cannot be greater than $k+2$. Thus, the $\phi_k(x)$ can be written in the form

$$\phi_k(x) = \sum_{m=1}^{k+2} c_m^{(k)}\, x^m\,. \tag{3.10}$$

Here, the constant terms $c_0^{(k)}$ have been omitted as they can only be determined later by normalization of the wave function $\psi(x)$. By inserting (3.10) into (3.9) for $k=1$, one finds

$$c_1^{(1)} = -\frac{A}{M\omega^2}\,, \qquad c_2^{(1)} = 0\,, \qquad c_3^{(1)} = -\frac{A}{3\hbar\omega}\,, \qquad \text{and } \epsilon_1 = 0\,. \tag{3.11}$$

For $k=2$, the solution reads

$$c_1^{(2)} = 0\,, \qquad c_2^{(2)} = \frac{7A^2}{8M^2\omega^4} - \frac{3B}{4M\omega^2}\,, \qquad c_3^{(2)} = 0\,, \qquad c_4^{(2)} = \frac{A^2}{8M\hbar\omega^3} - \frac{B}{4\hbar\omega}\,, \tag{3.12}$$

$$\text{and } \epsilon_2 = -\frac{11A^2\hbar^2}{8M^3\omega^4} + \frac{3B\hbar^2}{4M^2\omega^2}\,. \tag{3.13}$$

For the general case $k \geq 3$, it is helpful to rewrite (3.10) in the form

$$\phi_k(x) = \sum_{m=1}^{\infty} c_m^{(k)}\, x^m\,, \qquad \text{with } c_m^{(k)} \equiv 0 \quad \text{for } m > k+2\,, \tag{3.14}$$

as this allows the application of the Cauchy product rule to the product of the derivatives $\phi'_{k-l}(x)$ and $\phi'_l(x)$ in (3.9). The recursively determinable solution for the $\phi_k(x)$ and the energy corrections ϵ_k is then obtained as

$$\begin{aligned} c_m^{(k)} &= \frac{(m+2)(m+1)\hbar}{2mM\omega}\, c_{m+2}^{(k)} + \frac{\hbar}{2mM\omega} \sum_{l=1}^{k-1} \sum_{n=1}^{m+1} n(m+2-n)\, c_n^{(l)}\, c_{m+2-n}^{(k-l)}\,, \\ &\qquad \text{with } c_m^{(k)} \equiv 0 \quad \text{for } m > k+2\,, \end{aligned} \tag{3.15}$$

$$\epsilon_k = -\frac{\hbar^2}{M}\, c_2^{(k)} - \frac{\hbar^2}{2M} \sum_{l=1}^{k-1} c_1^{(l)}\, c_1^{(k-l)}\,. \tag{3.16}$$

Applying this result leads to the expansion coefficients and the energy correction in the third order of the coupling constant:

$$\begin{aligned} c_1^{(3)} = -\frac{5A^3\hbar}{M^4\omega^7} + \frac{6AB\hbar}{M^3\omega^5}\,, \qquad c_2^{(3)} = 0\,, \qquad c_3^{(3)} = -\frac{13A^3}{12M^3\omega^6} + \frac{3AB}{2M^2\omega^4}\,, \\ c_4^{(3)} = 0\,, \qquad c_5^{(3)} = -\frac{A^3}{10M^2\hbar\omega^5} + \frac{AB}{5M\hbar\omega^3}\,, \end{aligned} \tag{3.17}$$

$$\text{and } \epsilon_3 = 0\,. \tag{3.18}$$

And for the fourth order one obtains

$$\begin{aligned} c_1^{(4)} = 0\,, \qquad c_2^{(4)} = \frac{305A^4\hbar}{32M^5\omega^9} - \frac{123A^2B\hbar}{8M^4\omega^7} + \frac{21B^2\hbar}{8M^3\omega^5}\,, \qquad c_3^{(4)} = 0\,, \\ c_4^{(4)} = \frac{99A^4}{64M^4\omega^8} - \frac{47A^2B}{16M\omega^6} + \frac{11B^2}{16M^2\omega^4}\,, \qquad c_5^{(4)} = 0\,, \\ c_6^{(4)} = \frac{5A^4}{48M^3\hbar\omega^7} - \frac{A^2B}{4M^2\hbar\omega^5} + \frac{B^2}{12M\hbar\omega^3}\,, \end{aligned} \tag{3.19}$$

$$\text{and } \epsilon_4 = -\frac{465A^4\hbar^3}{32M^6\omega^9} + \frac{171A^2B\hbar^3}{8M^5\omega^7} - \frac{21B^2\hbar^3}{8M^4\omega^5}\,. \tag{3.20}$$

Comparing (3.13), (3.18), and (3.20) with (2.188), one sees that the result obtained by Bender-Wu recursion is indeed identical to the one obtained by explicitly evaluating Feynman diagrams. Since one wants to drive the expansion to higher orders, it is important to optimize the recursion formula with regard to its evaluation by a computer. To this end, it is helpful to introduce natural units, in which one has $\hbar = 1$, $M = 1$. Furthermore, since calculations on a computer can be performed more effectively when dealing with mere rational numbers, which are not afflicted with parameters like A, B, or ω, it is desirable to expand the coefficients $c_m^{(k)}$ and the energy corrections ϵ_k in products of powers of these parameters. Dimensional considerations lead to the following approaches for the coefficients $c_m^{(k)}$:

$$c_m^{(k)} = \sum_{\lambda=0}^{\lfloor k/2 \rfloor} \frac{A^{k-2\lambda}B^{\lambda}}{\omega^{5k/2-m/2-2\lambda}}\, c_{m,\lambda}^{(k)}\,, \qquad \text{with } c_{m,\lambda}^{(k)} \equiv 0 \quad \text{for } m > k+2\,, \tag{3.21}$$

and for the energy corrections ϵ_k:

$$\epsilon_k = \sum_{\lambda=0}^{\lfloor k/2 \rfloor} \frac{A^{k-2\lambda} B^\lambda}{\omega^{5k/2-1-2\lambda}} \, \epsilon_{k,\lambda} \, . \tag{3.22}$$

Similar to the procedure in (3.14), it is helpful to rewrite (3.21) in the form

$$c_m^{(k)} = \sum_{\lambda=0}^{\infty} \frac{A^{k-2\lambda} B^\lambda}{\omega^{5k/2-m/2-2\lambda}} \, c_{m,\lambda}^{(k)} \, , \qquad \text{with } c_{m,\lambda}^{(k)} \equiv 0 \quad \text{for } m > k+2 \text{ or } \lambda > \left\lfloor \frac{k}{2} \right\rfloor \, , \tag{3.23}$$

as this allows the application of the Cauchy product rule to the product of the coefficients $c_n^{(l)}$ and $c_{m+2-n}^{(k-l)}$ when inserting (3.23) into (3.15). Doing so and performing a coefficients comparison yields a recursion relation for the expansion coefficients $c_{m,\lambda}^{(k)}$:

$$c_{m,\lambda}^{(k)} = \frac{(m+2)(m+1)}{2m} \, c_{m+2,\lambda}^{(k)} + \frac{1}{2m} \sum_{l=1}^{k-1} \sum_{n=1}^{m+1} \sum_{\lambda'=0}^{\lambda} n(m+2-n) \, c_{n,\lambda-\lambda'}^{(l)} \, c_{m+2-n,\lambda'}^{(k-l)} \, ,$$
$$\text{with } c_{m,\lambda}^{(k)} \equiv 0 \quad \text{for } m > k+2 \text{ or } \lambda > \left\lfloor \frac{k}{2} \right\rfloor \, . \tag{3.24}$$

The starting values follow from comparing (3.11) and (3.12) with (3.21):

$$c_{1,0}^{(1)} = -1 \, , \qquad c_{2,0}^{(1)} = 0 \, , \qquad c_{3,0}^{(1)} = -\frac{1}{3} \, , \tag{3.25}$$

$$\begin{aligned} &c_{1,0}^{(2)} = 0 \, , \qquad c_{1,1}^{(2)} = 0 \, , \qquad c_{2,0}^{(2)} = \frac{7}{8} \, , \qquad c_{2,1}^{(2)} = -\frac{3}{4} \, , \\ &c_{3,0}^{(2)} = 0 \, , \qquad c_{3,1}^{(2)} = 0 \, , \qquad c_{4,0}^{(2)} = \frac{1}{8} \, , \qquad c_{4,1}^{(2)} = -\frac{1}{4} \, . \end{aligned} \tag{3.26}$$

The expansion coefficients $\epsilon_{k,\lambda}$ for the energy corrections ϵ_k are obtained by inserting (3.22) and (3.21) into (3.16) using natural units:

$$\epsilon_{k,\lambda} = -c_{2,\lambda}^{(k)} \; - \; \frac{1}{2} \sum_{l=1}^{k-1} \sum_{\lambda'=0}^{\lambda} c_{1,\lambda-\lambda'}^{(l)} \, c_{1,\lambda'}^{(k-l)} \, . \tag{3.27}$$

Table 3.1 shows the energy corrections ϵ_k up to the tenth order.

3.3 Ground-State Energy with External Current

In the presence of a constant external current j, the time-independent Schrödinger equation for the anharmonic oscillator (2.156) reads

$$-\frac{\hbar^2}{2M} \, \psi''(x) + \left(\frac{M}{2} \omega^2 x^2 + gAx^3 + g^2 B x^4 - jx \right) \psi(x) = E \, \psi(x) \, . \tag{3.28}$$

This problem can, for instance, be physically realized by taking the anharmonic oscillator into a constant electric field. The solution for the case of a vanishing coupling constant, $g = 0$, can be obtained analytically by introducing the new variables x' and E':

$$x' = x - \frac{j}{M\omega^2} \qquad \text{and} \qquad E' = \, E + \frac{j^2}{2M\omega^2} \, . \tag{3.29}$$

k	ϵ_k
1	0
2	$\dfrac{-11A^2+6B\omega^2}{8\omega^4}$
3	0
4	$-\dfrac{465A^4-684A^2B\omega^2+84B^2\omega^4}{32\omega^9}$
5	0
6	$\dfrac{-39709A^6+91014A^4B\omega^2-47308A^2B^2\omega^4+2664B^3\omega^6}{128\omega^{14}}$
7	0
8	$-3(6416935A^8-19945048A^6B\omega^2+18373480A^4B^2\omega^4$ $+4962400A^2B^3\omega^6 164720B^4\omega^8)/(2048\omega^{19})$
9	0
10	$(-2944491879A^{10}+11565716526A^8B\omega^2-15341262168A^6B^2\omega^4$ $+7905514480A^4B^3\omega^6-1320414512A^2B^4\omega^8+29335392B^5\omega^{10})/(8192\omega^{24})$

Table 3.1: Expansion coefficients for the ground-state energy of the anharmonic oscillator (3.4) up to the 10th order.

Performing these substitutions, the differential equation to be solved reduces to the case of the harmonic oscillator. Thus, in this section, for the wave function, the approach

$$\psi(x) = N\, e^{\phi(x)}\,, \qquad \text{with} \qquad \phi(x) = \frac{j}{\hbar\omega}x - \frac{M\omega}{2\hbar}x^2 + \sum_{k=1}^{\infty} g^k\, \phi_k(x)\,, \tag{3.30}$$

where N denotes a normalization constant, is chosen. Furthermore, the energy is expanded in the form

$$E(j) = \frac{\hbar\omega}{2} - \frac{j^2}{2M\omega^2} + \sum_{k=1}^{\infty} g^k\, \epsilon_k\,. \tag{3.31}$$

Inserting (3.30) and (3.31) into (3.28) and performing a coefficients comparison, one obtains an ordinary differential equation for the $\phi_k(x)$:

$$-\frac{\hbar^2}{2M}\phi_k''(x) - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1}\phi_{k-l}'(x)\,\phi_l'(x) + \left(\hbar\omega x - \frac{j\hbar}{M\omega}\right)\phi_k'(x) + \delta_{k,1}\,Ax^3 + \delta_{k,2}\,Bx^4 = \epsilon_k\,. \tag{3.32}$$

Under the assumption that $\phi_k(x)$ is a polynomial, it is, as before, possible to show by induction that the degree of $\phi_k(x)$ cannot be greater than $k+2$. Thus, the $\phi_k(x)$ can be written in the form (3.10). Again, the constant terms $c_0^{(k)}$ can only be determined by exploiting the normalization condition for the wave function. Inserting (3.10) into (3.32) allows the $\phi_k(x)$ to be determined recursively. First, one finds for $k=1$

$$c_1^{(1)} = -\frac{A}{M\omega^2} - \frac{j^2 A}{M^2\hbar\omega^5}\,, \qquad c_2^{(1)} = -\frac{jA}{2M\hbar\omega^3}\,, \qquad c_3^{(1)} = -\frac{A}{3\hbar\omega}\,, \tag{3.33}$$

$$\text{and } \epsilon_1 = \frac{3\hbar j A}{2M\omega^3} + \frac{j^3 A}{M^3\omega^6}\,. \tag{3.34}$$

And for $k=2$ one obtains

$$c_1^{(2)} = \frac{17jA^2}{4M^3\omega^6} + \frac{4j^3A^2}{M^4\hbar\omega^9} - \frac{5jB}{2M^2\omega^4} - \frac{j^3B}{M^3\hbar\omega^7}\,,$$

$$c_2^{(2)} = \frac{7A^2}{8M^2\omega^4} + \frac{3j^2A^2}{2M^3\hbar\omega^7} - \frac{3B}{4M\omega^2} - \frac{j^2B}{2M^2\hbar\omega^5}\,, \qquad c_3^{(2)} = \frac{jA^2}{2M^2\hbar\omega^5} - \frac{jB}{3M\hbar\omega^3}\,,$$

$$c_4^{(2)} = \frac{A^2}{8M\hbar\omega^3} - \frac{B}{4\hbar\omega}\,, \tag{3.35}$$

$$\text{and } \epsilon_2 = -\frac{11\hbar^2A^2}{8M^3\omega^4} - \frac{27\hbar j^2A^2}{4M^4\omega^7} - \frac{9j^4A^2}{2M^5\omega^{10}} + \frac{3\hbar^2B}{4M^2\omega^2} + \frac{3\hbar j^2B}{M^3\omega^5} + \frac{j^4B}{M^4\omega^8}\,. \tag{3.36}$$

Note that, for $j=0$, Eqs. (3.33) – (3.36) are identical with (3.11) – (3.13). Using the convention (3.14), one finds the solution for the general case $k \geq 3$:

$$\begin{aligned} c_m^{(k)} &= \frac{(m+2)(m+1)\hbar}{2mM\omega}\, c_{m+2}^{(k)} + \frac{\hbar}{2mM\omega} \sum_{l=1}^{k-1} \sum_{n=1}^{m+1} n(m+2-n)\, c_n^{(l)}\, c_{m+2-n}^{(k-l)} \\ &\quad + \frac{j(m+1)}{Mm\omega^2}\, c_{m+1}^{(k)}\,, \qquad \text{with } c_m^{(k)} \equiv 0 \quad \text{for } m > k+2\,, \end{aligned} \tag{3.37}$$

$$\epsilon_k = -\frac{j\hbar}{M\omega} c_1^{(k)} - \frac{\hbar^2}{M}\, c_2^{(k)} - \frac{\hbar^2}{2M} \sum_{l=1}^{k-1} c_1^{(l)}\, c_1^{(k-l)}\,. \tag{3.38}$$

Table 3.2 shows the energy corrections ϵ_k in the presence of an external current up to the sixth order using natural units, $\hbar = 1$, $M = 1$. Note that Tab. 3.2 reduces to Tab. 3.1 for a vanishing current.

According to Section 2.3, the knowledge of the ground-state energy $E(j)$ permits the calculation of the effective potential $V_{\text{eff}}(X)$ in the zero-temperature limit by performing a Legendre transformation with respect to the constant external current j. Since the free energy becomes the ground-state energy in the limit $T \to 0$, one has due to (2.36):

$$E(j(X)) = V_{\text{eff}}(X) - j(X)X\,. \tag{3.39}$$

Furthermore, due to (2.38), one has

$$j(X) = V'_{\text{eff}}(X)\,. \tag{3.40}$$

k	ϵ_k
1	$\frac{Aj(2j^2+3\omega^3)}{2\omega^6}$
2	$\frac{2B\omega^2(4j^4+12j^2\omega^3+3\omega^6)-A^2(36j^4+54j^2\omega^3+11\omega^6)}{8\omega^{10}}$
3	$\frac{Aj[3A^2(36j^4+63j^2\omega^3+22\omega^6)-2B\omega^2(24j^4+66j^2\omega^3+31\omega^6)]}{4\omega^{14}}$
4	$[36A^2B\omega^2(112j^6+324j^4\omega^3+212j^2\omega^6+19\omega^9)$ $-4B^2\omega^4(64j^6+264j^4\omega^3+248j^2\omega^6+21\omega^9)$ $-3A^4(2016j^6+4158j^4\omega^3+2112j^2\omega^6+155\omega^9)]/(32\omega^{10})$
5	$Aj[27A^4(1728j^6+4158j^4\omega^3+2816j^2\omega^6+465\omega^9)$ $+4B^2\omega^4(1536j^6+6408j^4\omega^3+7072j^2\omega^6+1683\omega^9)$ $-12A^2B\omega^2(3456j^6+10908j^4\omega^3+9176j^2\omega^6+1817\omega^9)]/(32\omega^{22})$
6	$[8B^3\omega^6(1536j^8+8544j^6\omega^3+14144j^4\omega^6+6732j^2\omega^9+333\omega^{12})$ $-4A^2B^2\omega^4(103680j^8+454032j^6\omega^3+584928j^4\omega^6+221706j^2\omega^9+11827\omega^{12})$ $+6A^4B\omega^2(285120j^8+991224j^6\omega^3+1024224j^4\omega^6+323544j^2\omega^9+15169\omega^{12})$ $-A^6(1539648j^8+4266108j^6\omega^3+3649536j^4\omega^6+979290j^2\omega^9+39709\omega^{12})]/(128\omega^{26})$

Table 3.2: Energy corrections for the ground-state energy of the oscillator with cubic and quartic anharmonicity in the presence of an external current up to the 6th order.

Thus, the effective potential is obtained by solving the differential equation

$$V_{\text{eff}}(X) = E\left(V'_{\text{eff}}(X)\right) + V'_{\text{eff}}(X)X\,. \tag{3.41}$$

To this end, the effective potential is expanded in the coupling constant,

$$V_{\text{eff}}(X) = \sum_{k=0}^{\infty} g^k V_k(X)\,, \tag{3.42}$$

and each order $V_k(X)$ is assumed to be a polynomial in the background X:

$$V_k(X) = \sum_{m=0}^{k+2} C_m^{(k)} X^m\,. \tag{3.43}$$

Using the result for the energy (3.31), where the first orders of ϵ_k are given by Tab. 3.2, and inserting the ansatz (3.42), (3.43) into the differential equation (3.41) permits us to obtain the effective potential by performing a coefficients comparison, first in the relevant order of the coupling constant g, and then for each order of X. It turns out that for k being even or

k	$V_k(X)$
0	$\frac{\omega}{2}+\frac{\omega^2}{2}X^2$
1	$AX^3+\frac{3A}{2\omega}X$
2	$\frac{-A^2(1+9\omega X^2)+B\omega^2(3+12\omega X^2+4\omega^2X^4)}{4\omega^4}$
3	$\frac{AX[3A^2(4+9\omega X^2)-2B\omega^2(13+18\omega X^2)]}{4\omega^6}$
4	$-[4B^2\omega^4(21+104\omega X^2+72\omega^2X^4)-12A^2B\omega^2(13+152\omega X^2+108\omega^2X^4)$ $+A^4(51+864\omega X^2+810\omega^2X^4)]/(32\omega^9)$
5	$3AX[9A^4(51+256\omega X^2+126\omega^2X^4)+4B^2\omega^4(209+544\omega X^2+216\omega^2X^4)$ $-4A^2B\omega^2(341+1296\omega X^2+540\omega^2X^4)]/(32\omega^{11})$
6	$[24B^3\omega^6(111+836\omega X^2+1088\omega^2X^4+288\omega^3X^6)$ $-36A^2B^2\omega^4(365+5654\omega X^2+8448\omega^2X^4+2160\omega^3X^6)$ $+6A^4B\omega^2(2129+46008\omega X^2+85248\omega^2X^4+22680\omega^3X^6)$ $-A^6(3331+90882\omega X^2+207360\omega^2X^4+61236\omega^3X^6)]/(128\omega^{14})$

Table 3.3: Effective potential of the anharmonic oscillator (3.4) up to the 6th order, expanded in the coupling constant g.

odd, also $V_k(X)$ is even or odd respectively, i.e. $C_m^{(k)}=\delta_{(-1)^{m+k},1}\,C_m^{(k)}$, where $\delta_{i,j}$ denotes the Kronecker symbol. Table 3.3 shows the first six orders of the effective potential, which have been obtained in this way.

Note that (3.42) and Tab. 3.3 represent an expansion in powers of the coupling constant g, whereas the previous result (2.170) together with (2.157) constitutes an expansion in $\hbar$. Re-expanding (2.157), (2.170) into a g-expansion, however, yields a result which is identical with (3.42), Tab. 3.3 up to the order g^4.

On the other hand, it is possible to convert the expansion (3.42) into an $\hbar$-expansion. In Section 2.8, an $\hbar$-expansion for the effective potential is obtained by applying the background method. Evaluating the generating functional (2.114) and the expansion (2.115) for the potential (3.4) at a constant background $X(\tau)\equiv X$ yields, by taking into account (2.137) and

(2.138),

$$Z = \oint \mathcal{D}\delta x \, \exp\Big\{ -\frac{1}{\hbar}\mathcal{A}(X) - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \Big[\frac{M}{2}\delta\dot{x}^2(\tau) + \frac{M}{2}\omega^2\left(1 + \frac{6gAX}{M\omega^2} + \frac{12g^2BX^2}{M\omega^2}\right)\delta x^2 + \big(gA + 4g^2BX\big)\,\delta x^3 + g^2B\delta x^4\Big]\Big\}\,, \tag{3.44}$$

where, according to the background method, the first order term has been omitted, and the integration runs over all fluctuations δx that are periodic in the imaginary time, i.e. $\delta x(0) = \delta x(\hbar\beta)$. Due to (2.37) and (2.127), one has the following relation between the partition function Z and the effective potential:

$$Z = \exp\left[-\beta V_{\rm eff}(X)\right]\,. \tag{3.45}$$

And by comparing (3.44) and (3.45), one obtains

$$\exp\left[-\beta V_{\rm eff}(X) + \beta V(X)\right] = \oint \mathcal{D}\delta x \, \exp\Big\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \times \Big[\frac{M}{2}\delta\dot{x}^2(\tau) + \frac{M}{2}\omega^2\left(1 + \frac{6gAX}{M\omega^2} + \frac{12g^2BX^2}{M\omega^2}\right)\delta x^2 + \big(gA + 4g^2BX\big)\,\delta x^3 + g^2B\delta x^4\Big]\Big\}\,. \tag{3.46}$$

In Section 2.7 and 2.8, we have evaluated the expression on the right-hand side of the last identity in the saddle-point approximation, i.e. we have performed an expansion in $\hbar$. However, in (3.46), the powers of the fluctuations δx are not related to the powers of the coupling constant g. Taking into account that the potential (3.4) vanishes at the origin, one obtains from (3.46)

$$\exp[-\beta V_{\rm eff}(X=0)] = \oint \mathcal{D}\delta x \, \exp\Big\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \Big[\frac{M}{2}\delta\dot{x}^2(\tau) + \frac{M}{2}\omega^2\delta x^2 + gA\delta x^3 + g^2B\delta x^4\Big]\Big\}\,. \tag{3.47}$$

Thus, the effective potential can be transformed according to

$$V_{\rm eff}(X) = V(X) + V_{\rm eff}(X=0)\Big|_{\omega^2=\Omega^2,\ A=A+4gBX}\,, \tag{3.48}$$

where Ω is defined by (2.157). It is important to note that in contrast to (3.46), there is a fixed relation between the powers of the fluctuations and the coupling constant in (3.47). Therefore, except for the tree-level, an expansion for the effective potential in the coupling constant g can be transformed into the corresponding $\hbar$-expansion by performing the substitutions

$$X \to 0\,, \qquad \omega \to \Omega\,, \qquad A \to A + 4gBX \tag{3.49}$$

in (3.42) and reintroducing $\hbar$ (and M) into Tab. 3.3. Evaluating (3.42), Tab. 3.3 in the second order of the coupling constant according to (3.49) reproduces (2.165). In the fourth order, one reobtains (2.170). In general, when the $\hbar$-expansion is given in the form

$$V_{\rm eff}(X) = \sum_{l=0}^{N} \hbar^l V^{(l)}(X) + \mathcal{O}(\hbar^{N+1})\,, \tag{3.50}$$

l	$V^{(l)}(X)$
0	$\frac{1}{2}\omega^2 X^2 + gAX^3 + g^2 BX^4$
1	$\frac{\Omega}{2}$
2	$\frac{3g^2B}{4\Omega^2} - \frac{g^2(A+4gBX)^2}{4\Omega^4}$
3	$-\frac{21g^4B^2}{8\Omega^5} + \frac{39g^4B(A+4gBX)^2}{8\Omega^7} - \frac{51g^4(A+4gBX)^4}{32\Omega^9}$
4	$-\frac{3285g^6B^2(A+4gBX)^2}{32\Omega^{10}} + \frac{6387g^6B(A+4gBX)^4}{64\Omega^{12}} - \frac{3331g^6(A+4gBX)^6}{128\Omega^{14}}$

Table 3.4: Effective potential of the anharmonic oscillator (3.4) up to the 4th order, expanded in the reduced Planck constant $\hbar$.

it is related to the g-expansion by

$$\sum_{l=0}^{N} \hbar^l V^{(l)}(X) = V(X) + \sum_{k=0}^{\lfloor N/2 \rfloor + 1} g^k V_k(X)\Big|_{X=0,\ \omega=\Omega,\ A=A+4gBX} . \tag{3.51}$$

Up to the fourth order, Tab. 3.4 shows the expansion coefficients $V^{(l)}(X)$, which have been obtained accordingly, for $M = 1$.

3.4 Effective Potential

The effective potential of the anharmonic oscillator can also be obtained directly by means of a recursion relation, which will be developed in this section. Using (3.39), (3.40) the Schrödinger equation (3.28) becomes

$$\begin{aligned} -\frac{\hbar^2}{2M}\,\psi''(x) + \left[\frac{M}{2}\omega^2 x^2 + gAx^3 + g^2Bx^4 - V'_{\text{eff}}(X)x\right]\psi(x) \\ = \left[V_{\text{eff}}(X) - V'_{\text{eff}}(X)X\right]\,\psi(x)\,. \end{aligned} \tag{3.52}$$

Since this equation has emerged from (3.28) by replacing the current j and the energy E according to (3.39), (3.40), the ansatz (3.30), (3.31) will have to be modified accordingly. To this end, consider the effective potential for a vanishing coupling constant, i.e. the harmonic oscillator's effective potential, which has been calculated in Section 2.4. In the zero-temperature limit, it is given by (2.67). Therefore, for $g = 0$ one has

$$j = M\omega^2 X\,. \tag{3.53}$$

Thus, the ansatz (3.30), (3.31) becomes

$$\psi(x) = N\, e^{\phi(x)}\,, \qquad \text{with} \qquad \phi(x) = \frac{M\omega X}{\hbar}x - \frac{M\omega}{2\hbar}x^2 + \sum_{k=1}^{\infty} g^k \phi_k(x)\,, \tag{3.54}$$

and

$$V_{\text{eff}}(X) = \frac{\hbar\omega}{2} + \frac{M}{2}\omega^2 X^2 + \sum_{k=1}^{\infty} g^k\, V_k(X)\,. \tag{3.55}$$

Inserting (3.54) and (3.55) into (3.52), one finds by coefficients comparison

$$-\frac{\hbar^2}{2M}\phi_k''(x) - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1}\phi_{k-l}'(x)\,\phi_l'(x) + \hbar\omega\,(x-X)\,\phi_k'(x) - xV_k'(X) + \delta_{k,1}\,Ax^3 + \delta_{k,2}\,Bx^4 = V_k(X) - V_k'(X)X\,. \tag{3.56}$$

As before, we use the approach (3.10), or rather (3.14), to solve this differential equation. First, for $k = 1$, one finds

$$c_1^{(1)} = \frac{A}{2M\omega^2} + \frac{2AX^2}{\hbar\omega}\,, \qquad c_2^{(1)} = -\frac{AX}{2\hbar\omega}\,, \qquad c_3^{(1)} = -\frac{A}{3\hbar\omega}\,, \tag{3.57}$$

$$\text{and } V_1(X) = \frac{3A\hbar}{2M\omega} + AX^3\,. \tag{3.58}$$

And for $k = 2$ one obtains

$$c_1^{(2)} = -\frac{13A^2X}{4M^2\omega^4} - \frac{2A^2X^3}{M\hbar\omega^3} + \frac{7BX}{2M\omega^2} + \frac{3BX^3}{\hbar\omega}\,,$$
$$c_2^{(2)} = \frac{A^2}{8M^2\omega^4} - \frac{3B}{4M\omega^2} - \frac{BX^2}{2\hbar\omega}\,, \qquad c_3^{(2)} = \frac{A^2X}{2M\hbar\omega^3} - \frac{BX}{3\hbar\omega}\,,$$
$$c_4^{(2)} = \frac{A^2}{8M\hbar\omega^3} - \frac{B}{4\hbar\omega}\,, \tag{3.59}$$

$$\text{and } V_2(X) = -\frac{\hbar^2A^2}{4M^3\omega^4} - \frac{9\hbar A^2X^2}{4M^2\omega^3} + \frac{3\hbar^2B}{4M^2\omega^2} + \frac{3\hbar BX^2}{M\omega} + BX^4\,. \tag{3.60}$$

For $k \geq 3$ one finds

$$c_m^{(k)} = \frac{(m+2)(m+1)\hbar}{2mM\omega}\,c_{m+2}^{(k)} + \frac{\hbar}{2mM\omega}\sum_{l=1}^{k-1}\sum_{n=1}^{m+1} n(m+2-n)\,c_n^{(l)}\,c_{m+2-n}^{(k-l)} + \frac{X(m+1)}{m}\,c_{m+1}^{(k)} \quad \text{for } m \geq 2 \quad \text{and with } c_m^{(k)} \equiv 0 \quad \text{for } m > k+2, \tag{3.61}$$

$$c_1^{(k)} = \frac{3\hbar}{M\omega}c_3^{(k)} + 2X\,c_2^{(k)} + \frac{\hbar}{M\omega}\sum_{l=1}^{k-1}\left(c_2^{(k-l)}c_1^{(l)} + c_1^{(k-l)}c_2^{(l)}\right) + \frac{1}{\hbar\omega}V_k'(X)\,, \tag{3.62}$$

$$V_k(X) = -\frac{\hbar^2}{M}\,c_2^{(k)} - \frac{3\hbar^2}{M}X\,c_3^{(k)} - 2\hbar\omega X^2\,c_2^{(k)} - \frac{\hbar^2}{M}X\sum_{l=1}^{k-1}\left(c_2^{(k-l)}c_1^{(l)} + c_1^{(k-l)}c_2^{(l)}\right) - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1}c_1^{(l)}\,c_1^{(k-l)}\,. \tag{3.63}$$

Using these results, the effective potential can be determined recursively. Indeed, one reobtains the results from Table 3.3.

Chapter 4

Variational Perturbation Theory

4.1 Basic Principles

The vast majority of physical systems cannot be treated exactly since the underlying equations cannot be solved analytically. A commonly applied method to obtain information on such a system approximatively is perturbation theory. This method is based upon the fact that in many cases a physical quantity f, e.g. the ground-state energy of a particle in some potential, is known exactly for a certain value g_0 of a coupling constant g, which is typically $g_0 = 0$. An approximation for the physical quantity f as a function of the coupling constant g is then obtained by expanding f in powers of g up to some order N:

$$f_N(g) = \sum_{n=0}^{N} a_n g^n \,. \tag{4.1}$$

A prominent example for this procedure is the calculation of the anomalous magnetic moment of the electron g_e in powers of the fine-structure constant $\alpha \approx 1/137$. This calculation has been done up to the order α^4, see Ref. [26], and yields a result, which coincides with the experimental value, $g_\mathrm{e} = 2.0023193043(74)$ [27], up to 9 digits. This impressive agreement has established quantum electrodynamics as the prototype of a relativistic quantum field theory.

However, as has been observed already by Freeman Dyson in 1952 [28], the quality of this agreement depends crucially on the smallness of the fine-structure constant. Dyson discovered that physical quantities in quantum electrodynamics have a vanishing convergence radius with respect to α. His argumentation was based on the observation that changing the sign of the fine-structure constant would be equivalent to repulsion between equal electric charges; resulting in a vacuum which disintegrates by spontaneous polarization. Thus, power series in the fine-structure constant α are not examples for convergent expansions, but, on the contrary, for expansions with a vanishing radius of convergence (see Fig. 4.1). Such divergent series might lead to reasonable results as long as the truncation number N is kept limited, as in the case of the calculation of the anomalous magnetic moment of the

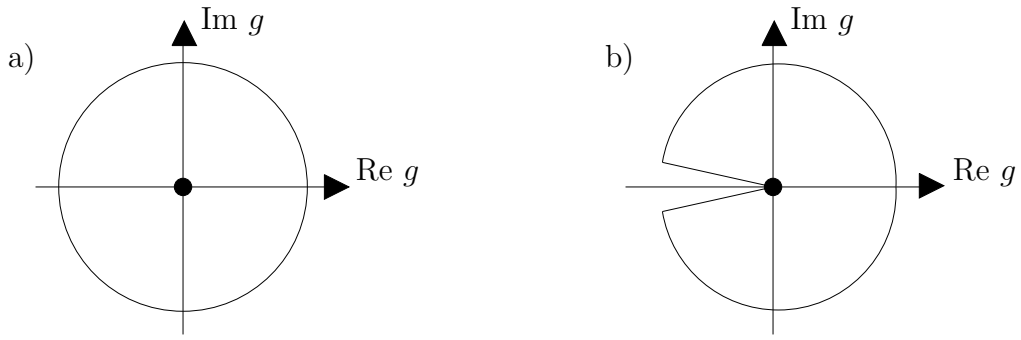


Figure 4.1: Schematic comparison of analytic properties of a) convergent and b) divergent series.

electron. However, once the expansion is driven past a certain order N, the result will cease to improve and will start to worsen. Eventually, for $N \to \infty$, the result of the expansion will diverge, no matter how small the coupling constant is.

To extract satisfying results for all values of the coupling constant, including the strong-coupling limit $g \to \infty$, from a divergent expansion of the form (4.1), it is thus necessary to resum (4.1). Padé approximants, which are derived by expanding a function as a ratio of two power series, constitute a crude method for such a resummation [29–31]. For quantum mechanical systems, physical results can be obtained by variational methods. For instance, the so-called δ-expansion allows the resummation of divergent perturbation series [32]. This method is based on introducing artificially a harmonic oscillator term in the potential and a subsequent optimization with respect to the trial-frequency of the artificial oscillator. This technique is called variational perturbation theory (VPT) [3–7]. It permits the evaluation of a divergent series of the form (4.1) for all values of the coupling constant g, including the strong-coupling limit, and yields a strong-coupling expansion of the generic form

$$f(g) = g^{p/q} \sum_{m=0}^{M} b_m \, g^{-2m/q} \, . \tag{4.2}$$

Here, p and q are real growth parameters and characterize the strong-coupling behavior. It turns out that due to dimensional reasons, for all quantum mechanical systems, p and q are integers, whereas, e.g., in the theory of critical phenomena p and q are irrational, as they are related to the critical exponents.

4.2 Arbitrary Coupling Strength

In this section, it is demonstrated how the resummation of a weak-coupling series is performed by applying VPT. To this end, we consider the perturbation series (4.1) of an arbi-

trary physical quantity f. Introducing a scaling parameter κ, which is afterwards set to one, Eq. (4.1) can be rewritten as

$$f_N(g) = \kappa^p \sum_{n=0}^{N} a_n \left(\frac{g}{\kappa^q}\right)^n \Bigg|_{\kappa=1} . \tag{4.3}$$

The parameters p and q will indeed determine the strong-coupling behavior of f as stated in (4.2). By performing Kleinert's square-root substitution [4, Ch. 5], i.e. by setting

$$\kappa = K\sqrt{1+gr}\,, \tag{4.4}$$

with

$$r = \frac{\kappa^2 - K^2}{gK^2}\,, \tag{4.5}$$

in (4.3), the variational parameter K is introduced into the perturbation series:

$$f_N(g) = \sum_{n=0}^{N} a_n g^n K^{p-nq} \left(1+gr\right)^{(p-nq)/2} \Big|_{\kappa=1} . \tag{4.6}$$

The Taylor series of the factor $(1+gr)^\alpha$ with $\alpha \equiv (p-nq)/2$ reads

$$(1+gr)^\alpha \Big|_{\kappa=1} = \sum_{k=0}^{N-n} \binom{\alpha}{k} \left(\frac{1}{K^2} - 1\right)^k + \mathcal{O}\left(g^{N-n+1}\right)\,, \tag{4.7}$$

where the generalized binomial coefficient is defined by

$$\binom{\alpha}{k} \equiv \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)}\,. \tag{4.8}$$

The series (4.7) is truncated after $k = N-n$ since the original function $f_N(g)$ is only known until the order g^N, and a later truncation would lead to terms of higher than this original perturbation order. As a result of this truncation, the function $f_N(g)$ becomes dependent on the variational parameter K:

$$f_N(g,K) = \sum_{n=0}^{N} a_n g^n K^{p-nq} \sum_{k=0}^{N-n} \binom{(p-nq)/2}{k} \left(\frac{1}{K^2} - 1\right)^k . \tag{4.9}$$

Since the dependence on the variational parameter K is merely due to the truncation of the Taylor expansion (4.7), one expects that the best approximation for the actual value of the physical quantity $f(g)$ can be obtained by minimizing the influence of K. In order to obtain an approximative result for $f(g)$, one will therefore evaluate the function $f_N(g,K)$ for that value of K for which its dependence on K becomes minimal. This concept is referred to as *principle of minimal sensitivity* [33]. In accordance with this principle, one seeks to minimize the influence of K by searching for local extrema, i.e. one determines K by solving

$$\frac{\partial f_N(g,K)}{\partial K}\Bigg|_{K=K^{(N)}(g)} = 0\,. \tag{4.10}$$

From the set of solutions to this conditional equation one will accept only the physical ones, e.g. the variational parameter might be required to be real and positive, in order to obtain a positive ground-state energy. In cases where (4.10) has no physical solutions, one looks for turning points instead, i.e. one will look for the solutions of

$$\left.\frac{\partial^2 f_N(g,K)}{\partial K^2}\right|_{K=K^{(N)}(g)} = 0\,. \tag{4.11}$$

In cases, where either (4.10) or (4.11) yields a multitude of physically acceptable solutions, one can apply different criteria for choosing a particular value of the variational parameter. It is possible, for instance, to choose the solution which is nearest to the solution of the previous order. Alternatively, one can look for solutions with as many vanishing derivatives as possible [34].

4.3 Strong-Coupling Limit

Even though VPT can be used to increase the precision of approximations obtained by evaluating weak-coupling series, its main purpose is the resummation of such series in cases of a large coupling constant or in the strong-coupling limit. In the theory of critical phenomena, for instance, reasonable results can only be obtained by resummation techniques, since the coupling constant typically diverges when approaching a critical point [5]. Thus, it is of particular interest to investigate the quality of the procedure introduced in the previous section for the strong-coupling limit. A careful analysis [5] of the conditions (4.10) and (4.11) for the function (4.9) shows that the variational parameter has the strong-coupling behavior

$$K^{(N)}(g) = g^{1/q}\left(K_0^{(N)} + K_1^{(N)} g^{-2/q} + K_2^{(N)} g^{-4/q} + \ldots\right)\,. \tag{4.12}$$

The power behavior of K is thus independent of the order N being considered and solely the coefficients $K_m^{(N)}$, $m = 0,\ 1,\ 2,\ \ldots$, depend on N. Inserting (4.12) into (4.9) yields the strong-coupling behavior of the approximation $f_N(g,K)$ for the physical quantity f:

$$\begin{aligned} &f_N\left(g, K^{(N)}(g)\right) \;= \\ &\quad g^{p/q}\left[b_0^{(N)}\left(K_0^{(N)}\right) + b_1^{(N)}\left(K_0^{(N)}, K_1^{(N)}\right) g^{-2/q} + b_2^{(N)}\left(K_0^{(N)}, K_1^{(N)}, K_2^{(N)}\right) g^{-4/q} + \ldots\right]\,. \end{aligned} \tag{4.13}$$

Therefore, also the power behavior of f is independent of the order N. The fraction p/q yields the leading power behavior in g, and $2/q$ indicates the approach to scaling. The leading-order strong-coupling coefficient turns out to be given by

$$b_0^{(N)}\left(K_0^{(N)}\right) = \sum_{n=0}^{N}\sum_{k=0}^{N-n}\binom{(p-nq)/2}{k}(-1)^k a_n (K_0^N)^{p-nq}\,, \tag{4.14}$$

where the inner sum can be further simplified by using [22, p. 3]

$$\sum_{k=0}^{m}(-1)^k\binom{\alpha}{k} = (-1)^m\binom{\alpha-1}{m}\,. \tag{4.15}$$

Thus, the leading strong-coupling coefficient reduces to

$$b_0^{(N)}(K_0^{(N)}) = \sum_{n=0}^{N}(-1)^{N-n}\binom{(p-nq)/2-1}{N-n}a_n\left(K_0^{(N)}\right)^{p-nq}\,, \tag{4.16}$$

and if one is only interested in the leading-order term of $f_N(g,K)$, it is sufficient to look for local extrema,

$$\left.\frac{\partial b_0^{(N)}(K)}{\partial K}\right|_{K=K_0^{(N)}} = 0\,, \tag{4.17}$$

or turning points,

$$\left.\frac{\partial^2 b_0^{(N)}(K)}{\partial K^2}\right|_{K=K_0^{(N)}} = 0\,, \tag{4.18}$$

of (4.16). Inserting the optimized $K_0^{(N)}$ into (4.16) then leads to the approximation $b_0^{(N)}(K_0^{(N)})$ of the leading strong-coupling coefficient b_0. A detailed analysis of the convergence behavior of $b_0^{(N)}$ shows that the VPT result approaches the exact value exponentially [5,35]:

$$\frac{|b_0^{(N)}-b_0|}{b_0} \propto \exp\left(-CN^{1-2/q}\right)\,. \tag{4.19}$$

4.4 Potential with Quartic Anharmonicity

In this section, the application of VPT to the anharmonic oscillator

$$V(x) = \frac{M}{2}\omega^2x^2 + gx^4 \tag{4.20}$$

will be demonstrated. The weak-coupling expansion for the ground-state energy of this system follows from the results of Section 3.2 for $A=0$, $B=1$, and $g\to\sqrt{g}$. Up to the third order it reads

$$E = \frac{\hbar\omega}{2} + g\,\frac{3\hbar^2}{4M^2\omega^2} - g^2\,\frac{21\hbar^3}{8M^4\omega^5} + g^3\,\frac{333\hbar^4}{16M^6\omega^8} + \dots\,, \tag{4.21}$$

which can also be written in the form

$$E = \omega\left(\frac{\hbar}{2} + g\,\frac{3\hbar^2}{4M^2\omega^3} - g^2\,\frac{21\hbar^3}{8M^4\omega^6} + g^3\,\frac{333\hbar^4}{16M^6\omega^9} + \dots\right)\,. \tag{4.22}$$

Comparing the last identity with (4.3) and identifying ω with the scaling parameter κ already indicates that for the anharmonic oscillator (4.20), one has $p=1$ and $q=3$. Now, the basic idea of VPT amounts to introducing an effective harmonic oscillator with trial frequency Ω according to

$$V(x) = \frac{M}{2}\,\Omega^2x^2 + gx^4 + \frac{M}{2}\left(\omega^2-\Omega^2\right)x^2 \tag{4.23}$$

and treating the deviation of the potential $V(x)$ from the harmonic oscillator with the trial frequency Ω as a perturbation. To this end, one rewrites the potential (4.23) as

$$V(x) = \frac{M}{2}\left(\Omega\sqrt{1+g\,\frac{\omega^2-\Omega^2}{g\Omega^2}}\right)^2 x^2 + gx^4\,. \tag{4.24}$$

Thus, if the weak-coupling expansion is available until some order N in the coupling constant g, one replaces the frequency ω according to

$$\omega \to \Omega\sqrt{1+gr}\,, \qquad \text{with} \qquad r = \frac{\omega^2-\Omega^2}{g\Omega^2}\,, \tag{4.25}$$

and then expands the resulting expression up to the order N in g. Equation (4.25) corresponds to the substitution (4.4), (4.5), and Ω plays the role of the variational parameter.

As an example, consider the first order of the weak-coupling expansion as given by (3.8) and (3.13):

$$E^{(1)} = \frac{\hbar\omega}{2} + g\,\frac{3\hbar^2}{4M^2\omega^2}\,. \tag{4.26}$$

Performing Kleinert's square-root substitution (4.25) and expanding until the first order in g then yields the ground-state energy as a function of the trial frequency Ω:

$$E^{(1)}(\Omega) = \frac{\hbar\Omega}{4} + \frac{\hbar\omega^2}{4\Omega} + g\,\frac{3\hbar^2}{4M^2\Omega^2}\,. \tag{4.27}$$

The principle of minimal sensitivity can be visualized by considering the function $E^{(N)}(\Omega)$. Figure 4.2 shows how $E^{(N)}(\Omega)$ depends on the variational parameter for $N = 1,\ 2,\ 3$ and for a certain value of the coupling constant. One sees indeed that a good approximation for the ground-state energy can be obtained by evaluating it at its minimum or turning point. For the first three orders, one thus has the conditional equations

$$\frac{\partial E^{(1)}(\Omega)}{\partial\Omega} = 0\,, \tag{4.28}$$

$$\frac{\partial^2 E^{(2)}(\Omega)}{\partial\Omega^2} = 0\,, \tag{4.29}$$

$$\frac{\partial E^{(3)}(\Omega)}{\partial\Omega} = 0\,, \tag{4.30}$$

the solutions of which, $\Omega^{(1)}$, $\Omega^{(2)}$, $\Omega^{(3)}$, then yield the corresponding approximations for the ground-state energy. In the first order, it follows from (4.27) and (4.28) that one has to solve

$$\frac{\hbar}{4} - \frac{\hbar\omega^2}{4(\Omega^{(1)})^2} - g\,\frac{3\hbar^2}{2M^2(\Omega^{(1)})^3} = 0\,, \tag{4.31}$$

which can be done analytically using Cardano's formula. The equations arising in higher orders must be solved numerically. From the multiple solutions to these equations, one accepts only those with a real and positive value of the variational parameter. It is particularly

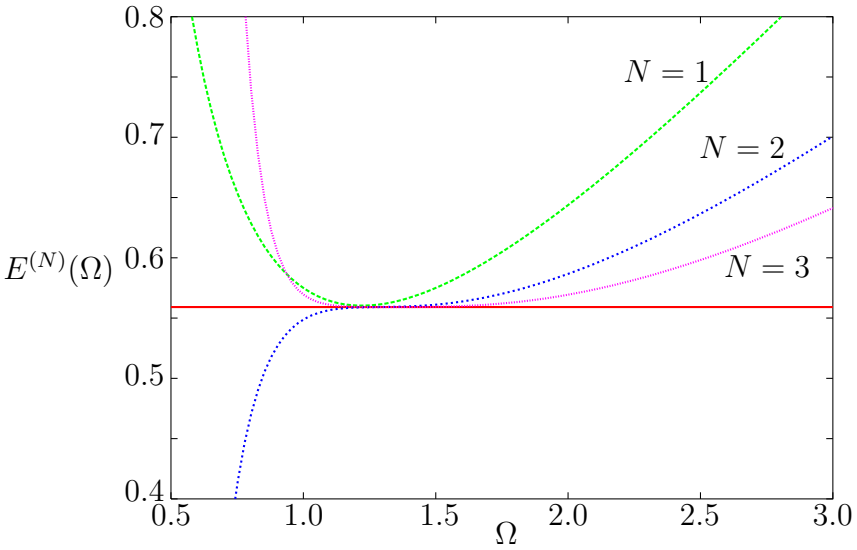


Figure 4.2: Trial function $E^{(N)}(\Omega)$ for $N = 1, 2, 3$ in natural units, $\hbar = M = \omega = 1$, and $g = 0.1$. The solid line represents the exact value for the ground-state energy, obtained by a numerical calculation using the shooting method, which is introduced in Appendix C.

interesting to examine the conditional equation (4.28), or rather (4.31), for the case of a large coupling constant g. Multiplying (4.31) with $(\Omega^{(1)})^3$ and inserting the approach

$$\Omega^{(1)} = \Omega_0^{(1)} g^{\alpha} + \Omega_1^{(1)} g^{\beta} + \Omega_2^{(1)} g^{\gamma} + \dots \,, \tag{4.32}$$

with

$$1 > \alpha > 0 > \beta > \gamma > \dots \,, \tag{4.33}$$

allows the determination of the strong-coupling behavior of the variational parameter. Here, condition (4.33) turns out to be self-consistent. One finds:

$$\alpha = \frac{1}{3} \,, \qquad \beta = -\frac{1}{3} \,, \qquad \gamma = -1 \,, \qquad \dots \,, \tag{4.34}$$

and

$$\Omega_0^{(1)} = \sqrt[3]{\frac{6\hbar}{M^2}} \,, \qquad \Omega_1^{(1)} = \frac{\omega^2}{3} \sqrt[3]{\frac{M^2}{6\hbar}} \,, \qquad \Omega_2^{(1)} = \frac{\omega^4 M^2}{324\hbar} \,, \qquad \dots \,. \tag{4.35}$$

Thus, the variational parameter can be written in the form

$$\Omega^{(1)} = g^{1/3} \left(\Omega_0^{(1)} + \Omega_1^{(1)} g^{-2/3} + \Omega_2^{(1)} g^{-4/3} + \dots \right) \,. \tag{4.36}$$

Inserting the last result into (4.27), one obtains the strong-coupling behavior of the ground-state energy:

$$E^{(1)} = g^{1/3} \left(b_0^{(1)} + b_1^{(1)} g^{-2/3} + b_2^{(1)} g^{-4/3} + \dots \right) \,, \tag{4.37}$$

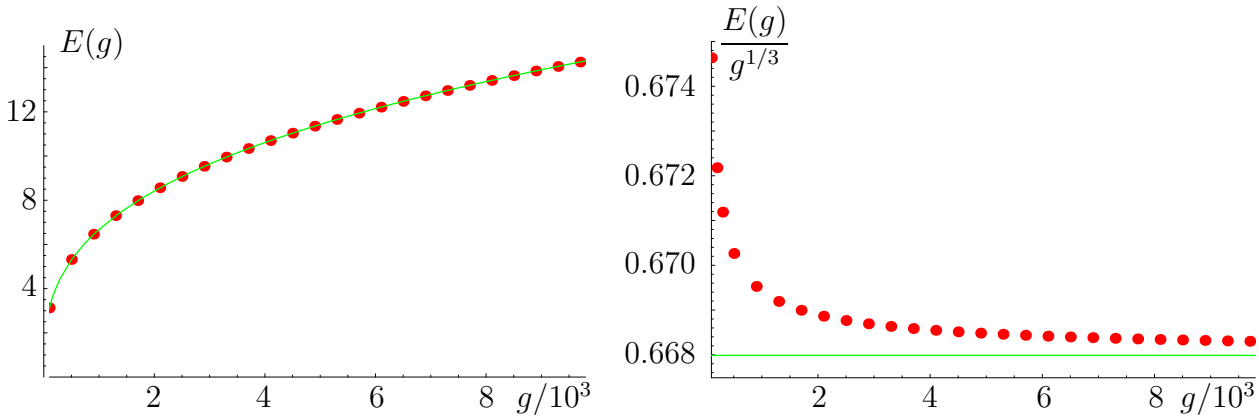


Figure 4.3: Numerical calculation of the ground-state energy for different values of the coupling constant obtained by applying the shooting method, introduced in Appendix C. In a) the solid line represents a fit assuming $E = b_0\, g^{1/3}$. In b) the solid line represents the high-precision value (4.40) for b_0 given by F. Vinette and J. Čížek [36].

where

$$b_0^{(1)} = \frac{3\hbar}{8}\sqrt[3]{\frac{6\hbar}{M^2}}\,, \qquad b_1^{(1)} = \frac{\hbar\omega^2}{4}\sqrt[3]{\frac{M^2}{6\hbar}}\,, \qquad b_2^{(1)} = -\frac{\omega^4 M^2}{144}\,, \qquad \ldots\,. \tag{4.38}$$

Thus, one has indeed an expansion of the form (4.2) with

$$p = 1 \qquad \text{and} \qquad q = 3\,, \tag{4.39}$$

as has already been stated in the remark after (4.22). Figure 4.3 shows a numerical calculation of the ground-state energy for different values of the coupling constant g. In natural units, $b_0^{(1)}$ has the numeric value $b_0^{(1)} \approx 0.68142$. The leading-order strong-coupling coefficient has been determined with extreme precision by F. Vinette and J. Čížek [36]:

$$b_0 = 0.667\,986\,259\,155\,777\,108\,270\,962\,016\,198\,601\,994\,304\,049\,36\ldots\,. \tag{4.40}$$

Thus, the relative deviation is

$$\frac{|b_0^{(1)} - b_0|}{b_0} \approx 2\%\,. \tag{4.41}$$

Following Refs. [8,9], Fig. 4.4 shows the logarithmic relative deviation of the leading strong-coupling coefficient calculated via VPT from the value given in Ref. [36] plotted, due to (4.19) and (4.39), versus the cubic root of the perturbation order. The values for $b_0^{(N)}$ have been obtained by optimizing (4.16) according to (4.17) and (4.18). The convergence of the calculation is found to be exponential. Fitting the logarithm of the relative error of the VPT result to a straight line yields

$$\ln\frac{|b_0^{(N)} - b_0|}{b_0} = -9.23(11)N^{1/3} + 5.50(34)\,. \tag{4.42}$$

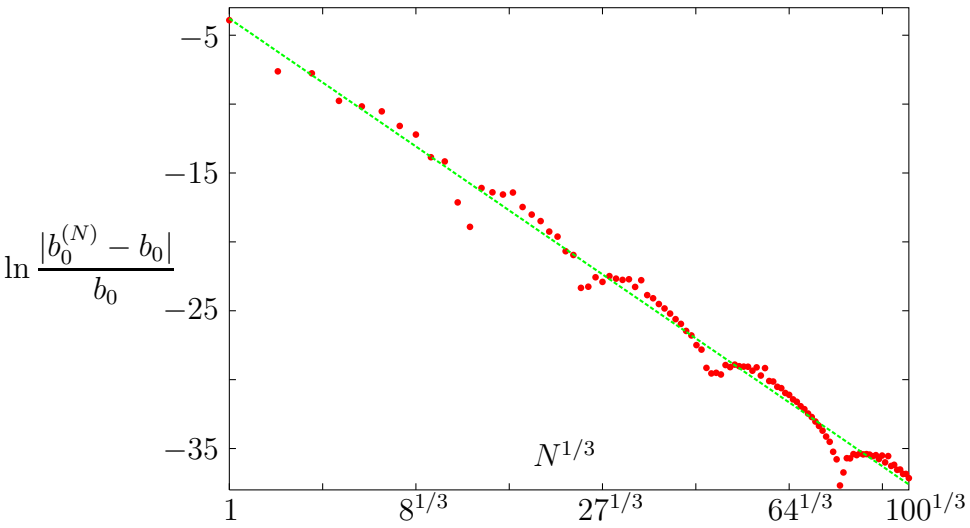


Figure 4.4: Logarithm of the relative deviation of the result for b_0 obtained via VPT from the value given in Ref. [36] versus the cubic root of the perturbation order up to the 100th order [8,9].

4.5 Potential with Cubic Anharmonicity

In this section, an oscillator with the potential

$$V(x) = \frac{M}{2}\omega^2 x^2 + igx^3 \tag{4.43}$$

is considered. The Hamiltonian

$$\mathcal{H} = p^2 - (ix)^n \tag{4.44}$$

has been examined thoroughly, see Refs. [10–14]. For $n = 2$, Eq. (4.44) reduces to the Hamiltonian of the harmonic oscillator. For $n > 1$, it turns out that with properly defined boundary conditions the spectrum of (4.44) is real and positive. Ordinarily, the boundary conditions that give quantized energy levels when considering the Schrödinger eigenvalue equation of a Hamiltonian are

$$|\psi(x)| \to 0 \qquad \text{as} \qquad |x| \to \infty\,. \tag{4.45}$$

In case of the Hamiltonian (4.44), this condition suffices when $1 < n < 4$. However, for arbitrary real n, the corresponding eigenvalue problem has to be continued into the complex x-plane, and the real x-axis is thus replaced by a contour in the complex plane. The spectrum of (4.44), obtained by imposing these boundary conditions, is shown in Fig. 4.5. The remarkable attribute of this generally non-Hermitian Hamiltonian (4.44) to possess a real and positive spectrum is attributed to its $\mathcal{PT}$-symmetry. Here, $\mathcal{P}$ and $\mathcal{T}$ are the operators of parity and time reversal, respectively:

$$\mathcal{P} \quad : \quad p \to -p\,, \qquad x \to -x\,, \tag{4.46}$$

$$\mathcal{T} \quad : \quad p \to -p\,, \qquad x \to x\,, \qquad i \to -i\,. \tag{4.47}$$

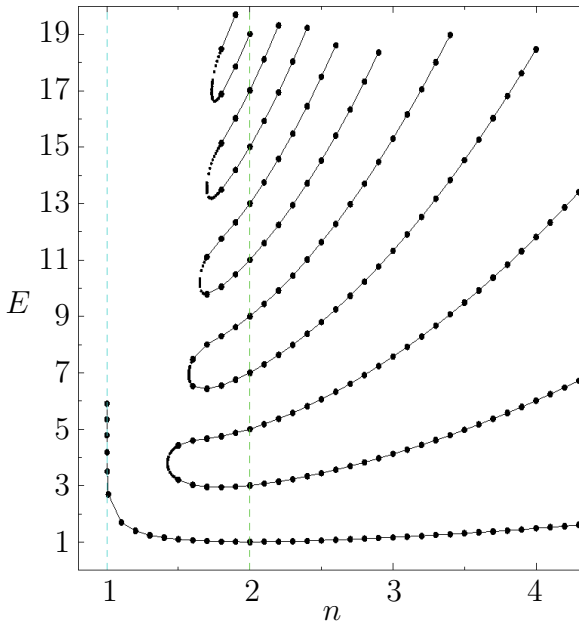


Figure 4.5: Spectrum of the Hamiltonian (4.44) [10].

Consider the time-independent Schrödinger equation for the potential (4.43) in natural units, $\hbar = M = 1$,

$$-\frac{1}{2}\,\frac{\partial^2}{\partial x^2}\,\psi(x) + \left(\frac{1}{2}\omega^2 x^2 + igx^3\right)\psi(x) = E\,\psi(x)\,. \tag{4.48}$$

Substituting

$$x \to \alpha x = g^{-1/5} x\,, \tag{4.49}$$

Eq. (4.48) becomes

$$-\frac{1}{2}\,\frac{\partial^2}{\partial x^2}\,\psi(x) + \left(\frac{1}{2}g^{-4/5}\omega^2 x^2 + ix^3\right)\psi(x) = g^{-2/5}E\,\psi(x)\,. \tag{4.50}$$

Expanding the wave function and the energy in terms powers of the coupling constant yields

$$\psi(x) = \psi_0(x) + g^{-4/5}\psi_1(x) + g^{-8/5}\psi_2(x) + \dots\,, \tag{4.51}$$

and

$$E = g^{2/5}b_0 + g^{-2/5}b_1 + g^{-6/5}b_2 + \dots\,. \tag{4.52}$$

Thus, by considering (4.50) in the strong-coupling limit one obtains the following relation between the leading strong-coupling coefficient b_0 and the energy eigenvalues of the Hamiltonian (4.44) for $n = 3$:

$$E(n=3) = 2^{3/5}\,b_0\,. \tag{4.53}$$

Here, the factor $2^{3/5}$ is due to the fact that in (4.44) the kinetic term is p^2 instead of $p^2/2$. A numerical value for the ground-state energy associated with the Hamiltonian (4.44) was given by C.M. Bender [10,37]:

$$E(n=3) = 1.15626707\ldots\,. \tag{4.54}$$

4.5.1 Resummation of Ground-State Energy

Due to (4.53), the ground-state energy associated with the Hamiltonian (4.44) can be obtained by determining the leading strong-coupling coefficient of the ground-state energy for the oscillator (4.43). To this end, one can resum the weak-coupling series obtained in Section 3.2 for $A = i$ and $B = 0$ via VPT. Up to the third order, the weak-coupling series reads

$$E = \frac{\hbar\omega}{2} + \tilde{g}\,\frac{11\hbar^2}{8M^3\omega^4} - \tilde{g}^2\,\frac{465\hbar^3}{32M^6\omega^9} + \tilde{g}^3\,\frac{39709\hbar^4}{128M^9\omega^{14}} + \ldots\,, \tag{4.55}$$

where we have replaced $g^2 \to \tilde{g}$ in order to facilitate the correct counting of each respective order in the coupling constant. Equation (4.55) can also be written in the form

$$E = \omega\left(\frac{\hbar}{2} + \tilde{g}\,\frac{11\hbar^2}{8M^3\omega^5} - \tilde{g}^2\,\frac{465\hbar^3}{32M^6\omega^{10}} + \tilde{g}^3\,\frac{39709\hbar^4}{128M^9\omega^{15}} + \ldots\right)\,. \tag{4.56}$$

As before, we compare the last identity with (4.3) and identify ω with the scaling parameter κ. Therefore, in the case of the anharmonic oscillator (4.43), we expect to obtain $p = 1$ and $q = 5$, and due to (4.13), the strong-coupling behavior of the ground-state energy of (4.43) will be of the form

$$E^{(N)} = \tilde{g}^{1/5}\left(b_0^{(N)} + b_1^{(N)}\tilde{g}^{-2/5} + b_2^{(N)}\tilde{g}^{-4/5} + \ldots\right)\,. \tag{4.57}$$

Thus, when reintroducing the original coupling constant, $\tilde{g} \to g^2$, we obtain the same strong-coupling behavior as in (4.52).

The first order of the weak-coupling expansion as given by (3.8), (3.13) reads

$$E^{(1)} = \frac{\hbar\omega}{2} + \tilde{g}\frac{11\hbar^2}{8M^3\omega^4}\,. \tag{4.58}$$

Performing Kleinert's square-root substitution (4.25) and re-expanding (4.58) in $\tilde{g}$ yields

$$E^{(1)}(\Omega) = \frac{\hbar\Omega}{4} + \frac{\hbar\omega^2}{4\Omega} + \tilde{g}\frac{11\hbar^2}{8M^3\Omega^4}\,. \tag{4.59}$$

Setting the first derivative with respect to the variational parameter Ω to zero and multiplying with $4\Omega^5/\hbar$, one obtains

$$(\Omega^{(1)})^5 - \omega^2(\Omega^{(1)})^3 - \tilde{g}\frac{22\hbar}{M^3} = 0\,. \tag{4.60}$$

Again, we consider this equation in the strong-coupling limit and solve it with an approach of the form (4.32), (4.33):

$$\Omega^{(1)} = \Omega_0^{(1)}\tilde{g}^{\alpha} + \Omega_1^{(1)}\tilde{g}^{\beta} + \Omega_2^{(1)}\tilde{g}^{\gamma} + \dots \,, \tag{4.61}$$

with

$$1 > \alpha > 0 > \beta > \gamma > \dots \,. \tag{4.62}$$

One obtains

$$\alpha = \frac{1}{5}\,, \qquad \beta = -\frac{1}{5}\,, \qquad \gamma = -\frac{3}{5}\,, \qquad \dots \,, \tag{4.63}$$

and

$$\Omega_0^{(1)} = \sqrt[5]{\frac{22\hbar}{M^3}}\,, \qquad \Omega_1^{(1)} = \frac{\omega^2}{5}\sqrt[5]{\frac{M^3}{22\hbar}}\,, \qquad \Omega_2^{(1)} = \frac{\omega^4 M}{25}\sqrt[5]{\frac{M^4}{10648\hbar^3}}\,, \qquad \dots \,. \tag{4.64}$$

Inserting this result into (4.59) yields the strong-coupling behavior of the ground-state energy:

$$E^{(1)} = \tilde{g}^{1/5}\left(b_0^{(1)} + b_1^{(1)}\tilde{g}^{-2/5} + b_2^{(1)}\tilde{g}^{-4/5} + \dots\right)\,, \tag{4.65}$$

where the coefficients read

$$b_0^{(1)} = \frac{5\hbar}{16}\sqrt[5]{\frac{22\hbar}{M^3}}\,, \qquad b_1^{(1)} = 4\hbar\omega^2\sqrt[5]{\frac{M^3}{22\hbar}}\,. \qquad b_2^{(1)} = -\frac{\hbar\omega^4}{100}\sqrt[5]{\frac{M^3}{22\hbar}}\,, \qquad \dots \,. \tag{4.66}$$

Thus, we have indeed an expansion of the form (4.2), with

$$p = 1 \qquad \text{and} \qquad q = 5\,, \tag{4.67}$$

and by reintroducing the original coupling constant $g = \sqrt{\tilde{g}}$ in (4.65) we reobtain (4.57) for $N = 1$.

However, it turns out that in the case of the potential with the cubic anharmonicity igx^3 the convergence of the VPT-result is not as satisfactory as in the case of the gx^4-oscillator. Whereas, according to (4.41), for the oscillator with the quartic anharmonicity the relative deviation of the first order result (4.38) from the exact value (4.40) is only in the order of a few percent, the first-order result (4.66) for the ground-state energy associated with the Hamiltonian (4.44) is much less precise:

$$\frac{|2^{3/5}b_0^{(1)} - E(n=3)|}{E(n=3)} \approx 24\%\,. \tag{4.68}$$

Figure 4.6 shows the logarithm of the relative deviation of the ground-state energy calculated by VPT from the value given by C.M. Bender up to the order $N = 20$. Due to (4.19) and (4.67) the plot is versus $N^{3/5}$. Fitting the logarithm of the relative deviation to a straight line yields

$$\ln\frac{|2^{3/5}b_0^{(N)} - E(n=3)|}{E(n=3)} = -0.96(11)N^{3/5} - 1.83(44)\,. \tag{4.69}$$

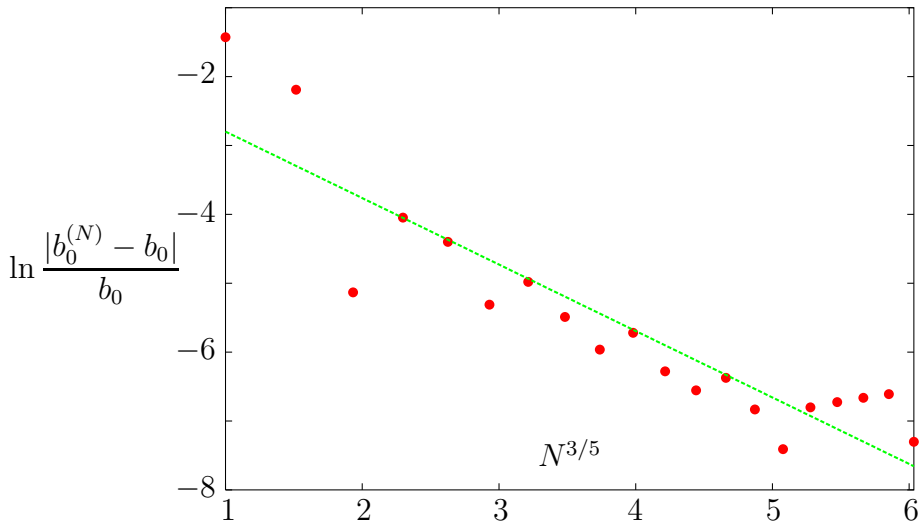


Figure 4.6: Logarithm of the relative deviation of the result for b_0, obtained via resummation of the corresponding weak-coupling series, from the value (4.54) given in Refs. [10,37] versus $N^{3/5}$. The dashed line represents a fit of the data to a straight line.

4.5.2 Resummation of Effective Potential

The convergence of the calculation in the previous section can be increased crucially by introducing a second variational parameter. This can be achieved naturally by combining two variational approaches: VPT and effective potential. The standard way of calculating the effective potential is the background method from field theory, which requires the evaluation of one-particle irreducible Feynman diagrams. Since the involved multiple imaginary-time integrals are not trivial to evaluate, only relatively low perturbation orders are accessible within the background method. Nevertheless, in Section 3.4 the effective potential for the potential (3.4) is obtained recursively by performing a Legendre transformation of the ground-state energy in presence of a constant external current. This expansion in g is then converted into an $\hbar$-expansion by (3.51), corresponding to the formalism of the background method. Table 4.1 shows the first five orders of the $\hbar$-expansion of the effective potential,

$$V_{\text{eff}}(X) = \sum_{l=0}^{\infty} \hbar^l V^{(l)}(X) \,, \tag{4.70}$$

for (4.43) obtained by setting

$$A \to i \,, \qquad B \to 0 \,, \qquad \text{and} \quad \Omega \to \sqrt{\omega^2 + \frac{6igX}{M}} \tag{4.71}$$

in Tab. 3.4. Now, $\hbar$ plays the role that was held before by the coupling constant g. Therefore, when performing Kleinert's square-root substitution (4.25), one needs to replace ω according to

$$\omega \to \Omega\sqrt{1 + \hbar r} \,, \qquad \text{with} \qquad r = \frac{\omega^2 - \Omega^2}{\hbar\Omega^2} \,. \tag{4.72}$$

l	$V^{(l)}(X)$
0	$\frac{M}{2}\omega^2 X^2 + igX^3$
1	$\frac{1}{2}\sqrt{\omega^2 + \frac{6igX}{M}}$
2	$\frac{g^2}{4M(M\omega^2 + 6igX)^2}$
3	$-\frac{51g^4}{32M^6\left(\omega^2 + \frac{6igX}{M}\right)^{9/2}}$
4	$\frac{3331g^6}{128M^2(M\omega^2 + 6igX)^7}$
5	$-\frac{1371477g^8}{2048M^{12}\left(\omega^2 + \frac{6igX}{M}\right)^{19/2}}$

Table 4.1: Coefficients for the effective potential (4.70) of the potential (4.43).

In the first order, one has

$$V_{\text{eff}}^{(1)}(X,\Omega) = \frac{M}{2}\omega^2 X^2 + igX^3 + \frac{\hbar}{2}\sqrt{\Omega^2 + \frac{6igX}{M}}\,. \tag{4.73}$$

In order to obtain an approximation for the ground-state energy, one has to combine the principle of minimal sensitivity (4.28) with condition (2.40). We thus seek to solve the coupled equations

$$\frac{\partial}{\partial\Omega}V_{\text{eff}}^{(1)}(X,\Omega)\bigg|_{X=X^{(1)},\,\Omega=\Omega^{(1)}} = 0 \tag{4.74}$$

and

$$\frac{\partial}{\partial X}V_{\text{eff}}^{(1)}(X,\Omega)\bigg|_{X=X^{(1)},\,\Omega=\Omega^{(1)}} = 0\,. \tag{4.75}$$

In this order, (4.74) merely leads to

$$\Omega^{(1)} = 0\,. \tag{4.76}$$

Thus, we obtain from (4.75):

$$X^{(1)} + \frac{M\omega^2}{3ig} + \frac{\hbar}{2\sqrt{6igM}(X^{(1)})^{3/2}} = 0\,. \tag{4.77}$$

1-loop VPT	1.12580003
2-loop VPT	1.15887214
3-loop VPT	1.15010079
4-loop VPT	1.15625481
5-loop VPT	1.15626432
Numerical	1.15626707

Table 4.2: Variational results for the ground-state energy of (4.44) for $n = 3$ compared to the numerical result (4.54) of Refs. [10,37].

This equation allows us to determine the strong-coupling behavior of X:

$$X^{(1)} = -ig^{-1/5}\left(X_0^{(1)} + X_1^{(1)} g^{-4/5} + X_2^{(1)} g^{-8/5} + \ldots\right) , \tag{4.78}$$

where the coefficients read

$$X_0^{(1)} = \sqrt[5]{\frac{\hbar^2}{24M}} , \qquad X_1^{(1)} = -\frac{2\omega^2 M}{15} , \qquad X_2^{(1)} = \frac{\omega^4 M^2}{75}\sqrt[5]{\frac{24M}{\hbar^2}} , \qquad \ldots . \tag{4.79}$$

As before, the power behavior of X does not depend on the order of the calculation, and only the coefficients $X_0^{(N)}$, $X_1^{(N)}$, $X_2^{(N)}$, ... are dependent on N. Since one has extremized the effective potential, inserting the results (4.76) and (4.77) into (4.73) yields the strong-coupling behavior of the ground-state energy:

$$E^{(1)} \;=\; g^{2/5}\left(b_0^{(1)} + b_1^{(1)} g^{-4/5} + b_2^{(1)} g^{-8/5} + \ldots\right) , \tag{4.80}$$

with

$$b_0^{(1)} = \frac{5\hbar}{2}\sqrt[5]{\frac{\hbar}{432M^3}} , \qquad b_1^{(1)} = -\frac{M\omega^2}{4}\sqrt[5]{\frac{\hbar^4}{18M^2}} , \qquad b_2^{(1)} = \frac{\omega^4 M^2}{15}\sqrt[5]{\frac{\hbar^2}{24M}} , \qquad \ldots . \tag{4.81}$$

The first-order result for the leading strong-coupling coefficient is already in good agreement with the numerical value (4.54) for the ground-state energy associated with the Hamiltonian (4.44) for $n = 3$:

$$\frac{|2^{3/5} b_0^{(1)} - E(n=3)|}{E(n=3)} \approx 3\% . \tag{4.82}$$

Thus, as comparison to (4.68) shows, the introduction of a second variational parameter has led to a significant improvement of the first-order result. In the second order, after performing Kleinert's square root substitution (4.72), the effective potential becomes

$$V_{\text{eff}}^{(2)}(X,\Omega) = \frac{M}{2}\omega^2 X^2 + igX^3 + \hbar\frac{M(\omega^2+\Omega^2) + 12igX}{4M\sqrt{\Omega^2 + 6igX/M}} + \hbar^2\frac{g^2}{4M(M\Omega^2 + 6igX)^2} . \tag{4.83}$$

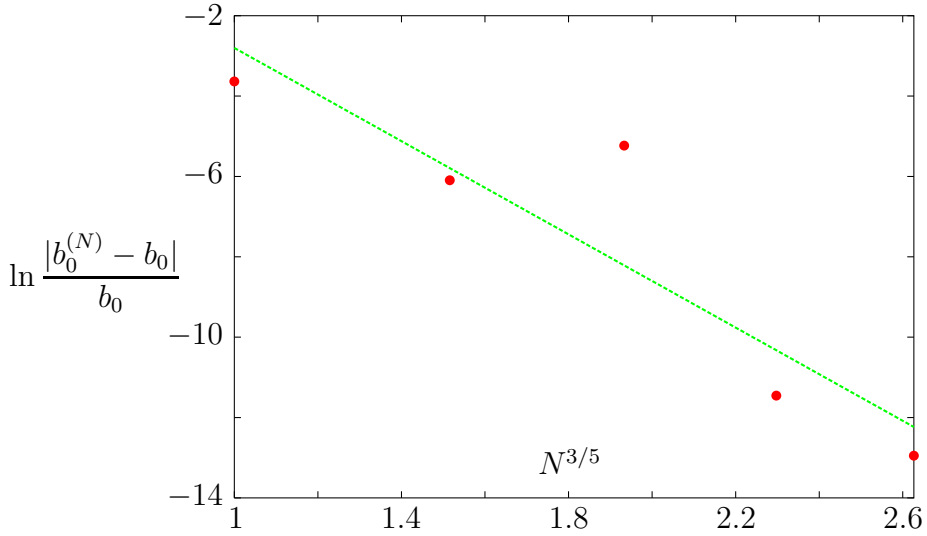


Figure 4.7: Logarithm of the relative deviation of the result for b_0, obtained via resummation of the effective potential, from the value (4.54) given in Refs. [10,37] versus $N^{3/5}$. The dashed line represents a fit of the data to a straight line.

Extremizing (4.83) in X and Ω allows the determining of the strong-coupling behavior of the variational parameter Ω:

$$\Omega^{(2)} = g^{2/5} \left(\Omega_0^{(2)} + \Omega_1^{(2)} g^{-4/5} + \Omega_2^{(2)} g^{-8/5} + \ldots \right) . \tag{4.84}$$

Table 4.2 summarizes the results for $2^{3/5}\, b_0^{(N)}$ until the fifth order. Figure 4.7 shows the logarithm of the relative deviation of the results obtained via VPT from the value (4.54) given by C.M. Bender up to the fifth order. In order to compare the quality of the convergence with that of the results from Section 4.5.1, the plot is again versus $N^{3/5}$. Fitting the logarithm of the relative deviation to a straight line yields

$$\ln \frac{|2^{3/5} b_0^{(N)} - E(n=3)|}{E(n=3)} = -5.8(1.6) N^{3/5} + 3.0(3.0) . \tag{4.85}$$

Comparing Fig. 4.6 and Fig. 4.7 or (4.69) and (4.85) shows that the convergence of the results obtained by resummation of the effective potential is significantly faster than that of the results obtained by resumming the weak-coupling series of the ground-state energy. Whereas the relative error of the 20th order result from Section 4.5.1 is still in the order of per mill,

$$\frac{|2^{3/5} b_0^{(20)} - E(n=3)|}{E(n=3)} \approx 0.6‰ , \tag{4.86}$$

already the fifth-order result obtained in this section is more than two orders of magnitude more precise:

$$\frac{|2^{3/5} b_0^{(5)} - E(n=3)|}{E(n=3)} \approx 2 \text{ ppm} . \tag{4.87}$$

Chapter 5

Extension to D Dimensions

5.1 Oscillator with Quartic Anharmonicity

In this section, we generalize the oscillator with quartic anharmonicity to D spatial dimensions. In Section 5.1.1, we obtain the weak-coupling series for its ground-state energy. In Section 5.1.2, we proceed to the strong-coupling limit and determine the leading strong-coupling expansion coefficients for $D = 2,\ 3,\ 10$. In Section 5.1.3, we introduce the method of large-D expansion.

5.1.1 Bender-Wu Recursion

In this section, a perturbation series for the ground-state energy of the D-dimensional anharmonic oscillator

$$V(\mathbf{x}) = \frac{M}{2}\omega^2\mathbf{x}^2 + g(\mathbf{x}^2)^2 \tag{5.1}$$

will be calculated recursively. In the following, x denotes the modulus of $\mathbf{x}$. Since the potential is rotationally symmetric, the ground-state wave function will depend on x only, and we identify $V(\mathbf{x}) \equiv V(x)$ and $\psi(\mathbf{x}) \equiv \psi(x)$. The time-independent Schrödinger equation reads

$$-\frac{\hbar^2}{2M}\Delta\,\psi(x) + \left(\frac{M}{2}\omega^2 x^2 + gx^4\right)\psi(x) = E\,\psi(x)\,. \tag{5.2}$$

In D dimensions, we choose an ansatz of the form

$$\psi(x) = \left(\frac{M\omega}{\pi\hbar}\right)^{D/4} \exp\left[-\frac{M\omega}{2\hbar}x^2 + \phi(x)\right]\,, \tag{5.3}$$

with

$$\phi(x) = \sum_{k=1}^{\infty} g^k \phi_k(x)\,, \tag{5.4}$$

and

$$E = D\frac{\hbar\omega}{2} + \sum_{k=1}^{\infty} g^k \epsilon_k \; . \tag{5.5}$$

Inserting (5.3) – (5.5) into (5.2) and comparing the coefficients yields a differential equation for the $\phi_k(x)$:

$$-\frac{\hbar^2}{2M}\phi_k''(x) + \hbar\omega\, x\, \phi_k'(x) - (D-1)\,\frac{\hbar^2}{2Mx}\,\phi_k'(x) - \frac{\hbar^2}{2M}\sum_{l=1}^{k-1}\phi_{k-l}'(x)\,\phi_l'(x) + \delta_{k,1}x^4 = \epsilon_k \; . \tag{5.6}$$

One can show by induction that if $\phi_k(x)$ is assumed to be a polynomial its degree cannot be greater than $2k+2$. The potential (5.1) is even in x, and this symmetry is passed on to the $\phi_k(x)$. Thus, the $\phi_k(x)$ can be written in the form

$$\phi_k(x) = \sum_{m=1}^{k+1} c_{2m}^{(k)}\, x^{2m} \; . \tag{5.7}$$

The constant terms $c_0^{(k)}$ can only be determined by normalizing the wave function. By inserting (5.7) into (5.6), one finds for $k = 1$

$$c_2^{(1)} = -\frac{2+D}{4M\omega^2} \; , \qquad c_4^{(1)} = -\frac{1}{4\hbar\omega} \; , \qquad \text{and } \; \epsilon_1 = \frac{D(2+D)\hbar^2}{4M^2\omega^2} \; . \tag{5.8}$$

In the general case, $k \geq 2$, one finds

$$c_m^{(k)} \;=\; \frac{(m+2)(m+1)+(D-1)(m+2)}{2mM\omega}\,\hbar c_{m+2}^{(k)} + \frac{\hbar}{2mM\omega}\sum_{l=1}^{k-1}\sum_{n=2}^{m} n(m+2-n)\, c_n^{(l)}\, c_{m+2-n}^{(k-l)} \; ,$$
$$\text{with } \; c_m^{(k)} \equiv 0 \quad \text{for } \; m > 2k+2 \; , \tag{5.9}$$

$$\epsilon_k \;=\; -D\,\frac{\hbar^2}{M}\,c_2^{(k)} \; . \tag{5.10}$$

As in Section 3.2, it is desirable to render the recursion relations (5.9), (5.10) dimensionless in order to achieve a more efficient numerical evaluation. To this end, one can use units in which $\hbar = M = 1$ and consider the approach (3.21), (3.22) for $A = 0$ and $B = 1$. One thus obtains the approach

$$c_m^{(k)} = \frac{\tilde{c}_m^{(k)}}{\omega^{3k-m/2}} \; , \tag{5.11}$$

and

$$\epsilon_k = \frac{\tilde{\epsilon}_k}{\omega^{3k-1}} \; . \tag{5.12}$$

k	ϵ_k
1	$\frac{D(2+D)}{4\omega^2}$
2	$-\frac{D(10+9D+2D^2)}{8\omega^5}$
3	$\frac{D(120+146D+59D^2+8D^3)}{16\omega^8}$
4	$-\frac{D(8840+12960D+7144D^2+1773D^3+168D^4)}{128\omega^{11}}$
5	$\frac{D(216960+360736D+241464D^2+82222D^3+14325D^4+1024D^5)}{256\omega^{14}}$

Table 5.1: Expansion coefficients for the ground-state energy of the anharmonic oscillator (5.1) up to the 5th order.

Inserting (5.7) together with (5.11) and (5.12) into (3.9) and setting $\hbar = M = 1$ yields for $k = 1$

$$\tilde{c}_2^{(1)} = -\frac{2+D}{4}\,, \qquad \tilde{c}_4^{(1)} = -\frac{1}{4}\,, \qquad \text{and } \tilde{\epsilon}_1 = \frac{D(2+D)}{4}\,. \tag{5.13}$$

In the general case, $k \geq 2$, one finds

$$\tilde{c}_m^{(k)} = [(m+2)(m+1)+(D-1)(m+2)]\frac{\tilde{c}_{m+2}^{(k)}}{2m} + \frac{1}{2m}\sum_{l=1}^{k-1}\sum_{n=2}^{m} n(m+2-n)\,\tilde{c}_n^{(l)}\,\tilde{c}_{m+2-n}^{(k-l)}\,, \quad \text{with } \tilde{c}_m^{(k)} \equiv 0 \quad \text{for } m > 2k+2\,, \tag{5.14}$$

$$\tilde{\epsilon}_k = -D\,\tilde{c}_2^{(k)}\,. \tag{5.15}$$

Using natural units, i.e. $\hbar = M = 1$, Tab. 5.1 shows the energy corrections ϵ_k up to the fifth order. For $D = 1$, it is identical with Table (3.1) when setting $A \to 0$, $B \to 1$, $g \to \sqrt{g}$.

5.1.2 Strong-Coupling Limit

In this section, we consider the strong-coupling limit for the anharmonic oscillator (5.1). Since the weak-coupling series of its ground-state energy is of the same form as in one dimension and the dimension D merely contributes to the weak-coupling coefficients ϵ_k, we can use the same formalism as in Section 4.4. As to our knowledge the strong-coupling coefficient $b_0^{(N)}(D)$ has not yet been calculated for $D \neq 1$, we will first examine how a numerical value for $b_0^{(N)}(D)$ can be obtained for $D = 2,\ 3,\ 10$. In Appendix C, the shooting

$b_0(D=2)$	1.4771497535779972(31)
$b_0(D=3)$	2.3936440164822970(37)
$b_0(D=10)$	10.758265165443755(69)

Table 5.2: Numerical results for the leading strong-coupling coefficient b_0 for the ground-state energy of (5.1).

method is introduced. We have applied this method to determine numerically the ground-state energy of the anharmonic oscillator (5.1) for different values of the coupling-constant g. The strong-coupling behavior (4.37) can be rewritten in the form

$$\frac{E(g)}{g^{1/3}} = b_0 + b_1\, g^{-2/3} + b_2\, g^{-4/3} + \dots\,, \tag{5.16}$$

and when substituting

$$y = \frac{E(g)}{g^{1/3}} \qquad \text{and} \qquad x = g^{-2/3}\,, \tag{5.17}$$

one obtains

$$y = b_0 + b_1\, x + b_2\, x^2 + \dots\,. \tag{5.18}$$

In order to obtain a numerical value for the leading strong-coupling coefficient b_0, we will thus fit our data to a function of the form (5.18). In doing so, a hierarchy of approximations is obtained by choosing polynomials of increasing degree as functions for fitting the data. Once the results for b_0 cease to converge, the value for b_0 from the preceding order is taken as the result of the fitting procedure, and its error is estimated by considering the difference to the result of the previous order. Table 5.2 summarizes our numerical results, which have been obtained accordingly.

In the following, we show how the leading strong-coupling coefficient can be calculated by applying a formalism analogous to the one used in Section 4.4. As an example, we again consider the resummation of the first order of the weak-coupling series. In D dimensions, the first-order result (5.5), (5.8) reads

$$E^{(1)} = D\frac{\hbar\omega}{2} + g\frac{D(D+2)\hbar^2}{4M^2\omega^2}\,. \tag{5.19}$$

Performing Kleinert's square-root substitution (4.25) and expanding again in the coupling constant g, the last identity becomes

$$E^{(1)}(\Omega) = D\frac{\hbar\Omega}{4} + D\frac{\hbar\omega^2}{4\Omega} + g\frac{D(D+2)\hbar^2}{4M^2\Omega^2}\,. \tag{5.20}$$

According to the principal of minimal sensitivity, we thus seek to solve the conditional equation

$$D\frac{\hbar}{4} - D\frac{\hbar\omega^2}{4(\Omega^{(1)})^2} - g\frac{D(D+2)\hbar^2}{2M^2(\Omega^{(1)})^3} = 0\,. \tag{5.21}$$

$b_0(D=2)$	1.477149753577994356(33)
$b_0(D=3)$	2.3936440164823030895(77)
$b_0(D=10)$	10.75826516544379740809 1(18)

Table 5.3: VPT results for the leading-order strong-coupling coefficient b_0 for the ground-state energy of (5.1).

In order to solve (5.21), we use, as before, an ansatz of the form (4.32), (4.33) and obtain

$$\Omega^{(1)} = g^{1/3}\left(\Omega_0^{(1)} + \Omega_1^{(1)} g^{-2/3} + \Omega_2^{(1)} g^{-4/3} + \dots\right) , \tag{5.22}$$

with

$$\Omega_0^{(1)} = \sqrt[3]{\frac{2(D+2)\hbar}{M^2}} , \qquad \Omega_1^{(1)} = \frac{\omega^2}{3}\sqrt[3]{\frac{M^2}{2(D+2)\hbar}} , \qquad \Omega_2^{(1)} = \frac{\omega^4 M^2}{108(D+2)\hbar} , \quad \dots . \tag{5.23}$$

Inserting (5.22), (5.23) into (5.19) yields the strong-coupling behavior of the ground-state energy:

$$E^{(1)} = g^{1/3}\left(b_0^{(1)} + b_1^{(1)} g^{-2/3} + b_2^{(1)} g^{-4/3} + \dots\right) , \tag{5.24}$$

with

$$b_0^{(1)} = \frac{3D\hbar}{8}\sqrt[3]{\frac{2(D+2)\hbar}{M^2}} , \quad b_1^{(1)} = \frac{D\hbar\omega^2}{4}\sqrt[3]{\frac{M^2}{2(D+2)\hbar}} , \quad b_2^{(1)} = -\frac{D\omega^4 M^2}{48(D+2)} , \quad \dots . \tag{5.25}$$

Note that for $D = 1$ Eqs. (5.23), (5.25) pass into the earlier results (4.35), (4.37). Due to the exponential convergence of VPT, it turns out that the accuracy of our numerical results for the leading strong-coupling coefficients b_0 is not sufficient for useful examination of the convergence behavior of VPT in high orders. Therefore, we use our results from the 80th VPT order as a more precise approximation for b_0. Table 5.3 summarizes our results, where in each case the uncertainty of b_0 has been estimated by examining the deviation from the result of the previous order. For $D = 2$ and $D = 10$, the VPT results lie within the error margins of the numerical results. However, this is not the case for $D = 3$, where the VPT result lies just outside of the corresponding numerical error margins. We attribute this discrepancy to an overly optimistic error estimation for the numerical result. The precision of the results shown in Tab. 5.3 improves with increasing dimension, which already indicates that the calculation converges faster in higher dimensions. Figure 5.1 shows the convergence of the VPT results for the three different cases. Fitting the data to straight lines yields

$$\ln \frac{|b_0^{(N)}(D=2) - b_0(D=2)|}{b_0(D=2)} = -9.89(23) N^{1/3} + 5.98(72) , \tag{5.26}$$

$$\ln \frac{|b_0^{(N)}(D=3) - b_0(D=3)|}{b_0(D=3)} = -10.67(15) N^{1/3} + 7.43(48) , \tag{5.27}$$

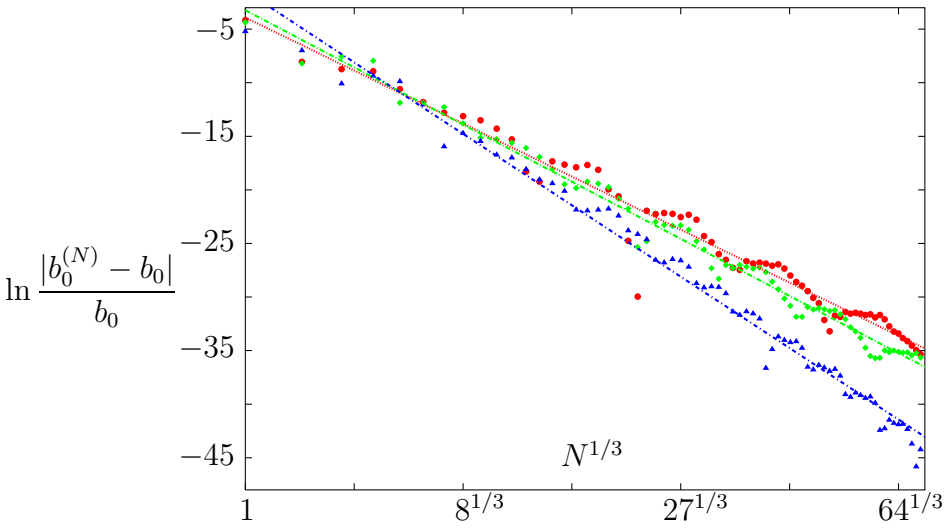


Figure 5.1: Logarithm of the relative deviation of the result for the leading strong-coupling coefficient $b_0(D)$ for $D = 2$ (circles), $D = 3$ (diamonds), and $D = 10$ (triangles) versus the cubic root of the perturbation order up to the 70th order. The dashed lines represent fits of the data to straight lines.

$$\ln \frac{|b_0^{(N)}(D=10) - b_0(D=10)|}{b_0(D=10)} = -13.33(20)N^{1/3} + 11.89(63)\,. \tag{5.28}$$

Thus, we find that the convergence of the VPT result improves with increasing dimension. But this tendency does not come as a surprise since for $D \to \infty$ the oscillator with quartic anharmonicity is exactly solvable [38, Ch. 14].

5.1.3 Large-D Expansion

In quantum mechanics, the large-D expansion is equivalent to the large-N expansion of field theory, where N denotes the number of field components, see e.g. Ref. [39]. For the ground-state energy of the anharmonic oscillator (5.1), the large-D expansion can be derived by applying the Hubbard-Stratonovich transformation, which is given by the functional identity

$$\oint \mathcal{D}\sigma \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\ \left[\frac{1}{g}\sigma^2(\tau) + 2i\mathbf{x}^2(\tau)\sigma(\tau)\right]\right\} = \exp\left\{-\frac{g}{\hbar}\int_0^{\hbar\beta} d\tau\ \left[\mathbf{x}^2(\tau)\right]^2\right\}\,, \tag{5.29}$$

and which can be considered the continuum limit of the discretized expression

$$\prod_i \frac{1}{\sqrt{\pi\hbar g}} \int_{-\infty}^{\infty} d\sigma_i\ \exp\left[-\frac{1}{\hbar}\left(\frac{1}{g}\sigma_i^2 + 2i\mathbf{x}_i^2\sigma_i\right)\right] = \prod_i \exp\left[-\frac{g}{\hbar}\left(\mathbf{x}_i^2\right)^2\right]\,. \tag{5.30}$$

In this section, for the leading strong-coupling coefficient b_0 of the ground-state energy of the anharmonic oscillator (5.1), we demonstrate how the large-D expansion can be obtained approximately by resumming the corresponding weak-coupling series via VPT and considering the large-D limit.

The partition function of the D-dimensional anharmonic oscillator (5.1) reads

$$Z_D(g) = \oint \mathcal{D}\mathbf{x} \, \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{\mathbf{x}}^2(\tau) + \frac{M}{2}\omega^2\mathbf{x}^2(\tau) + g\left[\mathbf{x}^2(\tau)\right]^2\right]\right\} . \tag{5.31}$$

Using (5.29) in order to rewrite (5.31), one obtains

$$\begin{aligned} Z_D(g) &= \oint \mathcal{D}\sigma \exp\left[-\frac{1}{\hbar g}\int_0^{\hbar\beta} d\tau\, \sigma^2(\tau)\right] \\ &\times \oint \mathcal{D}\mathbf{x} \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{\mathbf{x}}^2(\tau) + \frac{M}{2}\left(\omega^2 + \frac{4i\sigma(\tau)}{M}\right)\mathbf{x}^2(\tau)\right]\right\} . \end{aligned} \tag{5.32}$$

The $\mathbf{x}(\tau)$-path integral factorizes into D one-dimensional path integrals for a harmonic oscillator with the frequency

$$\Omega(\tau) := \omega\sqrt{1 + \frac{4i}{M\omega^2}\sigma(\tau)} \tag{5.33}$$

and can be evaluated using the results from Appendix A. One obtains

$$Z_D(g) = \oint \mathcal{D}\sigma \exp\left\{-D\mathcal{A}[\sigma]\right\} , \tag{5.34}$$

where the action

$$\mathcal{A}[\sigma] := \frac{1}{\hbar D g}\int_0^{\hbar\beta} d\tau\sigma^2(\tau) + \frac{1}{2}\mathrm{Tr}\, \ln\left[-\frac{d^2}{d\tau^2} + \omega^2 + \frac{4i}{M}\sigma(\tau)\right] \tag{5.35}$$

has been introduced. Thus, in analogy to (2.114) and (3.45) we define the effective potential according to

$$Z_D(g) = \exp\left[-\beta V_{\mathrm{eff}}(\sigma_0)\right] \tag{5.36}$$

and evaluate the path integral (5.34) by applying the background method. Since now D plays the role that was held before by $1/\hbar$, we thus consider the limit $D \to \infty$. The ground-state energy can then be obtained by extremizing the effective potential $V_{\mathrm{eff}}(\sigma_0)$ with respect to the background σ_0. According to the background method, the zeroth loop-order approximation of the effective potential is given by the tree-level:

$$V_{\mathrm{eff}}^{(l=0)}(\sigma_0) = D\left(\frac{\sigma_0^2}{\tilde{g}} + \frac{\hbar}{2}\sqrt{\omega^2 + \frac{4i}{M}\sigma_0}\right) , \tag{5.37}$$

with $\tilde{g} := gD$. Introducing $\tilde{\sigma}_0$ according to

$$\sigma_0 = -i\tilde{\sigma}_0 , \tag{5.38}$$

the extremization condition reads

$$\frac{\partial V_{\mathrm{eff}}^{(l=0)}(\tilde{\sigma}_0)}{\partial\tilde{\sigma}_0} = D\left(-\frac{2\tilde{\sigma}_0}{\tilde{g}} + \frac{\hbar}{M\sqrt{\omega^2 + 4\tilde{\sigma}_0/M}}\right) = 0 . \tag{5.39}$$

In the strong-coupling limit, $\tilde{g} \to \infty$, one obtains the solution

$$\tilde{\sigma}_0 \approx \tilde{g}^{2/3} \frac{1}{4} \sqrt[3]{\frac{4\hbar^2}{M}} \,, \tag{5.40}$$

which leads to the following strong-coupling behavior of the ground-state energy:

$$E^{(l=0)} \approx D\tilde{g}^{1/3} \frac{3\hbar}{8} \sqrt[3]{\frac{2\hbar}{M^2}} \,. \tag{5.41}$$

Reintroducing the original coupling constant, the last identity becomes

$$E^{(l=0)} = g^{1/3} D^{4/3} \frac{3\hbar}{8} \sqrt[3]{\frac{2\hbar}{M^2}} \,. \tag{5.42}$$

However, this result can also be obtained directly by considering the large-D limit for the leading strong-coupling coefficient obtained in Section 5.1.2. Our VPT-result in the first order (5.25) reads

$$b_0^{(1)} = \frac{3D\hbar}{8} \sqrt[3]{\frac{2(D+2)\hbar}{M^2}} \,, \tag{5.43}$$

and in the leading order of D we obtain immediately

$$b_0^{(1)} \approx D^{4/3} \frac{3\hbar}{8} \sqrt[3]{\frac{2\hbar}{M^2}} \,, \tag{5.44}$$

which is in accordance with (5.42). Up to the second order of the coupling constant, the weak-coupling series reads

$$E^{(2)} = D\frac{\hbar\omega}{2} + g\frac{D(D+2)\hbar^2}{4M^2\omega^2} - g^2 \frac{D(10+9D+2D^2)\hbar^3}{8M^4\omega^5} \,. \tag{5.45}$$

The leading strong-coupling coefficient as a function of the variational parameter Ω can be obtained from the weak-coupling series by applying (4.16):

$$b_0^{(2)}(\Omega) = D\frac{3\hbar\Omega}{16} + \frac{D(D+2)\hbar^2}{2M^2\Omega^2} - \frac{D(10+9D+2D^2)\hbar^3}{8M^4\Omega^5} \,. \tag{5.46}$$

Here, we have identified the parameter κ from (4.3) with ω and have thus again found $p = 1$ and $q = 3$. Consequently, the extremization condition (4.17) reads

$$3M^4\hbar(\Omega^{(2)})^6 - 16(D+2)\hbar^2 M^2 (\Omega^{(2)})^3 + 10(10+9D+2D^2)\hbar^3 = 0 \,. \tag{5.47}$$

In order to solve this equation, we use the approach

$$\Omega^{(2)} = D^{1/3} \left(C_0 + C_1 \frac{1}{D} + \dots \right) \tag{5.48}$$

and obtain

$$C_0 = \sqrt[3]{\frac{2\hbar}{M^2}} \,, \qquad C_1 = \frac{13}{12} \sqrt[3]{\frac{2\hbar}{M^2}} \,, \qquad \dots \,. \tag{5.49}$$

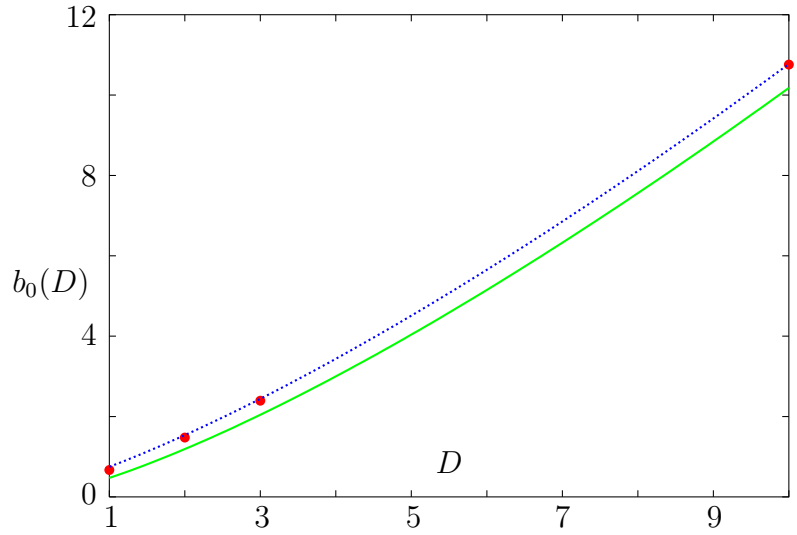


Figure 5.2: Leading strong-coupling coefficient $b_0(D)$ versus the dimension D. The solid line represents the first-order result (5.44). The dotted line is the second-order result (5.50). The circles represent the quasi-exact values, obtained from the 80th VPT order, as given in Tab. 5.3.

Inserting this result into (5.46), we find

$$b_0^{(2)} = D^{4/3}\left(\frac{3\hbar}{8}\sqrt[3]{\frac{2\hbar}{M^2}} + \frac{7\hbar}{32D}\sqrt[3]{\frac{2\hbar}{M^2}} + \dots\right) . \tag{5.50}$$

This procedure can easily be driven to higher orders. Figure 5.2 shows the leading strong-coupling coefficients $b_0^{(1)}$ and $b_0^{(2)}$ as given by (5.44) and (5.50) versus the dimension D. The relative deviation of these results from the 80th VPT order results is shown in Fig. 5.3.

5.2 Background Method for Effective Potential

In this section, the calculation of the effective potential from Sections 2.7 and 2.8 is generalized to the case of a rotationally symmetric potential in D spatial dimensions. Unless otherwise stated, throughout this section, we use sum convention, i.e. when an index occurs twice on one side of an equation the respective summation sign is omitted. Thus, we write e.g.

$$\sum_{i=1}^{D} X_i Y_i \equiv X_i Y_i \, . \tag{5.51}$$

Consider the partition function

$$Z = \oint \mathcal{D}\mathbf{x} \, \exp\left\{-\mathcal{A}[\mathbf{x}]/\hbar\right\} \, , \tag{5.52}$$

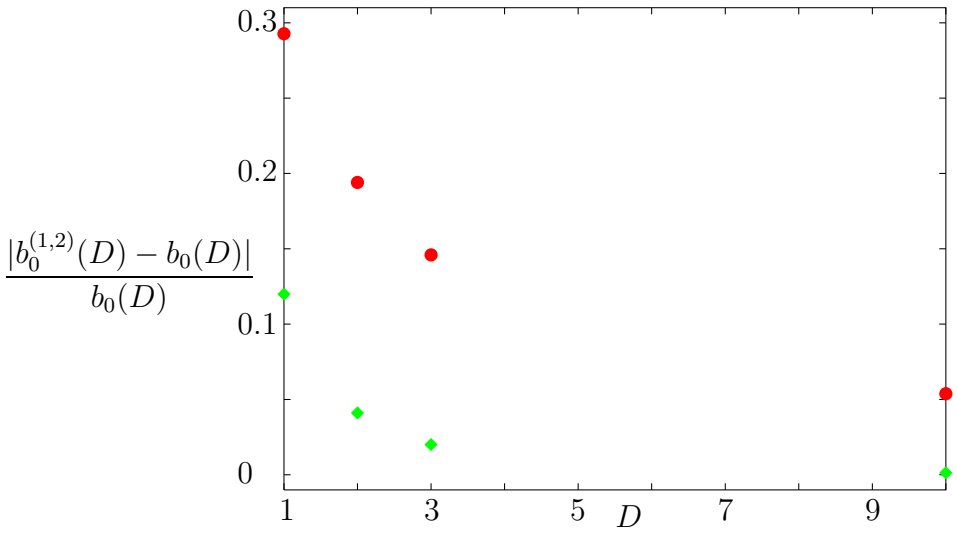


Figure 5.3: Relative deviation of the leading strong-coupling coefficients $b_0^{(1,2)}(D)$ from the quasi-exact values, obtained from the 80th VPT order, as given in Tab. 5.3. The circles represent the relative deviation of the result (5.44). The relative error of the result (5.50) is represented by diamonds.

where $\mathcal{A}[\mathbf{x}]$ is the D-dimensional generalization of the imaginary-time action (2.14):

$$\mathcal{A}[\mathbf{x}] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{\mathbf{x}}^2(\tau) + V(\mathbf{x}(\tau)) \right] . \tag{5.53}$$

Within the background method, the position variable $\mathbf{x}$ is expanded around some background $\mathbf{X}(\tau)$, according to $\mathbf{x}(\tau) = \mathbf{X}(\tau) + \delta\mathbf{x}(\tau)$. Since in this chapter we are only interested in the effective potential and not in the effective action, all calculations are done for a τ-independent background: $\mathbf{X}(\tau) \equiv \mathbf{X}$. A functional Taylor expansion of the imaginary-time action (5.53) yields

$$\begin{aligned}
\mathcal{A}[\mathbf{X}+\delta\mathbf{x}] \;=\; & \mathcal{A}[\mathbf{X}]\Big|_{\mathbf{X}(\tau)\equiv\mathbf{X}} + \int_0^{\hbar\beta} d\tau_1 \, \frac{\delta\mathcal{A}[\mathbf{X}]}{\delta X_i(\tau_1)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} \delta x_i(\tau_1) \\
& + \frac{1}{2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, \frac{\delta^2\mathcal{A}[\mathbf{X}]}{\delta X_i(\tau_1)\delta X_j(\tau_2)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} \delta x_i(\tau_1)\delta x_j(\tau_2) \\
& + \frac{1}{6}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \, \frac{\delta^3\mathcal{A}[\mathbf{X}]}{\delta X_i(\tau_1)\delta X_j(\tau_2)\delta X_k(\tau_3)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} \delta x_i(\tau_1)\delta x_j(\tau_2)\delta x_k(\tau_3) \\
& + \frac{1}{24}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \int_0^{\hbar\beta} d\tau_4 \\
& \qquad \times \frac{\delta^4\mathcal{A}[\mathbf{X}]}{\delta X_i(\tau_1)\delta X_j(\tau_2)\delta X_k(\tau_3)\delta X_l(\tau_4)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} \delta x_i(\tau_1)\delta x_j(\tau_2)\delta x_k(\tau_3)\delta x_l(\tau_4) + \ldots \, .
\end{aligned} \tag{5.54}$$

As in Section 2.7, the first-order term will be neglected, and terms that are of higher than second order define the interaction part

$$\mathcal{A}^{(\mathrm{int})}[\delta\mathbf{x}] = \frac{1}{6}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \, \frac{\delta^3\mathcal{A}[\mathbf{X}]}{\delta X_i(\tau_1)\delta X_j(\tau_2)\delta X_k(\tau_3)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} \delta x_i(\tau_1)\delta x_j(\tau_2)\delta x_k(\tau_3)$$
$$+ \frac{1}{24}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \int_0^{\hbar\beta} d\tau_4$$
$$\times \frac{\delta^4\mathcal{A}[\mathbf{X}]}{\delta X_i(\tau_1)\delta X_j(\tau_2)\delta X_k(\tau_3)\delta X_l(\tau_4)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} \delta x_i(\tau_1)\delta x_j(\tau_2)\delta x_k(\tau_3)\delta x_l(\tau_4) + \dots \,. \quad (5.55)$$

Thus, by changing the functional integration variable in (5.52) from $\mathbf{x}$ to $\delta\mathbf{x}$, one obtains

$$Z = \exp\left\{-\frac{1}{\hbar}\mathcal{A}[\mathbf{X}]\Big|_{\mathbf{X}(\tau)\equiv\mathbf{X}}\right\} \oint \mathcal{D}\delta\mathbf{x} \, \exp\left\{-\mathcal{A}^{(1)}[\delta\mathbf{x}]/\hbar - \mathcal{A}^{(\mathrm{int})}[\delta\mathbf{x}]/\hbar\right\}, \quad (5.56)$$

with

$$\mathcal{A}^{(1)}[\delta\mathbf{x}] = \frac{1}{2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, \frac{\delta^2\mathcal{A}[\mathbf{X}]}{\delta X_i(\tau_1)\delta X_j(\tau_2)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} \delta x_i(\tau_1)\delta x_j(\tau_2) \,. \quad (5.57)$$

The second functional derivative of the imaginary-time action (5.53), the integral kernel, reads

$$\frac{\delta^2\mathcal{A}[\mathbf{X}]}{\delta X_i(\tau_1)\delta X_j(\tau_2)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} \equiv G^{-1}_{ij}(\tau_1,\tau_2) = \left[-M\frac{d^2}{d\tau_2^2}\delta_{ij} + \frac{\partial^2 V(X)}{\partial X_i(\tau_1)\partial X_j(\tau_2)}\right]\bigg|_{\mathbf{X}(\tau)=\mathbf{X}} \delta(\tau_2-\tau_1) \,. \quad (5.58)$$

Here and in the following, it is assumed that the potential is rotationally symmetric, and the modulus of the background variable, $|\mathbf{X}|$, is denoted by X. Consequently, we identify $V(\mathbf{X}) \equiv V(X)$. Evaluating the second derivative of the potential yields

$$\frac{\partial^2 V(X(\tau))}{\partial X_i(\tau)\partial X_j(\tau)}\bigg|_{\mathbf{X}(\tau)\equiv\mathbf{X}} = P^L_{ij}\, V''(X) + P^T_{ij}\, \frac{V'(X)}{X} \,, \quad (5.59)$$

where the longitudinal and transversal projection operators $P^{L/T}_{ij}$ are defined by

$$P^T_{ij} = \frac{X_i X_j}{X^2} \qquad \text{and} \qquad P^T_{ij} = \delta_{ij} - P^L_{ij} \,. \quad (5.60)$$

Note that these projection operators have the following properties:

$$P^L_{ij}P^L_{jk} = P^L_{ik} \,, \qquad P^T_{ij}P^T_{jk} = P^T_{ik} \,, \quad (5.61)$$

$$P^L_{ij}P^L_{ij} = 1 \,, \qquad P^T_{ij}P^T_{ij} = D-1 \,, \qquad P^L_{ij}P^T_{jk} = P^T_{ij}P^L_{jk} = 0 \,, \quad (5.62)$$

$$P^L_{ij}X_j = X_i \,, \qquad P^T_{ij}X_j = 0 \,. \quad (5.63)$$

Introducing the operator

$$\hat{O}_{ij}(\tau) = M\left[-\frac{d^2}{d\tau^2}\delta_{ij} + \frac{1}{M}P^L_{ij}\,V''(X) + \frac{1}{M}P^T_{ij}\,\frac{V'(X)}{X}\right], \tag{5.64}$$

inserting (5.58) and (5.59) into (5.57), and performing the τ_2-integration, one obtains the intermediate result

$$\mathcal{A}^{(1)}[\delta\mathbf{x}] = \frac{1}{2}\int_0^{\hbar\beta} d\tau\;\delta x_i(\tau)\hat{O}_{ij}(\tau)\delta x_j(\tau)\,. \tag{5.65}$$

Consider the eigenvalue problem of $\hat{O}_{ij}(\tau)$:

$$\hat{O}_{ij}(\tau)v_j^{(m,n)}(\tau) = M\lambda^{(m)}v_i^{(m,n)}(\tau) \qquad \text{and} \qquad \mathbf{v}^{(m,n)}(0) = \mathbf{v}^{(m,n)}(\hbar\beta)\,, \tag{5.66}$$

$$\text{for } n = 1,\,2,\,\ldots,\,D\,. \tag{5.67}$$

The approach

$$v_j^{(m,1)}(\tau) = X_j\,e^{-i\omega_m\tau}\,, \tag{5.68}$$

with ω_m being the Matsubara frequencies

$$\omega_m = \frac{2\pi}{\hbar\beta}\,m\,, \quad m = 0,\,\pm1,\,\pm2,\,\ldots\,, \tag{5.69}$$

leads to the eigenvalue

$$\lambda_L^{(m)} = \omega_m^2 + \frac{V''(X)}{M}\,. \tag{5.70}$$

On the other hand, the approach

$$v_j^{(m,n)}(\tau) = Y_j^{(n)}\,e^{-i\omega_m\tau}\,, \qquad \text{with} \qquad X_jY_j^{(n)} = 0 \qquad \text{and} \qquad Y_j^{(n)} = \left(Y_j^{(n)}\right)^*\,, \tag{5.71}$$

$$\text{for } n = 2,\,3,\,\ldots D, \tag{5.72}$$

leads to the $(D-1)$-fold degenerate eigenvalue

$$\lambda_T^{(m)} = \omega_m^2 + \frac{V'(X)}{MX}\,. \tag{5.73}$$

Thus, defining the longitudinal and transversal frequencies

$$\omega_L^2 = \frac{V''(X)}{M} \qquad \text{and} \qquad \omega_T^2 = \frac{V'(X)}{MX}\,, \tag{5.74}$$

the eigenvalues of the operator $\hat{O}_{ij}(\tau)$ read

$$\lambda_L^{(m)} = \omega_m^2 + \omega_L^2 \qquad \text{and} \qquad \lambda_T^{(m)} = \omega_m^2 + \omega_T^2\,. \tag{5.75}$$

And without loss of generality

$$\{\mathbf{v}^{(m,n)}(\tau)\mid m = 0,\,\pm1,\,\pm2,\,\ldots\,;n = 1,\,2,\ldots,\,D\} \tag{5.76}$$

can assumed to be an orthonormal basis of the solution space to (5.66), where

$$\hat{O}_{ij}(\tau)v_j^{(m,1)}(\tau) = M\lambda_L^{(m)}v_i^{(m,1)}(\tau)\,, \tag{5.77}$$

and

$$\hat{O}_{ij}(\tau)v_j^{(m,n)}(\tau) = M\lambda_T^{(m)}v_i^{(m,n)}(\tau) \qquad \text{for} \qquad n = 2,\,3,\,\ldots\,,D\,. \tag{5.78}$$

Then, the fluctuations $\delta\mathbf{x}(\tau)$ can be expressed in the form

$$\delta\mathbf{x}(\tau) = \sum_{m=-\infty}^{\infty} c^{(m,n)}\mathbf{v}^{(m,n)}(\tau)\,, \tag{5.79}$$

and the orthonormality condition reads

$$\int_0^{\hbar\beta} d\tau\; v_i^{(m,n)}v_i^{(m',n')*} = \delta_{m,m'}\delta_{n,n'}\hbar\beta\,. \tag{5.80}$$

Since $\mathbf{X}$ and $\mathbf{Y}^{(n)}$ are real, definitions (5.68) and (5.71) allow the rewriting of the last identity in the form

$$\int_0^{\hbar\beta} d\tau\; v_i^{(m,n)}v_i^{(m',n')} = \delta_{m,-m'}\delta_{n,n'}\hbar\beta\,. \tag{5.81}$$

In addition, the fluctuations $\delta\mathbf{x}(\tau)$ must be real. Therefore, the expansion coefficients $c^{(m,n)}$ in (5.79) must obey the condition

$$c^{(m,n)} = c^{(-m,n)*}\,, \tag{5.82}$$

and their real and imaginary parts are even and odd, respectively:

$$\mathrm{Re}\,c^{(m,n)} = \mathrm{Re}\,c^{(-m,n)}\,, \qquad \mathrm{Im}\,c^{(m,n)} = -\mathrm{Im}\,c^{(-m,n)}\,. \tag{5.83}$$

Inserting the decomposition (5.79) into (5.65) and using the properties (5.77) and (5.78) of the operator $\hat{O}_{ij}(\tau)$ yields

$$\begin{aligned}\mathcal{A}^{(1)}[\delta\mathbf{x}] \;&=\; \frac{1}{2}\int_0^{\hbar\beta} d\tau \sum_{m,m'=-\infty}^{\infty}\sum_{n=1}^{D} c^{(m,n)}v_i^{(m,n)} \\ &\quad\times M\left(\lambda_L^{(m')}c^{(m',1)}v_i^{(m',1)} + \lambda_T^{(m')}\sum_{n'=2}^{D} c^{(m',n')}v_i^{(m',n')}\right)\,,\end{aligned} \tag{5.84}$$

where for reasons of clarity the use of sum convention has been set aside. Exploiting the orthonormality relation (5.81) and the symmetry (5.82) of the coefficients $c^{(m,n)}$, one obtains the result

$$\begin{aligned}\mathcal{A}^{(1)}[\delta\mathbf{x}] \;&=\; \frac{M\hbar\beta}{2}\Bigg[\lambda_L^{(0)}\left|c^{(0,1)}\right|^2 + \lambda_T^{(0)}\sum_{n=2}^{D}\left|c^{(0,n)}\right|^2 \\ &\quad + 2\sum_{m=1}^{\infty}\left(\lambda_L^{(m)}\left|c^{(m,1)}\right|^2 + \lambda_T^{(m)}\sum_{n=2}^{D}\left|c^{(m,n)}\right|^2\right)\Bigg]\,.\end{aligned} \tag{5.85}$$

This result can be applied to evaluate the partition function

$$Z^{(1)}(X) = \oint \mathcal{D}\delta\mathbf{x} \, \exp\left\{-\mathcal{A}^{(1)}[\delta\mathbf{x}]/\hbar\right\} \, . \tag{5.86}$$

As in Appendix A, the path integral measure $\mathcal{D}\delta\mathbf{x}$ is replaced by an infinite product of integrals

$$\oint \mathcal{D}\delta\mathbf{x} \, \rightarrow \, \prod_{n=1}^{D} \left[N_0 \int_{-\infty}^{\infty} dc^{(0,n)} \, \prod_{m=1}^{\infty} \left(N_m \int_{-\infty}^{\infty} d \, \mathrm{Re} \, c^{(m,n)} \int_{-\infty}^{\infty} d \, \mathrm{Im} \, c^{(m,n)} \right) \right] \, , \tag{5.87}$$

where the normalization constants N_0 and N_m are obtained by comparison with the known result [4, Ch. 5] for the D-dimensional harmonic oscillator, i.e. $\omega_L^2 = \omega_T^2 = \omega^2$. One thus obtains as in Appendix A

$$N_0 = \sqrt{\frac{M}{2\pi\hbar^2\beta}} \, , \qquad N_m = \frac{M\omega_m^2\beta}{\pi} \, , \tag{5.88}$$

and

$$Z^{(1)}(X) = \frac{1}{2\sinh(\hbar\beta\omega_L/2)} \left(\frac{1}{2\sinh(\hbar\beta\omega_T/2)} \right)^{D-1} \, . \tag{5.89}$$

In Appendix A, it is shown that $Z^{(1)}(X)$ can also be written in the form

$$Z^{(1)}(X) = \exp\left(-\frac{1}{2} \, \mathrm{Tr} \ln G^{-1} \right) \, , \tag{5.90}$$

with

$$\mathrm{Tr} \ln G^{-1} = \sum_{m=-\infty}^{\infty} \left(\ln \lambda_L^{(m)} + (D-1) \ln \lambda_T^{(m)} \right) \, . \tag{5.91}$$

In the one-dimensional case the effective action is given by (2.129), which remains valid in D dimensions. Therefore, by evaluating (2.129) for a constant background and dividing by $\hbar\beta$, one obtains

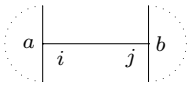
$$V_{\mathrm{eff}}(X) = V(X) + \frac{1}{2\beta} \mathrm{Tr} \ln G^{-1} + V_{\mathrm{eff}}^{(\mathrm{int})}(X) \, . \tag{5.92}$$

As before, the interaction part of the effective potential $V_{\mathrm{eff}}^{(\mathrm{int})}(X)$ is expanded in the form

$$V_{\mathrm{eff}}^{(\mathrm{int})} = -\hbar \sum_{l=2}^{\infty} V_{\mathrm{eff}}^{(l)}(X) \, , \tag{5.93}$$

where each loop order $V_{\mathrm{eff}}^{(l)}(X)$ consists of all one-particle irreducible Feynman diagrams with l loops. In the case of a D-dimensional rotationally symmetric potential the Feynman rules for a constant background read:

- The vertices of the diagram are numbered arbitrarily.
- All outgoing lines of all vertices are denoted by an arbitrary index.
- A line between the ath and bth vertex connecting the lines i and j stands for the propagator $G_{ij}(\tau_a, \tau_b)$:



$$\equiv \; G_{ij}(\tau_a, \tau_b) \; , \tag{5.94}$$

  where the propagator $G_{ij}(\tau_a, \tau_b)$ is defined by the identity

$$\int_0^{\hbar\beta} d\tau_a \, G^{-1}_{ij}(\tau_c, \tau_a) G_{jk}(\tau_a, \tau_b) \equiv \hbar \, \delta_{ik} \, \delta(\tau_c - \tau_b) \; . \tag{5.95}$$

- The resulting product of propagators is integrated. Let the ath vertex be of degree n with $n \geq 3$ and have the n outgoing lines i, j, k, $\ldots$, m; then it leads to the integration:

$$\rightarrow \; -\frac{1}{\hbar} \, \frac{\partial^n V(X)}{\partial X_i \, \partial X_j \, \partial X_k \, \ldots \, \partial X_m} \int_0^{\hbar\beta} d\tau_a \; . \tag{5.96}$$

The diagrams contributing to the second loop order and their respective weights are given by (2.109). The diagram  thus stands for

$$= \; \frac{1}{\hbar^2} \, \frac{\partial^3 V(X)}{\partial X_i \partial X_j \partial X_k} \, \frac{\partial^3 V(X)}{\partial X_l \partial X_m \partial X_n} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, G_{il}(\tau_1, \tau_2) G_{jm}(\tau_1, \tau_2) G_{kn}(\tau_1, \tau_2) \; . \tag{5.97}$$

And the diagram  is given by

$$= \; -\frac{1}{\hbar} \, \frac{\partial^4 V(X)}{\partial X_i \partial X_j \partial X_k \partial X_l} \int_0^{\hbar\beta} d\tau \, G_{ij}(\tau, \tau) G_{kl}(\tau, \tau) \; . \tag{5.98}$$

From (5.58) – (5.60) and (5.74), it follows that the integral kernel $G^{-1}_{ij}(\tau_1, \tau_2)$ is given by

$$G^{-1}_{ij}(\tau_1, \tau_2) = M \left[P^L_{ij} \left(-\frac{d^2}{d\tau_1^2} + \omega_L^2 \right) + P^T_{ij} \left(-\frac{d^2}{d\tau_1^2} + \omega_T^2 \right) \right] \delta(\tau_2 - \tau_1) \; . \tag{5.99}$$

Its Matsubara decomposition reads

$$G^{-1}_{ij}(\tau_1, \tau_2) = \sum_{m=-\infty}^{\infty} G^{-1(m)}_{ij} e^{-i\omega_m(\tau_1 - \tau_2)} \; , \tag{5.100}$$

and $G^{-1(m)}_{ij}$ is given by Fourier inversion

$$G^{-1(m)}_{ij} = \frac{1}{\hbar\beta} \int_0^{\hbar\beta} d\tau \, G^{-1}_{ij}(\tau, 0) \, e^{+i\omega_m \tau} = \frac{M}{\hbar\beta} \left[P^L_{ij}(\omega_m^2 + \omega_L^2) + P^T_{ij}(\omega_m^2 + \omega_T^2) \right] \; . \tag{5.101}$$

Expressing the integral kernel $G_{ij}^{-1}(\tau_1,\tau_2)$, the propagator $G_{jk}(\tau_2,\tau_3)$, and the delta function by their Matsubara decompositions, Eq. (5.95) becomes

$$\int_0^{\hbar\beta} d\tau_2 \sum_{m=-\infty}^{\infty} G_{ij}^{-1(m)} e^{-i\omega_m(\tau_1-\tau_2)} \sum_{m'=-\infty}^{\infty} G_{jk}^{(m')} e^{-i\omega_{m'}(\tau_2-\tau_3)} \equiv \hbar\delta_{ik} \sum_{m=-\infty}^{\infty} \frac{1}{\hbar\beta} e^{-i\omega_m(\tau_1-\tau_3)} . \tag{5.102}$$

After performing the integration and comparing the coefficients one obtains

$$G_{ij}^{-1(m)} G_{jk}^{(m)} = \frac{1}{\hbar\beta^2}\,\delta_{ik} . \tag{5.103}$$

This equation can be solved by the approach

$$G_{jk}^{(m)} = P_{jk}^L A^{(m)} + P_{jk}^T B^{(m)} . \tag{5.104}$$

Inserting (5.101), (5.104) into (5.103) and using the properties (5.61), (5.62) yields

$$\frac{M}{\hbar\beta}\left[P_{ik}^L A^{(m)}(\omega_m^2+\omega_L^2) + P_{ik}^T B^{(m)}(\omega_m^2+\omega_T^2)\right] = \frac{1}{\hbar\beta^2}\left(P_{ik}^L + P_{ik}^T\right) . \tag{5.105}$$

From the last identity and (5.104), it follows that

$$G_{jk}^{(m)} = \frac{1}{M\beta}\left(P_{jk}^L \frac{1}{\omega_m^2+\omega_L^2} + P_{jk}^T \frac{1}{\omega_m^2+\omega_T^2}\right) . \tag{5.106}$$

Thus, the Matsubara decomposition of the propagator becomes

$$G_{jk}(\tau_1,\tau_2) = \frac{1}{M\beta} \sum_{m=-\infty}^{\infty} \left(P_{jk}^L \frac{1}{\omega_m^2+\omega_L^2} + P_{jk}^T \frac{1}{\omega_m^2+\omega_T^2}\right) e^{-i\omega_m(\tau_1-\tau_2)} . \tag{5.107}$$

The series is evaluated in Appendix A, and the propagator $G_{ij}(\tau_1,\tau_2)$ can be decomposed into a longitudinal and a transversal part, yielding

$$G_{jk}(\tau_1,\tau_2) = P_{jk}^L G_L(\tau_1,\tau_2) + P_{jk}^T G_T(\tau_1,\tau_2) , \tag{5.108}$$

with

$$G_L(\tau_1,\tau_2) = \frac{\hbar}{2M\omega_L} \frac{\cosh(\omega_L|\tau_1-\tau_2| - \hbar\beta\omega_L/2)}{\sinh(\hbar\beta\omega_L/2)} , \tag{5.109}$$

and

$$G_T(\tau_1,\tau_2) = \frac{\hbar}{2M\omega_T} \frac{\cosh(\omega_T|\tau_1-\tau_2| - \hbar\beta\omega_T/2)}{\sinh(\hbar\beta\omega_T/2)} . \tag{5.110}$$

In order to evaluate the twofold integral (5.97) and the integral (5.98) we calculate the third and fourth derivative of the potential. First, using (5.59), we find

$$\frac{\partial^3 V(X)}{\partial X_i \partial X_j \partial X_k} = P_{ijk}^L V'''(X) + P_{ijk}^T \left[\frac{V''(X)}{X} - \frac{V'(X)}{X^2}\right] , \tag{5.111}$$

where the operators P^L_{ijk} and P^T_{ijk} are given by

$$P^L_{ijk} = \frac{X_i X_j X_k}{X^3}\,, \qquad \text{and} \qquad P^T_{ijk} = \delta_{ij}\frac{X_k}{X} + \delta_{ik}\frac{X_j}{X} + \delta_{jk}\frac{X_i}{X} - 3P^L_{ijk}\,. \tag{5.112}$$

Furthermore, the fourth derivative reads

$$\frac{\partial^4 V(X)}{\partial X_i \partial X_j \partial X_k \partial X_l} = P^L_{ijkl} V^{(4)}(X) + P^T_{ijkl}\frac{V'''(X)}{X} + P^E_{ijkl}\left[\frac{V''(X)}{X^2} - \frac{V'(X)}{X^3}\right], \tag{5.113}$$

where the following abbreviations have been introduced:

$$P^L_{ijkl} = \frac{X_i X_j X_k X_l}{X^4}\,, \tag{5.114}$$

$$P^T_{ijkl} = \delta_{ij}\frac{X_k X_l}{X^2} + \delta_{ik}\frac{X_j X_l}{X^2} + \delta_{il}\frac{X_j X_k}{X^2} + \delta_{jk}\frac{X_i X_l}{X^2} + \delta_{jl}\frac{X_i X_k}{X^2} + \delta_{kl}\frac{X_i X_k}{X^2} - 6P^L_{ijkl}\,, \tag{5.115}$$

$$P^E_{ijkl} = \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - 3P^L_{ijkl} - 3P^T_{ijkl}\,. \tag{5.116}$$

Note that the operators $P^{L/T}_{ij}$, $P^{L/T}_{ijk}$, $P^{L/T/E}_{ijkl}$ are all totally symmetric tensors. The definitions (5.60), (5.112), and (5.114) – (5.116) directly lead to the following relations:

$$\frac{X_i}{X}P^L_{ijk} = P^L_{jk}\,, \qquad \frac{X_i}{X}P^T_{ijk} = P^T_{jk}\,; \tag{5.117}$$

$$P^L_{ij}P^L_{ikl} = P^L_{jkl}\,, \quad P^T_{ij}P^T_{ikl} = \frac{X_k}{X}P^T_{jl} + \frac{X_l}{X}P^T_{jk}\,, \quad P^L_{ij}P^T_{ikl} = \frac{X_j}{X}P^T_{kl}\,, \quad P^T_{ij}P^L_{ikl} = 0\,; \tag{5.118}$$

$$P^L_{hij}P^L_{hkl} = P^L_{ijkl}\,, \qquad P^T_{hij}P^T_{hkl} = P^T_{ij}P^T_{kl} + P^L_{ik}P^T_{jl} + P^L_{il}P^T_{jk} + P^L_{jk}P^T_{il} + P^L_{jl}P^T_{ik}\,, \tag{5.119}$$

$$P^L_{hij}P^T_{hkl} = P^L_{ij}P^T_{kl}\,, \qquad P^T_{hij}P^L_{hkl} = P^T_{ij}P^L_{kl}\,; \tag{5.120}$$

$$P^L_{ij}P^L_{ijkl} = P^L_{kl}\,, \qquad P^T_{ij}P^T_{ijkl} = (D-1)P^L_{kl}\,, \tag{5.121}$$

$$P^L_{ij}P^T_{ijkl} = P^T_{kl}\,, \qquad P^T_{ij}P^L_{ijkl} = 0\,, \tag{5.122}$$

$$P^L_{ij}P^E_{ijkl} = -2P^T_{kl}\,, \qquad P^T_{ij}P^E_{ijkl} = (D+1)P^T_{kl} - 2(D-1)P^L_{kl}\,. \tag{5.123}$$

Using the results (5.108), (5.111), the relations (5.61), (5.62), and (5.117) – (5.120), one obtains the intermediate result for the twofold integral (5.97)

$$\begin{aligned} \text{⟲} \;=\; & \frac{1}{\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \left\{ G_L^3(\tau_1,\tau_2)\,[V'''(X)]^2 \right. \\ & \left. + 3(D-1)G_L(\tau_1,\tau_2)G_T^2(\tau_1,\tau_2)\left[\frac{V''(X)}{X} - \frac{V'(X)}{X^2}\right]^2 \right\}. \end{aligned} \tag{5.124}$$

The remaining integrals are solved in Appendix B, and one obtains

$$\begin{aligned}
\ominus \quad &= \frac{2\hbar^2\beta}{\omega_L}\frac{1}{(2M\omega_L)^3}[V'''(X)]^2\left[\frac{1}{3}+\frac{1}{\sinh^2(\hbar\beta\omega_L/2)}\right] \\
&+\frac{6\hbar^2\beta(D-1)}{2\omega_T+\omega_L}\frac{1}{2M\omega_L}\frac{1}{(2M\omega_T)^2}\left[\frac{V''(X)}{X}-\frac{V'(X)}{X^2}\right]^2 \\
&\times\left[\coth^2(\hbar\beta\omega_T/2)+\frac{\omega_T}{\omega_L}\frac{1}{\sinh^2(\hbar\beta\omega_T/2)}+\frac{\omega_T}{2\omega_T-\omega_L}\frac{\sinh(\hbar\beta(\omega_T-\omega_L/2))}{\sinh(\hbar\beta\omega_L/2)\sinh^2(\hbar\beta\omega_T/2)}\right].
\end{aligned} \tag{5.125}$$

The integral (5.98) can be evaluated by using the results (5.108), (5.113) and the relations (5.62) and (5.121) – (5.123). In this case, the integration is trivial as it only leads to a factor $\hbar\beta$. One obtains

$$\begin{aligned}
\bigcirc\!\!\bigcirc \quad &= -\beta\left\{G_L^2(\tau,\tau)V^{(4)}(X)+\,(D^2-1)\,G_T^2(\tau,\tau)\left[\frac{V''(X)}{X^2}-\frac{V'(X)}{X^3}\right]\right. \\
&\left.+\,2(D-1)\,G_L(\tau,\tau)G_T(\tau,\tau)\left[\frac{V'''(X)}{X}-\frac{2V''(X)}{X^2}+\frac{2V'(X)}{X^3}\right]\right\}.
\end{aligned} \tag{5.126}$$

And when explicitly inserting the result for the propagator (5.109), (5.110), one has

$$\begin{aligned}
\bigcirc\!\!\bigcirc \quad &= -\frac{\hbar^2\beta}{(2M)^2}\left\{\frac{1}{\omega_L^2}\coth^2(\hbar\beta\omega_L/2)V^{(4)}(X)\right. \\
&+\frac{D^2-1}{\omega_T^2}\coth^2(\hbar\beta\omega_T/2)\left[\frac{V''(X)}{X^2}-\frac{V'(X)}{X^3}\right] \\
&\left.+\frac{2(D-1)}{\omega_L\omega_T}\coth(\hbar\beta\omega_L/2)\coth(\hbar\beta\omega_T/2)\left[\frac{V'''(X)}{X}-\frac{2V''(X)}{X^2}+\frac{2V'(X)}{X^3}\right]\right\}.
\end{aligned} \tag{5.127}$$

Thus, using the results (5.89), (5.90), (5.92), (5.125), and (5.127) and taking into account (2.109), (2.144), and (5.93), one obtains the temperature-dependent effective potential for a rotationally symmetric potential in D spatial dimensions up to the second loop order:

$$\begin{aligned}
V_{\text{eff}}(X) &= V(X)+\frac{1}{\beta}\big\{\ln\left[2\sinh(\hbar\beta\omega_L/2)\right]+(D-1)\ln\left[2\sinh(\hbar\beta\omega_T/2)\right]\big\} \\
&+\frac{\hbar^2}{8(2M)^2}\left\{\frac{1}{\omega_L^2}\coth^2(\hbar\beta\omega_L/2)V^{(4)}(X)+\frac{D^2-1}{\omega_T^2}\coth^2(\hbar\beta\omega_T/2)\left[\frac{V''(X)}{X^2}-\frac{V'(X)}{X^3}\right]\right. \\
&\left.+\frac{2(D-1)}{\omega_L\omega_T}\coth(\hbar\beta\omega_L/2)\coth(\hbar\beta\omega_T/2)\left[\frac{V'''(X)}{X}-\frac{2V''(X)}{X^2}+\frac{2V'(X)}{X^3}\right]\right\} \\
&-\frac{\hbar^2}{6(2M)^3}\left\{\frac{1}{\omega_L^4}[V'''(X)]^2\left[\frac{1}{3}+\frac{1}{\sinh^2(\hbar\beta\omega_L/2)}\right]+\frac{3(D-1)}{2\omega_T+\omega_L}\frac{1}{\omega_L\omega_T^2}\left[\frac{V''(X)}{X}-\frac{V'(X)}{X^2}\right]^2\right. \\
&\left.\times\left[\coth^2(\hbar\beta\omega_T/2)+\frac{\omega_T}{\omega_L}\frac{1}{\sinh^2(\hbar\beta\omega_T/2)}+\frac{\omega_T}{2\omega_T-\omega_L}\frac{\sinh(\hbar\beta(\omega_T-\omega_L/2))}{\sinh(\hbar\beta\omega_L/2)\sinh^2(\hbar\beta\omega_T/2)}\right]\right\} \\
&+\mathcal{O}(\hbar^3).
\end{aligned} \tag{5.128}$$

In the zero-temperature limit this simplifies to

$$\lim_{\beta\to\infty} V_{\rm eff}(X) = V(X) + \frac{\hbar\omega_L}{2} + (D-1)\,\frac{\hbar\omega_T}{2} + \frac{\hbar^2}{8(2M)^2}\left\{\frac{1}{\omega_L^2}V^{(4)}(X)\right.$$
$$\left. + \frac{D^2-1}{\omega_T^2}\left[\frac{V''(X)}{X^2} - \frac{V'(X)}{X^3}\right] + \frac{2(D-1)}{\omega_L\omega_T}\left[\frac{V'''(X)}{X} - \frac{2V''(X)}{X^2} + \frac{2V'(X)}{X^3}\right]\right\}$$
$$- \frac{\hbar^2}{6(2M)^3}\left\{\frac{1}{3\omega_L^4}[V'''(X)]^2 + \frac{3(D-1)}{2\omega_T+\omega_L}\,\frac{1}{\omega_L\omega_T^2}\left[\frac{V''(X)}{X} - \frac{V'(X)}{X^2}\right]^2\right\} + \mathcal{O}(\hbar^3)\,. \quad (5.129)$$

Note that for $D = 1$ (5.128) and (5.129) pass into the earlier results (2.151) and (2.152), respectively.

Chapter 6

Outlook

In this chapter, we examine how the methods presented in this work can be applied to further problems. In Section 6.1, we show how the recursion relations for the ground-state energy developed in Chapter 3 could be generalized to the free energy for finite temperatures. Furthermore, the effective mass is introduced in Section 6.2.

6.1 Finite Temperature

In Chapter 3, we have obtained recursion relations for the ground-state energy of an anharmonic oscillator. At finite temperatures, thermal fluctuations become relevant in addition to the quantum fluctuations. These temperature dependent fluctuations can be taken into account by considering the free energy of a system. In imaginary-time, $\tau = it$, the time-dependent Schrödinger equation for the imaginary-time evolution amplitude $(x_b\,\tau|x_a\,0)$ reads

$$-\hbar\frac{\partial}{\partial\tau}(x_b\,\tau|x_a\,0) = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x_b^2}(x_b\,\tau|x_a\,0) + V(x_b)(x_b\,\tau|x_a\,0)\,, \tag{6.1}$$

with the initial condition

$$(x_b\,0|x_a\,0) = \delta(x_b - x_a)\,. \tag{6.2}$$

According to (2.13) and (2.15), the partition function for a quantum-mechanical system can be obtained by integrating over the diagonal elements of the imaginary-time evolution amplitude evaluated at $\tau = \hbar\beta$:

$$Z = \int_{-\infty}^{\infty} dx\,(x\,\hbar\beta|x\,0)\,. \tag{6.3}$$

The partition function, and therefore the free-energy of a system, can thus be obtained by solving (6.1). In Ref. [24] the following ansatz for the imaginary-time evolution amplitude for the potential (1.1) is made:

$$(x_b\,\tau|x_a\,0) = (x_b\,\tau|x_a\,0)_\omega\,A(x_b, x_a, \tau)\,, \tag{6.4}$$

where the imaginary-time evolution amplitude of the harmonic oscillator, $(x_b\,\tau|x_a\,0)_\omega$, is modified by the function $A(x_b, x_a, \tau)$. The approach (6.4) leads to a partial differential equation for the amplitude $A(x_b, x_a, \tau)$, which is then solved by expanding $A(x_b, x_a, \tau)$ in the coupling constant g, in x_b, and in x_a with τ-dependent expansion coefficients

$$A\left(x_b, x_a, \tau\right) = \sum_{k=0}^{\infty} \sum_{m=0}^{2k} \sum_{n=0}^{2m} g^k \frac{c^{(k)}_{2m|n}(\tau)}{\sinh^n \omega\tau}\, x_a^{2m-n} x_b^n \,. \tag{6.5}$$

This procedure constitutes a generalization of the Bender-Wu recursion method introduced in Chapter 3. There, it was used to solve the time-independent Schrödinger equation, and the expansion coefficients were determined by solving algebraic recursion relations. In Ref. [24], however, a recursive set of first-order ordinary differential equations is solved in order to determine the expansion coefficients $c^{(k)}_{2m|n}(\tau)$. The resulting weak-coupling series is then resummed via VPT, and the free energy of the anharmonic oscillator (1.1) is calculated up to the fifth order for arbitrary temperatures.

The recursion relation for the ground-state energy of the anharmonic oscillator with cubic anharmonicity (1.3), which has been obtained in Section 3.2, could now be generalized in a similar way. By combining the methods from Chapter 3 and Ref. [24] it should thus be possible to perturbatively calculate the free energy for the anharmonic oscillator (1.3) to high orders.

6.2 Effective Mass

In the zeroth order, the effective action $\Gamma[X]$ reduces to the tree-level, i.e. the imaginary-time action evaluated at the background $X(\tau)$,

$$\Gamma^{(0)}[X] = \mathcal{A}[X] = \int_0^{\hbar\beta} d\tau \, \left[\frac{M}{2}\, \dot{X}^2(\tau) + V(X(\tau))\right] \,. \tag{6.6}$$

The self energy is defined as the second functional derivative of the effective action, evaluated at a constant background:

$$\Sigma(\tau_1, \tau_2) = \left.\frac{\delta^2\Gamma[X]}{\delta X(\tau_1)\delta X(\tau_2)}\right|_{X(\tau)\equiv X} \,. \tag{6.7}$$

In the zeroth order, it thus reduces to

$$\Sigma^{(0)}(\tau_1, \tau_2) = \left.\frac{\delta^2\Gamma^{(0)}[X]}{\delta X(\tau_1)\delta X(\tau_2)}\right|_{X(\tau)\equiv X} = \left[-M\frac{d^2}{d\tau_1^2} + V''(X)\right]\delta(\tau_1 - \tau_2) \,. \tag{6.8}$$

The Matsubara decomposition of the self energy in the zeroth order is given by

$$\Sigma^{(0)}(\tau_1, \tau_2) = \frac{1}{\hbar\beta} \sum_{m=-\infty}^{\infty} \Sigma^{(0)}(\omega_m) e^{-i\omega_m(\tau_1 - \tau_2)} \,, \tag{6.9}$$

with the Matsubara frequencies ω_m as specified in (A.3). Taking into account the Matsubara decomposition of the delta function (A.20), one obtains from (6.8) and (6.9):

$$\Sigma^{(0)}(\omega_m) = M\omega_m^2 + V''(X) \,. \tag{6.10}$$

The identity

$$M = \left.\frac{\partial\Sigma^{(0)}(\omega_m)}{\partial\omega_m^2}\right|_{\omega_m=0} \tag{6.11}$$

then motivates the definition of the effective mass:

$$M_{\text{eff}} = \left.\frac{\partial\Sigma(\omega_m)}{\partial\omega_m^2}\right|_{\omega_m=0} \,. \tag{6.12}$$

In Ref. [40] the effective mass is calculated for an arbitrary potential in the first-loop order, yielding the result

$$M_{\text{eff}} = M + \hbar\frac{M^{1/2}[V'''(X)]^2}{32[V''(X)]^{5/2}} + \mathcal{O}(\hbar^2) \,. \tag{6.13}$$

In order to extend this calculation to higher orders, it would be desirable to develop a recursion relation for the effective mass, as for the effective potential in Section 3.4.

Appendix A

Harmonic Generating Functional

In this section, the generating functional (2.48) for the harmonic oscillator (2.47) is evaluated. The path integration in (2.48) is performed over all paths $x(\tau)$ which are periodic in the imaginary time τ, i.e.

$$x(0) = x(\hbar\beta) \,. \tag{A.1}$$

Thus, these paths $x(\tau)$ can be continued periodically and possess a Fourier decomposition. In the context of the imaginary-time formalism, the decomposition of paths is referred to as their *Matsubara decomposition*. It reads

$$x(\tau) = \sum_{m=-\infty}^{\infty} x_m e^{-i\omega_m \tau} \,, \tag{A.2}$$

with the *Matsubara frequencies*

$$\omega_m = \frac{2\pi}{\hbar\beta}\, m \,, \quad m = 0,\, \pm 1,\, \pm 2,\, \ldots \,. \tag{A.3}$$

Note that the periodicity of the paths $x(\tau)$ is passed on to their derivatives $\dot{x}(\tau)$:

$$\dot{x}(0) = \dot{x}(\hbar\beta) \,. \tag{A.4}$$

Furthermore, the Matsubara amplitudes x_m in (A.2) are restricted by the condition that the path $x(\tau)$ be real. From $x^*(\tau) = x(\tau)$ one concludes

$$x_m = x^*_{-m} \,, \tag{A.5}$$

so the real and imaginary parts of the Matsubara amplitude x_m are even and odd, respectively:

$$\mathrm{Re}\, x_m = \mathrm{Re}\, x_{-m} \,, \qquad \mathrm{Im}\, x_m = -\mathrm{Im}\, x_{-m} \,. \tag{A.6}$$

The Matsubara decomposition of the paths $x(\tau)$ permits us to rewrite the generating functional of the harmonic oscillator (2.48). The path integral measure in (2.48) will have to be

replaced by an infinite product of integrals. Due to (A.6), real and imaginary part of the Matsubara amplitude x_m with negative m are fixed by those with positive m. Thus, the path $x(\tau)$ can be determined by specifying all x_m with positive m and the zero mode x_0. Furthermore, as a consequence of (A.6), x_0 is real. Consequently, the following approach for the path integral measure can be implemented:

$$\oint \mathcal{D}x \;\to\; N_0 \int_{-\infty}^{\infty} dx_0 \prod_{m=1}^{\infty} \left(N_m \int_{-\infty}^{\infty} d\,\mathrm{Re}\, x_m \int_{-\infty}^{\infty} d\,\mathrm{Im}\, x_m \right) , \tag{A.7}$$

where N_0 and N_m denote normalization constants. They will be determined by comparing the harmonic oscillator's partition function within the path integral formalism (2.15) with the quantum statistical partition function (2.6). The latter can be determined by considering the occupation number representation of the eigenstates of the harmonic oscillator's Hamiltonian and is given by

$$Z_\omega = \mathrm{Tr}\left(e^{-\beta \hat{H}} \right) = \frac{1}{2 \sinh \hbar\beta\omega/2} \, . \tag{A.8}$$

Applying (A.2) and using (A.7), the generating functional for the harmonic oscillator (2.48) – (2.50) takes the form

$$\begin{aligned} Z_\omega[j] \;&=\; N_0 \int_{-\infty}^{\infty} dx_0 \prod_{m=1}^{\infty} \left(N_m \int_{-\infty}^{\infty} d\,\mathrm{Re}\, x_m \int_{-\infty}^{\infty} d\,\mathrm{Im}\, x_m \right) \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \right. \\ &\times \left. \left[\frac{M}{2} \sum_{m=-\infty}^{\infty} \sum_{m'=-\infty}^{\infty} x_m x_{m'} (\omega^2 + \omega_m^2)\, e^{-i(\omega_m + \omega_{m'})\tau} - j(\tau) \sum_{m=-\infty}^{\infty} x_m e^{-i\omega_m \tau} \right] \right\} . \end{aligned} \tag{A.9}$$

The first part of the τ-integral can be evaluated by using the result

$$\int_0^{\hbar\beta} d\tau \, e^{-i(\omega_m + \omega_{m'})\tau} = \hbar\beta \delta_{m,-m'} \, . \tag{A.10}$$

Taking into account (A.5), one obtains

$$\begin{aligned} Z_\omega[j] \;&=\; N_0 \int_{-\infty}^{\infty} dx_0 \prod_{m=1}^{\infty} \left(N_m \int_{-\infty}^{\infty} d\,\mathrm{Re}\, x_m \int_{-\infty}^{\infty} d\,\mathrm{Im}\, x_m \right) \\ &\times \exp\left[-\frac{M}{2} \sum_{m=-\infty}^{\infty} |x_m|^2 (\omega^2 + \omega_m^2)\beta + \frac{1}{\hbar} \sum_{m=-\infty}^{\infty} x_m \int_0^{\hbar\beta} d\tau \, j(\tau) e^{-i\omega_m \tau} \right] . \end{aligned} \tag{A.11}$$

By separating the zero mode and using (A.3), (A.6), one obtains

$$\begin{aligned} Z_\omega[j] \;&=\; N_0 \int_{-\infty}^{\infty} dx_0 \, \exp\left[-\frac{M}{2} x_0^2 \omega^2 \beta + \frac{x_0}{\hbar} \int_0^{\hbar\beta} d\tau \, j(\tau) \right] \\ &\times \prod_{m=1}^{\infty} \left\{ N_m \int_{-\infty}^{\infty} d\,\mathrm{Re}\, x_m \, \exp\left[-M\beta \left(\mathrm{Re}\, x_m \right)^2 (\omega^2 + \omega_m^2) + \frac{2\,\mathrm{Re}\, x_m}{\hbar} \int_0^{\hbar\beta} d\tau \, j(\tau) \cos\left(\omega_m \tau\right) \right] \right. \\ &\times \left. \int_{-\infty}^{\infty} d\,\mathrm{Im}\, x_m \, \exp\left[-M\beta \, \left(\mathrm{Im}\, x_m \right)^2 (\omega^2 + \omega_m^2) + \frac{2\,\mathrm{Im}\, x_m}{\hbar} \int_0^{\hbar\beta} d\tau \, j(\tau) \sin\left(\omega_m \tau\right) \right] \right\} . \end{aligned} \tag{A.12}$$

Evaluating the x_0-, Re x_m-, and Im x_m-integrals by using the result

$$\int_{-\infty}^{\infty} dx\ \exp(-p^2x^2+qx) = \frac{\sqrt{\pi}}{p}\exp\left(\frac{q^2}{4p^2}\right) \qquad [p>0]\,, \tag{A.13}$$

one obtains

$$Z_\omega[j] = Z_w\ \exp\left[\frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, G_\omega(\tau_1,\tau_2) j(\tau_1) j(\tau_2)\right]\,, \tag{A.14}$$

where the partition function Z_ω reads

$$Z_\omega[0] \equiv Z_\omega = N_0\sqrt{\frac{2\pi}{M\omega^2\beta}}\left(\prod_{m=1}^{\infty}\frac{N_m\pi}{M\beta(\omega^2+\omega_m^2)}\right)\,, \tag{A.15}$$

and the harmonic propagator $G_\omega(\tau_1,\tau_2)$ is given by

$$G_\omega(\tau_1,\tau_2) := \frac{1}{M\beta}\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m(\tau_1-\tau_2)}}{\omega^2+\omega_m^2}\,. \tag{A.16}$$

On the other hand, the partition function (A.8) can be expressed in the form [22, p. 37]

$$Z_\omega = \frac{1}{\hbar\beta\omega}\prod_{m=1}^{\infty}\frac{4m^2\pi^2}{\hbar^2\beta^2\omega^2+4m^2\pi^2}\,. \tag{A.17}$$

Comparing (A.15) and (A.17) yields the normalization constants

$$N_0 = \sqrt{\frac{M}{2\pi\hbar^2\beta}} \qquad \text{and} \qquad N_m = \frac{M\omega_m^2\beta}{\pi}\,. \tag{A.18}$$

Furthermore, by considering the identity

$$\int_0^{\hbar\beta} d\tau\ M\left(-\frac{d^2}{d\tau_1^2}+\omega^2\right)\delta(\tau_1-\tau)\,\frac{1}{M\beta}\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m(\tau-\tau_2)}}{\omega^2+\omega_m^2} = \frac{1}{\beta}\sum_{m=-\infty}^{\infty}e^{-i\omega_m(\tau_1-\tau_2)} \tag{A.19}$$

and comparing it with the Matsubara decomposition of the delta function,

$$\delta(\tau_1,\tau_2) = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}e^{-i\omega_m(\tau_1-\tau_2)}\,, \tag{A.20}$$

and with the definition of the integral kernel (2.50), one reads off that the propagator defined by (A.16) satisfies the relation (2.54). In the following it will be demonstrated that the harmonic propagator (A.16) can indeed be expressed in the form (2.55). Poisson's summation formula implies the identity [4, Sec. 2.16]

$$\sum_{m=-\infty}^{\infty} f(m) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} e^{-2\pi i\mu n} f(\mu)\,. \tag{A.21}$$

Using (A.21), one proves that

$$\frac{1}{M\beta}\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m(\tau_1-\tau_2)}}{\omega^2+\omega_m^2}=\frac{\hbar}{2\pi M}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}d\omega_m\,\frac{e^{-i\omega_m(\tau_1-\tau_2+n\hbar\beta)}}{\omega^2+\omega_m^2}\,. \tag{A.22}$$

The ω_m-integral on the right-hand side of the last equation can be evaluated by applying Cauchy's residue theorem. The result is found in Ref. [22, p. 312]. Together with (A.16) one thus obtains from the last identity

$$G_\omega(\tau_1,\tau_2)=\frac{\hbar}{2M\omega}\sum_{n=-\infty}^{\infty}e^{-\omega|\tau_1-\tau_2+n\hbar\beta|}\,. \tag{A.23}$$

Since both, τ_1 and τ_2, lie within the interval $[0,\,\hbar\beta]$, one has $|\tau_1-\tau_2|\le\hbar\beta$, and the sum on the right-hand side of (A.23) can be decomposed:

$$G_\omega(\tau_1,\tau_2)=\frac{\hbar}{2M\omega}\left\{e^{-\omega|\tau_1-\tau_2|}+\sum_{n=1}^{\infty}\left[e^{-\omega(\tau_1-\tau_2+n\hbar\beta)}+e^{-\omega(\tau_2-\tau_1+n\hbar\beta)}\right]\right\}\,. \tag{A.24}$$

Evaluating the geometric series that stem from (A.24), the harmonic propagator takes the form (2.55):

$$G_\omega(\tau_1,\tau_2)=\frac{\hbar}{2M\omega}\,\frac{\cosh(\omega|\tau_1-\tau_2|-\hbar\beta\omega/2)}{\sinh(\hbar\beta\omega/2)}\,. \tag{A.25}$$

Finally, we show that the function $f(\omega)$, defined by

$$f(\omega)=\exp\left(-\frac{1}{2}\mathrm{Tr}\ln G_\omega^{-1}\right)\,, \tag{A.26}$$

with

$$\mathrm{Tr}\ln G_\omega^{-1}=\sum_{m=-\infty}^{\infty}\ln\left(\omega^2+\omega_m^2\right)\,, \tag{A.27}$$

is identical to the partition function (A.8). Note that the eigenvalue problem of the integral kernel (2.50) ,

$$\int_0^{\hbar\beta}d\tau_2\,G^{-1}(\tau_1,\tau_2)x_m(\tau_2)=M\lambda_m x_m(\tau_1)\,, \tag{A.28}$$

with

$$x_m(0)=x_m(\hbar\beta)\,, \tag{A.29}$$

can be solved using the approach

$$x_m(\tau)=x_m e^{-i\omega_m\tau} \tag{A.30}$$

and that the eigenvalues of $G^{-1}(\tau_1, \tau_2)$ are given by

$$\lambda_m = \omega^2 + \omega_m^2 \,. \tag{A.31}$$

Forming the logarithmic derivative of $f(\omega)$ with respect to ω and taking into account (A.16), (A.25), and (A.27) yields

$$\frac{\partial}{\partial\omega} \ln f(\omega) = -\frac{\hbar\beta}{2} \coth(\hbar\beta\omega/2) = -\frac{\partial}{\partial\omega} \ln\sinh(\hbar\beta\omega/2) \,. \tag{A.32}$$

Integrating the last identity with respect to ω, one obtains

$$f(\omega) = \frac{c}{\sinh(\hbar\beta\omega/2)} \,, \tag{A.33}$$

where c does not depend on ω. It remains to demonstrate that $c = 1/2$. To this end, we show that for $\omega \ll 1$ one has

$$f(\omega) \approx \frac{1}{\hbar\beta\omega} \,. \tag{A.34}$$

For $\omega \ll 1$ one can approximate

$$\sum_{m=-\infty}^{\infty} \ln(\omega^2 + \omega_m^2) = \ln\omega^2 + 2\sum_{m=1}^{\infty} \ln(\omega^2 + \omega_m^2) \overset{\omega\ll 1}{\approx} \ln\omega^2 + 2\sum_{m=1}^{\infty} \ln\omega_m^2 \,. \tag{A.35}$$

Note that in the limit $\omega \to 0$ both terms on the right hand side of the last identity are divergent. This divergence will be treated by means of zeta-function regularization [4, Ch. 2]. Using definition (A.3), one obtains

$$\sum_{m=-\infty}^{\infty} \ln(\omega^2 + \omega_m^2) \overset{\omega\ll 1}{\approx} \ln\omega^2 + 2\ln\left(\frac{2\pi}{\hbar\beta}\right)^2 \sum_{m=1}^{\infty} 1 + 2\sum_{m=1}^{\infty} \ln m^2 \,. \tag{A.36}$$

For $n \neq 1$, the Riemann zeta function can be given by

$$\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n} \,. \tag{A.37}$$

In Ref. [22, p. 1074] the values

$$\zeta(0) = -\frac{1}{2} \qquad \text{and} \qquad \zeta'(0) = -\frac{1}{2}\ln 2\pi \tag{A.38}$$

of the zeta function are given. Thus, considering the identity

$$\ln m = -\frac{d}{dx} m^{-x}\Big|_{x=0} \tag{A.39}$$

and identifying

$$\sum_{m=1}^{\infty} 1 = \zeta(0) \qquad \text{and} \qquad \sum_{m=1}^{\infty} \ln m = -\zeta'(0), \tag{A.40}$$

one obtains from (A.26), (A.27), and (A.36)

$$f(\omega) \overset{\omega\ll 1}{\approx} \exp\left[-\left(\ln\omega + \ln\hbar\beta\right)\right] \,, \tag{A.41}$$

which is identical to (A.34).

Appendix B

Standard Integrals

Calculating the effective potential up to $l = 2$, 3 loops necessitates the evaluation of the one-particle irreducible vacuum diagrams (2.109), (2.110), which are specified by the Feynman rules (2.146), (2.147), and where the propagator $G_\Omega(\tau_1, \tau_2)$ is given by (2.140), (2.141). The ground-state energy of the anharmonic oscillator (2.156) can be determined by evaluating the Feynman diagrams (2.186) in the zero-temperature limit. The temperature-dependent free energy in the second loop order is given by (2.181), where the propagator $G_\omega(\tau_1, \tau_2)$ is specified in (2.55). In D spatial dimensions, the effective potential up to $l = 2$ loops is obtained by evaluating the diagrams (2.109), where the Feynman rules (5.94), (5.96) apply, and where the propagator is given by (5.108) – (5.110). When performing these calculations, certain multiple-integrals arise. The evaluation of these standard integrals will be demonstrated in this appendix.

B.1 Integrals for Arbitrary Temperatures

The harmonic propagator $G_\omega(\tau_1, \tau_2)$ is given by (2.55):

$$G_\omega(\tau_1, \tau_2) = \frac{\hbar}{2M\omega} \, \frac{\cosh(\omega|\tau_1 - \tau_2| - \hbar\beta\omega/2)}{\sinh(\hbar\beta\omega/2)} \, . \tag{B.1}$$

Evaluating the second-order free energy (2.181) leads to the twofold integral

$$I_1 := \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, \cosh(\omega|\tau_1 - \tau_2| - \hbar\beta\omega/2) \, . \tag{B.2}$$

In order to evaluate this integral, it can be decomposed into two twofold integrals:

$$\begin{aligned} I_1 \;\; = \;\; & \int_0^{\hbar\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \, \cosh(\omega(\tau_1 - \tau_2) - \hbar\beta\omega/2) \\ & + \int_0^{\hbar\beta} d\tau_2 \int_0^{\tau_2} d\tau_1 \, \cosh(\omega(\tau_2 - \tau_1) - \hbar\beta\omega/2) \, . \end{aligned} \tag{B.3}$$

Renaming τ_1 to τ_2 and τ_2 to τ_1 in the second twofold integral yields

$$I_1 = 2\int_0^{\hbar\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \, \cosh(\omega(\tau_1-\tau_2)-\hbar\beta\omega/2) = \frac{2\hbar\beta}{\omega}\sinh(\hbar\beta\omega/2)\,. \tag{B.4}$$

The propagator the in case of an arbitrary potential (2.141) is obtained by introducing the new frequency (2.140). It has the same form as the propagator for the harmonic oscillator (2.55). Therefore, the following results can be applied to calculate the effective potential (2.148) and the free energy (2.181). In both cases, a twofold integral of the form

$$I_2 := \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, \cosh^3(\Omega|\tau_1-\tau_2|-\hbar\beta\Omega/2) \tag{B.5}$$

has to be evaluated. In order to do so, it can, as above, be decomposed into two twofold integrals:

$$I_2 = 2\int_0^{\hbar\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \, \cosh^3(\Omega(\tau_1-\tau_2)-\hbar\beta\Omega/2)\,. \tag{B.6}$$

The remaining integrals can be solved subsequently. Their solution is, for example, given in Ref. [22, p. 94f]. One obtains

$$I_2 = \frac{2\hbar\beta}{\Omega}\left[\sinh(\hbar\beta\Omega/2)+\frac{1}{3}\sinh^3(\hbar\beta\Omega/2)\right]\,. \tag{B.7}$$

This result permits the evaluation of the diagrams (2.109) for arbitrary temperatures and the calculation of the free energy (2.181).

Calculating the effective potential for a rotationally symmetric potential in D spatial dimension leads to a twofold integral over a product of propagators with different frequencies:

$$I_3 := \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \, \cosh(\omega_L|\tau_1-\tau_2|-\hbar\beta\omega_L/2)\cosh^2(\omega_T|\tau_1-\tau_2|-\hbar\beta\omega_T/2)\,. \tag{B.8}$$

Again, it can be decomposed into two twofold integrals,

$$I_3 = 2\,\frac{1}{\omega_T}\int_0^{\hbar\beta} d\tau_1 \int_{-\hbar\beta\omega_T/2}^{\omega_T\tau_1-\hbar\beta\omega_T/2} d\xi \, \cosh^2\xi \, \cosh\left(\frac{\omega_L}{\omega_T}\xi\right)\,, \tag{B.9}$$

where the substitution

$$\tau_2(\xi) = \tau_1 - \frac{\xi}{\omega_T} - \hbar\beta/2 \tag{B.10}$$

has been performed. The ξ-integral can be solved by using results from Ref. [22, p. 102, p. 105]. One obtains

$$\begin{aligned} I_3 \;=\; & \frac{2}{2\omega_T+\omega_L}\Bigg\{\hbar\beta\Big[\cosh^2(\hbar\beta\omega_T/2)\sinh(\hbar\beta\omega_L/2)+\frac{\omega_T}{\omega_L}\sinh(\hbar\beta\omega_L/2) \\ & \qquad +\frac{\omega_T}{2\omega_T-\omega_L}\sinh(\hbar\beta(\omega_T-\omega_L/2))\Big] \\ & +\int_{-\hbar\beta\omega_T/2}^{\hbar\beta\omega_T/2} d\zeta \, \left[\cosh^2\zeta\sinh\left(\frac{\omega_L}{\omega_T}\zeta\right)+\frac{\omega_T}{\omega_L}\sinh\left(\frac{\omega_L}{\omega_T}\zeta\right)+\frac{\omega_T}{2\omega_T-\omega_L}\sinh\left(2\zeta-\frac{\omega_L}{\omega_T}\zeta\right)\right]\Bigg\}\,, \end{aligned} \tag{B.11}$$

where the substitution

$$\tau_1(\zeta) = \frac{\zeta}{\omega_T} + \hbar\beta/2 \tag{B.12}$$

has been performed. Since all components of the ζ-integral are odd, and since the integration limits are symmetric with respect to the origin, the ζ-integral vanishes, and one obtains the result

$$\begin{aligned} I_3 \;=\; & \frac{2\hbar\beta}{2\omega_T+\omega_L}\Big[\cosh^2(\hbar\beta\omega_T/2)\sinh(\hbar\beta\omega_L/2) + \frac{\omega_T}{\omega_L}\sinh(\hbar\beta\omega_L/2) \\ & + \frac{\omega_T}{2\omega_T-\omega_L}\sinh(\hbar\beta(\omega_T-\omega_L/2))\Big]\,. \end{aligned} \tag{B.13}$$

Note that due to $\cosh^2 z - \sinh^2 z = 1$, the result (B.13) becomes (B.7) for $\omega_L = \omega_T = \Omega$.

B.2 Integrals in the Zero-Temperature Limit

In the zero-temperature limit, the propagator $G_\Omega(\tau_1,\tau_2)$ is given by (2.142):

$$\lim_{T\to 0} G_\Omega(\tau_1,\tau_2) = \frac{\hbar}{2M\Omega}\, e^{-\Omega|\tau_1-\tau_2|}\,. \tag{B.14}$$

Determining the effective potential in this limit up to $l=3$ loops by evaluating the Feynman diagrams (2.110), which are specified by (2.146), (2.147), leads to standard multiple-integrals. These integrals arise also when calculating the anharmonic oscillator's ground-state energy (2.186). Here, the diagrams are specified by the Feynman rules (2.182) – (2.184). For both calculations the multiplicity of an integration is determined by the number of vertices in the corresponding diagram. When evaluating a diagram with two vertices, the twofold integral

$$I(n_{12}) := \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\; \exp\left(-n_{12}\Omega|\tau_1-\tau_2|\right) \tag{B.15}$$

arises. A diagram with three vertices leads to the threefold integral

$$\begin{aligned} I(n_{12},n_{13},n_{23}) \;:=\; & \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \\ & \times \exp\left(-n_{12}\Omega|\tau_1-\tau_2| - n_{13}\Omega|\tau_1-\tau_3| - n_{23}\Omega|\tau_2-\tau_3|\right)\,. \end{aligned} \tag{B.16}$$

And in order to calculate a diagram with four vertices the fourfold integral

$$\begin{aligned} I(n_{12},n_{13},n_{14},n_{23},n_{24},n_{34}) \;:=\; & \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \int_0^{\hbar\beta} d\tau_4\; \exp(-n_{12}\Omega|\tau_1-\tau_2| \\ & -n_{13}\Omega|\tau_1-\tau_3| - n_{14}\Omega|\tau_1-\tau_4| - n_{23}\Omega|\tau_2-\tau_3| - n_{24}\Omega|\tau_2-\tau_4| - n_{34}\Omega|\tau_3-\tau_4|) \end{aligned} \tag{B.17}$$

has to be evaluated. The number n_{ij} turns out to denote the number of lines connecting the vertices i and j. In the following, (B.15) – (B.17) will be calculated in the leading order for

$\beta \to \infty$. Decomposing the integral (B.15) into $2! = 2$ contributions,

$$\begin{aligned} I(n_{12}) &:= \int_0^{\hbar\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \, \exp\left[-n_{12}\Omega(\tau_1 - \tau_2)\right] \\ &\quad + \int_0^{\hbar\beta} d\tau_2 \int_0^{\tau_2} d\tau_1 \, \exp\left[-n_{12}\Omega(\tau_2 - \tau_1)\right] \, , \end{aligned} \tag{B.18}$$

and renaming the integration variables of the second twofold integral yields the result

$$I(n_{12}) = \frac{2}{n_{12}\Omega}\left[\hbar\beta + \frac{1}{n_{12}\Omega}\left(e^{-n_{12}\hbar\beta\Omega} - 1\right)\right] \stackrel{\beta\to\infty}{\longrightarrow} \frac{2\hbar\beta}{n_{12}\Omega} \, . \tag{B.19}$$

Correspondingly, the threefold integral (B.16) can be decomposed into $3! = 6$ contributions

$$\begin{aligned} I(n_{12}, n_{13}, n_{23}) &= J(n_{12}, n_{13}, n_{23}) + J(n_{12}, n_{23}, n_{13}) + J(n_{13}, n_{12}, n_{23}) \\ &\quad + J(n_{13}, n_{23}, n_{12}) + J(n_{23}, n_{12}, n_{13}) + J(n_{23}, n_{13}, n_{12}) \, , \end{aligned} \tag{B.20}$$

where the evaluation of

$$\begin{aligned} J(n_{12}, n_{13}, n_{23}) &:= \int_0^{\hbar\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \int_0^{\tau_2} d\tau_3 \\ &\quad \times \exp\left[-n_{12}\Omega(\tau_1 - \tau_2) - n_{13}\Omega(\tau_1 - \tau_3) - n_{23}\Omega(\tau_2 - \tau_3)\right] \end{aligned} \tag{B.21}$$

leads to

$$J(n_{12}, n_{13}, n_{23}) \stackrel{\beta\to\infty}{\longrightarrow} \frac{\hbar\beta}{\Omega^2(n_{12} + n_{13})(n_{13} + n_{23})} \, . \tag{B.22}$$

Thus, inserting (B.22) into (B.20) leads to the result

$$I(n_{12}, n_{13}, n_{23}) \stackrel{\beta\to\infty}{\longrightarrow} \frac{4\hbar\beta}{\Omega^2} \frac{n_{12} + n_{13} + n_{23}}{(n_{12} + n_{13})(n_{12} + n_{23})(n_{13} + n_{23})} \, . \tag{B.23}$$

The fourfold integral (B.17) is solved in a similar way, but it has to be decomposed into $4! = 24$ contributions, which correspond to the possibilities to order the imaginary times $\tau_1, \tau_2, \tau_3, \tau_4$:

$$\begin{aligned} I(n_{12}, n_{13}, n_{14}, n_{23}, n_{24}, n_{34}) &:= \int_0^{\hbar\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \int_0^{\tau_2} d\tau_3 \int_0^{\tau_3} d\tau_4 \, \exp[-n_{12}\Omega(\tau_1 - \tau_2) \\ &- n_{13}\Omega(\tau_1 - \tau_3) - n_{14}\Omega(\tau_1 - \tau_4) - n_{23}\Omega(\tau_2 - \tau_3) - n_{24}\Omega(\tau_2 - \tau_4) - n_{34}\Omega(\tau_3 - \tau_4)] \\ &+ 23 \text{ fourfold integrals.} \end{aligned} \tag{B.24}$$

The first contribution, which corresponds to the case $\tau_1 \geq \tau_2 \geq \tau_3 \geq \tau_4$, yields:

$$\begin{aligned} &\int_0^{\hbar\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \int_0^{\tau_2} d\tau_3 \int_0^{\tau_3} d\tau_4 \, \exp[-n_{12}\Omega(\tau_1 - \tau_2) - n_{13}\Omega(\tau_1 - \tau_3) - n_{14}\Omega(\tau_1 - \tau_4) \\ &\qquad -n_{23}\Omega(\tau_2 - \tau_3) - n_{24}\Omega(\tau_2 - \tau_4) - n_{34}\Omega(\tau_3 - \tau_4)] \\ &\stackrel{\beta\to\infty}{\longrightarrow} \frac{\hbar\beta}{\Omega^3(n_{12} + n_{13} + n_{14})(n_{14} + n_{24} + n_{34})(n_{13} + n_{14} + n_{23} + n_{24})} \, . \end{aligned} \tag{B.25}$$

Evaluating the remaining 23 fourfold integrals by suitably renaming the integration variables τ_1, τ_2, τ_3, τ_4 and the indices n_{ij} yields the final result

$$
\begin{aligned}
&I(n_{12},n_{13},n_{14},n_{23},n_{24},n_{34}) \overset{\beta\to\infty}{\longrightarrow} \\
&\quad\frac{2\hbar\beta}{\Omega^3}\left\{\frac{1}{n_{12}+n_{13}+n_{24}+n_{34}}\left[\frac{1}{n_{12}+n_{13}+n_{14}}\left(\frac{1}{n_{12}+n_{23}+n_{24}}+\frac{1}{n_{13}+n_{23}+n_{34}}\right)\right.\right. \\
&\qquad\left.+\frac{1}{n_{14}+n_{24}+n_{34}}\left(\frac{1}{n_{12}+n_{23}+n_{24}}+\frac{1}{n_{13}+n_{23}+n_{34}}\right)\right] \\
&\qquad+\frac{1}{n_{12}+n_{14}+n_{23}+n_{34}}\left[\frac{1}{n_{12}+n_{23}+n_{24}}\left(\frac{1}{n_{12}+n_{13}+n_{14}}+\frac{1}{n_{13}+n_{23}+n_{34}}\right)\right. \\
&\qquad\left.+\frac{1}{n_{14}+n_{24}+n_{34}}\left(\frac{1}{n_{12}+n_{13}+n_{14}}+\frac{1}{n_{13}+n_{23}+n_{34}}\right)\right] \\
&\qquad+\frac{1}{n_{13}+n_{14}+n_{23}+n_{24}}\left[\frac{1}{n_{13}+n_{23}+n_{34}}\left(\frac{1}{n_{12}+n_{13}+n_{14}}+\frac{1}{n_{12}+n_{23}+n_{24}}\right)\right. \\
&\qquad\left.\left.\left.+\frac{1}{n_{14}+n_{24}+n_{34}}\left(\frac{1}{n_{12}+n_{13}+n_{14}}+\frac{1}{n_{12}+n_{23}+n_{24}}\right)\right]\right\}.
\end{aligned}
\tag{B.26}
$$

In Section 2.8, the following integrals are needed:

$$I(2,1,2) \overset{\beta\to\infty}{\longrightarrow} \frac{5\hbar\beta}{9\Omega^2}\,, \tag{B.27}$$

$$I(1,2,1) \overset{\beta\to\infty}{\longrightarrow} \frac{8\hbar\beta}{9\Omega^2}\,, \tag{B.28}$$

$$I(1,1,1,1,1,1) \overset{\beta\to\infty}{\longrightarrow} \frac{2\hbar\beta}{3\Omega^3}\,, \tag{B.29}$$

$$I(1,2,2,1,0,0) \overset{\beta\to\infty}{\longrightarrow} \frac{22\hbar\beta}{27\Omega^3}\,. \tag{B.30}$$

In Section 2.10, one needs additionally:

$$I(1,3,0) \overset{\beta\to\infty}{\longrightarrow} \frac{4\hbar\beta}{3\Omega^2}\,, \tag{B.31}$$

$$I(1,2,0) \overset{\beta\to\infty}{\longrightarrow} 2\frac{\hbar\beta}{\Omega^2}\,, \tag{B.32}$$

$$I(1,1,0) \overset{\beta\to\infty}{\longrightarrow} 4\frac{\hbar\beta}{\Omega^2}\,, \tag{B.33}$$

$$I(1,1,1,2,0,0) \overset{\beta\to\infty}{\longrightarrow} \frac{16\hbar\beta}{9\Omega^3}\,, \tag{B.34}$$

$$I(1,2,1,0,0,0) \overset{\beta\to\infty}{\longrightarrow} 4\frac{\hbar\beta}{\Omega^3}\,, \tag{B.35}$$

$$I(1,1,1,0,0,0) \overset{\beta\to\infty}{\longrightarrow} 8\frac{\hbar\beta}{\Omega^3}\,. \tag{B.36}$$

Appendix C

Shooting Method

In this section, it will be demonstrated how the time-independent Schrödinger equation (3.5) can be solved by using the so-called shooting method. In natural units, $\hbar = 1$, $M = 1$, Eq. (3.5) reads

$$-\frac{1}{2}\,\psi''(x) + \left(\frac{1}{2}\omega^2 x^2 + gAx^3 + g^2Bx^4\right)\psi(x) = E\,\psi(x)\,. \tag{C.1}$$

In order to illustrate the application of the shooting method, we consider this equation without the cubic nonlinearity, i.e. $A = 0$, and for arbitrary positive but fixed values of ω^2 and g^2B. For any preassigned value of E, the wave function $\psi(x)$ can be obtained numerically, e.g. with the aid of the Runge-Kutta method. Since the differential equation (C.1) is of second order, the starting values $\psi(x_s)$ and $\psi'(x_s)$ need to be known in order to obtain a unique solution. For $A = 0$, the anharmonic potential is even, and the eigenfunctions have defined parity. The ground-state wave function has no zeros and is thus even. Therefore, choosing $x_s = 0$, one obtains the starting value $\psi'(0) = 0$ and $\psi(0)$ is fixed by the normalization condition. Initially, one can choose $\psi(0) = 1$. The ground-state energy E_0 can be

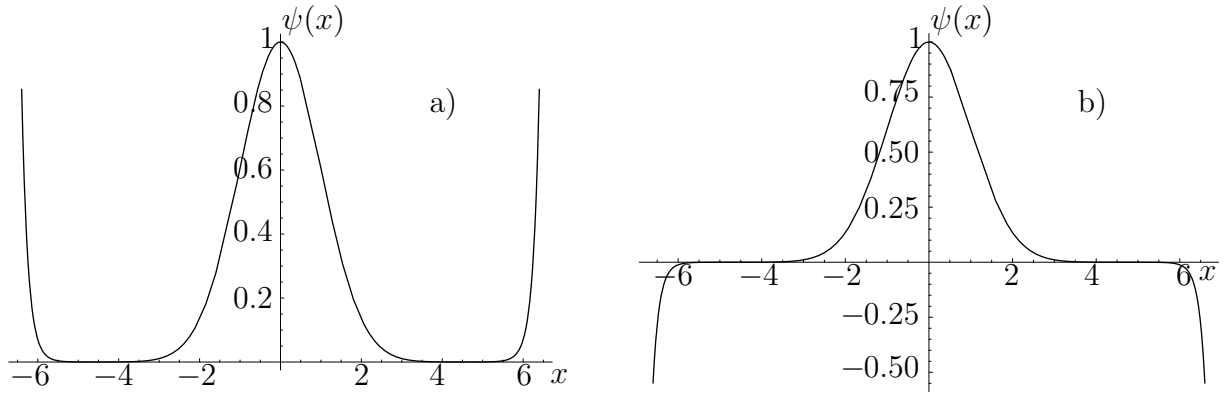


Figure C.1: Numerical Solution of (C.1) for a) $\omega = 1$, $A = 0$, $B = 1$, $g = 0.01$, E = 0.5007468224 and b) $\omega = 1$, $A = 0$, $B = 1$, $g = 0.01$, E = 0.5007468283.

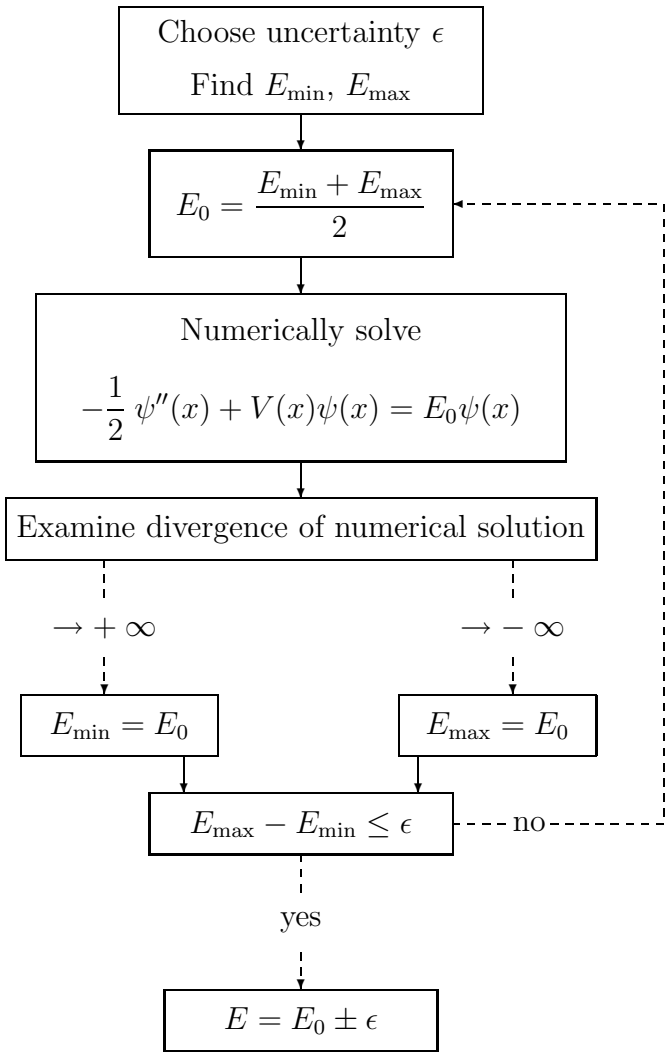


Figure C.2: Algorithmic procedure of the shooting method.

determined iteratively since the numerical solution of the differential equation (C.1) will diverge towards positive infinity when an energy value is chosen that is greater than the actual ground-state energy ($E < E_{\text{real}}$), but it will diverge towards negative infinity when an energy value is chosen that is smaller than the actual ground-state energy ($E > E_{\text{real}}$). Figure C.1 a) and b) show examples for the two cases. In this way, one deduces that the actual ground state energy for the potential $V(x) = 0.5x^2 + 10^{-4}x^4$ is between $E_{\min} = 0.5007468224$ and $E_{\max} = 0.5007468283$. Figure C.2 shows a flow chart of the algorithmic procedure of the shooting method.

For $A \neq 0$, one can no longer assume $\psi'(0) = 0$. The shooting method can, nevertheless, still be applied; but now two quantities, E_0 and $\psi'(0)$, have to be determined iteratively. For an arbitrarily chosen pair of values of E_0 and $\psi'(0)$, the numerical solution of (C.1) might diverge towards towards positive infinity for $x \to \infty$ and towards negative infinity for

$x \to -\infty$, or vice-versa. Thus, when applying the shooting method as illustrated in Fig. C.2, the type of divergence has to be determined for $x > 0$ *or* for $x < 0$; and depending on which of the possibilities is chosen, one obtains different values for the ground-state energy. The correct value of the ground-state energy, however, is obtained for that particular value of $\psi'(0)$ that leads to identical results when examining the solution's divergence for $x > 0$ and $x < 0$.

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