Part III

Variational Perturbation Theory in Quantum Statistics

Chapter 7

Introduction

The exact calculation of path integrals is only possible, if they are or can be transformed in a Gaussian shape. In Part II of this thesis, we have considered a very general Gaussian action (3.1) and calculated the quantum-statistical properties of systems governed by such an action. All Euclidean systems, where the action only contains terms of the form $x^m(\tau)p^n(\tau)$ with $(m,n) \in \{(2,0),(1,1),(0,2)\}$, belong to this class of exactly solvable problems. An example is a particle in a harmonic potential and influenced by external sources which linearly couple to particle position or momentum. In order to motivate the general theory in Part II, we have investigated the quantum statistics of the one-dimensional problem in detail. Another system in this class is a charged particle in static electric and/or magnetic field, since the scalar potential of the electric field couples linearly to the position, and the vector potential of the magnetic field is minimally coupled to the momentum. We will consider an application in this part, where we investigate the quantum-statistical properties of hydrogen in uniform magnetic field. As a warm-up exercise, we will treat there the exactly solvable problem of a single electron in magnetic field at arbitrary temperature. It is worth noting that the calculation of the path amplitude for the three-dimensional hydrogen atom is also exactly done after mapping it to a four-dimensional oscillator [4].

Nevertheless, most of the interesting systems have nontrivial interactions, which prevent an exact evaluation of quantum-statistical quantities. A characteristic property of such systems is that they are usually governed by potentials, which "disturb" the Gaussian shape of the action, for example the x^4 term of the anharmonic oscillator, its pendant in the field theory of critical phenomena, ϕ^4, or the interaction $\bar{\psi}\gamma_\mu\psi A^\mu$ between matter fields $\bar{\psi}$, ψ and electromagnetic field A_μ in quantum electrodynamics (QED). The coupling strength between these fields in QED is rather small, it is the fine structure constant $\alpha = e^2/4\pi\varepsilon_0\hbar c \approx 1/137$. In cases, where the coupling constant is small, it is useful to expand the time evolution operator (or the corresponding action exponential in the functional integral) into a Taylor series and to calculate perturbative corrections to the result of the exactly solvable unperturbed system. Since it is usually impossible to evaluate the corrections in all orders, the perturbation series must be broken up after any order n. For weak coupling, the first contributing perturbative order yields already satisfactory results for many systems. There is no guarantee, however, that, despite a small coupling constant, the perturbative series converges. The reason is that the number of terms contributing to a certain order of perturbation is extremely increasing from order to order. A practical quantity for checking the convergence of a series is its radius of convergence, which is defined as the infinite-order limit of the absolute ratio of contributions

a_n of successive orders:

$$R = \lim_{n\to\infty} \left| \frac{a_n}{a_{n+1}} \right| . \tag{7.1}$$

The series *converges*, if $R > 1$, and *diverges* for $R < 1$. Since in nth order $a_n = c_n g^n$, where c_n is the expansion coefficient and g the coupling constant, we find

$$R = \frac{r}{g}, \qquad r = \lim_{n\to\infty} \left| \frac{c_n}{c_{n+1}} \right| . \tag{7.2}$$

In this relation, the competitive character of expansion coefficients and coupling strength turns out clearly. Thus, a perturbative series converges, if $r > g$, since the overall contribution decreases for successive orders of perturbation. A diverging series is characterized by $r < g$. Unfortunately, the radius of convergence can only be evaluated exactly, if a recursion equation for the perturbative coefficients exists, which relates c_n and c_{n+1}. For most problems, it is not possible to exactly determine R, and one can only make an extrapolation estimated from successive low orders, for which the coefficients c_n are known. Following Dyson [42], even perturbative series in QED will diverge for orders of perturbation higher than the inverse fine structure constant, i.e. $n > 1/\alpha$.

In order to obtain finite results from truncated perturbative expansions, it is necessary to apply methods, which perform an approximate summation of the series. It is even possible to use such summation methods for strong-coupling series, where the perturbations are not small in comparison with the unperturbed contribution. Well-known summation methods were developed by Euler, Borel, and Padé. The applicabiltiy of such methods is usually restricted to series obeying some requirements regarding the growth of the expansion coefficients for large orders [43]. Alternative promising procedures are based on nonlinear transformations, e.g. sequence transformations [44], for accelerating the convergence of originally diverging series.

We use a different powerful method for the summation of perturbative series, which is called *variational perturbation theory* [4, Chap. 5]. A first approach was used by Feynman in 1954 for discussing the polaron problem [45]. This procedure was improved by Feynman and Kleinert [8] and, independently, by Giachetti and Tognetti [9] in 1985/86. In this approach, the action of a harmonic oscillator with trial frequency $\Omega(x_0)$ serves as trial system and the remainder as perturbation. The correctly treated zero-frequency mode x_0 of the path by a separate x_0-integration makes it possible to reexpress the quantum-statistical partition function by an integral over a classically looking Boltzmann factor, which contains the *effective classical potential*. Based on the Jensen-Peierls inequality, variation with respect to the trial frequency $\Omega(x_0)$ yields an upper bound for the effective classical potential. Meanwhile, this method is denoted as *variational approach*, since a systematic extension to higher-order variational perturbation theory was developed by Kleinert [4,46,47]. We will review the fundamentals of the approach and the systematic theory in the following sections.

In the following chapters, we present generalizations of this theory, which enable us to enlarge the range of applicability of variational perturbation theory. We develop variational perturbation theory for density matrices [20] and calculate the density of a particle in the double-well potential. Furthermore, we investigate the pair-distribution function for hydrogen, which is a characteristic quantity of hydrogen plasma. By extending variational perturbation theory for applications in phase space, where we practically introduce the *effective classical Hamiltonian*, we calculate the quantum-statistical properties of hydrogen in magnetic fields [18,19]. The zero-temperature limit of the effective classical Hamiltonian yields the binding energy. This quantity possesses quite different asymptotic behaviors for weak and strong magnetic fields. We investigate these limits in detail, and the results confirm the power of the variational summation method. Finally, in Part IV of this thesis, we turn to membrane physics, where we calculate the fluctuation pressure which fluid membranes exert upon hard walls [48,49]. By an analytic strong-coupling calculation, we evaluate the constants occuring in Helfrich's ideal-gas-like pressure law [50] to such a high accuracy that their values lie well within the error bounds of Monte-Carlo simulations. Aside from the very successful calculation of critical exponents in ϕ^4 theory [5], the results for the fluctuating membranes show that variational perturbation theory is also applicable for the summation of perturbation series arising from field theories.

7.1 Variational Approach via Jensen-Peierls Inequality

We review the variational approach [4,8,45] for the calculation of the quantum-statistical partition function Z in the more general phase space representation. As shown in Eq. (4.29), we express the partition function (4.28) as an integral of the restricted partition function $Z^{\mathbf{p}_0\mathbf{x}_0}$ over the zero-frequency phase space coordinates $\mathbf{p}_0$ and $\mathbf{x}_0$. The relation between $Z^{\mathbf{p}_0\mathbf{x}_0}$ and the effective classical Hamiltonian $H_{\text{eff}}(p_0, x_0)$ is given by Eq. (4.31). We write the restricted partition function for any system with an dimensionless action $\mathcal{A}[\mathbf{p}, \mathbf{x}]$ as a path integral over the phase space coordinates $\mathbf{w}^T = (\mathbf{x}^T, \mathbf{p}^T)$ as

$$Z^{\mathbf{w}_0} = (2\pi\hbar)^d \oint \mathcal{D}^{2d}w\, \delta(\mathbf{w}_0 - \overline{\mathbf{w}(\tau)})\, e^{-\mathcal{A}[\mathbf{w}]/\hbar}. \tag{7.3}$$

In general, this quantity cannot be calculated exactly, and therefore we decompose the action $\mathcal{A}[\mathbf{w}]$ into a part $\mathcal{A}_\Omega^{\mathbf{w}_0}[\mathbf{w}]$, for which the restricted partition function is known, and a remainder, which we call the interaction term $\mathcal{A}_{\text{int}}[\mathbf{w}]$:

$$\mathcal{A}[\mathbf{w}] = \mathcal{A}_\Omega^{\mathbf{w}_0}[\mathbf{w}] + \mathcal{A}_{\text{int}}[\mathbf{w}]. \tag{7.4}$$

The action of the exactly solvable system shall be expressed as

$$\mathcal{A}_\Omega^{\mathbf{w}_0}[\mathbf{w}] = \frac{\hbar}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \left(\mathbf{w}^T(\tau) - \mathbf{w}_0^T\right) S_\Omega(\tau,\tau') \left(\mathbf{w}(\tau') - \mathbf{w}_0\right), \tag{7.5}$$

where we have subtracted the zero-frequency mode from the phase space coordinates. The elements of the symmetric matrix S_Ω are of the form $S_{\Omega,ij} = \Omega_{ij} S_{ij}$, where the $2d^2 + d$ parameters $\Omega_{ij} = \Omega_{ji}$ are still undetermined. The matrix S shall be of the form (3.10), which makes it possible to exactly calculate the corresponding restricted partition function:

$$\begin{aligned} Z_\Omega^{\mathbf{w}_0} &= (2\pi\hbar)^d \oint \mathcal{D}^{2d}w\, \delta(\mathbf{w}_0 - \overline{\mathbf{w}(\tau)}) \exp\left\{-\frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \left(\mathbf{w}^T(\tau) - \mathbf{w}_0^T\right) S_\Omega(\tau,\tau') \left(\mathbf{w}(\tau') - \mathbf{w}_0\right)\right\} \\ &= \frac{1}{\sqrt{\det_{\text{ps}} S_{\Omega,0}^{-1} \det S_\Omega}}\,. \end{aligned} \tag{7.6}$$

Here, we have made use of the calculation for the restricted partition function in Section 4.2, with the result (4.52). The exponential function occurring in (4.52) is absent in Eq. (7.6) due to the subtraction of the zero-frequency modes of the phase space path in the action of Eq. (7.5). In analogy to Eq. (4.53), we use the path integral (7.6) to define expectation values

$$\begin{aligned} \langle O_1(\mathbf{w}(\tau_1)) O_2(\mathbf{w}(\tau_2)) \cdots \rangle_\Omega^{\mathbf{w}_0} &= (2\pi\hbar)^d \left[Z_\Omega^{\mathbf{w}_0}\right]^{-1} \oint \mathcal{D}^{2d}w\, \delta(\mathbf{w}_0 - \overline{\mathbf{w}(\tau)}) \\ &\quad \times O_1(\mathbf{w}(\tau_1)) O_2(\mathbf{w}(\tau_2)) \cdots e^{-\mathcal{A}_\Omega^{\mathbf{w}_0}[\mathbf{w}]/\hbar}. \end{aligned} \tag{7.7}$$

By adding and subtracting the trial action (7.5) to the full action in the Boltzmann factor of expression (7.3), we obtain

$$Z^{\mathbf{w}_0} = (2\pi\hbar)^d \oint \mathcal{D}^{2d}w\, \delta(\mathbf{w}_0 - \overline{\mathbf{w}(\tau)})\, e^{-\mathcal{A}_\Omega^{\mathbf{w}_0}[\mathbf{w}]/\hbar} \exp\left\{-\left(\mathcal{A}[\mathbf{w}] - \mathcal{A}_\Omega^{\mathbf{w}_0}[\mathbf{w}]\right)/\hbar\right\}. \tag{7.8}$$

With the definition (7.7), the right-hand side of this equation can be written as expectation value of the exponential function containing the perturbation $\mathcal{A}[\mathbf{w}] - \mathcal{A}_\Omega^{\mathbf{w}_0}[\mathbf{w}] \equiv \mathcal{A}_{\text{int}}[\mathbf{w}]$:

$$Z^{\mathbf{w}_0} = Z_\Omega^{\mathbf{w}_0} \left\langle e^{-\mathcal{A}_{\text{int}}[\mathbf{w}]/\hbar} \right\rangle_\Omega^{\mathbf{w}_0}. \tag{7.9}$$

With the help of the Jensen-Peierls inequality,

$$\left\langle e^{-O} \right\rangle \geq e^{-\langle O \rangle}, \tag{7.10}$$

we can estimate Eq. (7.9) by

$$Z^{\mathbf{w}_0} \geq Z_\Omega^{\mathbf{w}_0} e^{-\langle \mathcal{A}_{\rm int}[\mathbf{w}]/\hbar \rangle_\Omega^{\mathbf{w}_0}}. \tag{7.11}$$

Since the restricted partition functions are related to the effective classical Hamiltonians via

$$Z^{\mathbf{w}_0} = e^{-\beta H_{\rm eff}(\mathbf{w}_0)}, \qquad Z_\Omega^{\mathbf{w}_0} = e^{-\beta H_{{\rm eff},\Omega}(\mathbf{w}_0)}, \tag{7.12}$$

the inequality (7.11) can be written as

$$H_{\rm eff}(\mathbf{w}_0) \leq H_{{\rm eff},\Omega}(\mathbf{w}_0) + \frac{1}{\hbar\beta} \langle \mathcal{A}_{\rm int}[\mathbf{w}] \rangle_\Omega^{\mathbf{w}_0} \equiv \mathcal{H}_\Omega^{(1)}(\mathbf{w}_0). \tag{7.13}$$

We express the action $\mathcal{A}_{\rm int}[\mathbf{w}]$ as a time integral over an interaction potential $V_{\rm int}(\mathbf{w}(\tau))$,

$$\mathcal{A}_{\rm int}[\mathbf{w}] = \int_0^{\hbar\beta} d\tau \, V_{\rm int}(\mathbf{w}(\tau)). \tag{7.14}$$

The invariance of the expectation value under time translations makes the time integral trivial and the expectation value of the action becomes

$$\langle \mathcal{A}_{\rm int}[\mathbf{w}] \rangle_\Omega^{\mathbf{w}_0} = \int_0^{\hbar\beta} d\tau \, \langle V_{\rm int}(\mathbf{w}(\tau)) \rangle_\Omega^{\mathbf{w}_0} = \hbar\beta \, \langle V_{\rm int}(\mathbf{w}) \rangle_\Omega^{\mathbf{w}_0}. \tag{7.15}$$

Thus the estimate $\mathcal{H}_\Omega^{(1)}(\mathbf{w}_0)$ can be written as

$$\mathcal{H}_\Omega^{(1)}(\mathbf{w}_0) = H_{{\rm eff},\Omega}(\mathbf{w}_0) + \langle V_{\rm int}(\mathbf{w}) \rangle_\Omega^{\mathbf{w}_0}. \tag{7.16}$$

This quantity is now optimized with respect to the set of parameters Ω_{ij} to yield the optimal upper bound for the effective classical Hamiltonian:

$$\frac{\partial \mathcal{H}_\Omega^{(1)}(\mathbf{w}_0)}{\partial \Omega_{ij}} \stackrel{!}{=} 0. \tag{7.17}$$

Let us denote the set of optimal parameters satisfying these $2d^2 + d$ equations as $\Omega_{ij}^{(1)}(\mathbf{w}_0)$. Inserting these results into (7.16), the optimal upper bound for the effective classical Hamiltonian is given by

$$\mathcal{H}^{(1)}(\mathbf{w}_0) = \mathcal{H}_{\Omega^{(1)}}^{(1)}(\mathbf{w}_0). \tag{7.18}$$

If more than one solution to the equations (7.17) exist, the smallest must be chosen, since the effective Hamiltonian (which can also be considered as a local free energy $F^{\mathbf{w}_0}$) must be minimal in the equilibrium state of the system. Should no solutions exist, the parameters are chosen from the flattest region, i.e. where $\mathcal{H}_{\Omega^{(1)}}^{(1)}(\mathbf{w}_0)$ depends *minimally* on the parameters Ω_{ij}. This is the principle of minimal sensitivity, which states that the best estimate possesses the least dependence of the variational parameters [51]. This is a conclusion of the independence of the exact effective classical Hamiltonian from these parameters.

The simplest case for the trial action (7.5) is the usual harmonic oscillator in one dimension

$$\mathcal{A}_\Omega^{p_0 x_0}[p,x] = \int_0^{\hbar\beta} d\tau \left\{ \frac{1}{2M}[p(\tau) - p_0]^2 + \frac{1}{2} M\Omega^2 [x(\tau) - x_0]^2 \right\}, \tag{7.19}$$

where only the potential contains a trial parameter Ω.

7.2 Variational Perturbation Theory to Any Order

A Taylor expansion of the exponential function in the expectation value of Eq. (7.9) in powers of the interaction $\mathcal{A}_{\rm int}[\mathbf{w}]$ makes it possible to systematically improve the variational approach. Since the summations of perturbative expansions truncated in different orders of perturbation can yield approximations for the effective classical Hamiltonian, which alternate around the exact result, the inequality (7.10) does not hold in general.

Performing the Taylor expansion, Eq. (7.9) becomes

$$Z^{\mathbf{w}_0} = Z_\Omega^{\mathbf{w}_0} \sum_{n=0}^{\infty} \frac{(-1)^n}{\hbar^n n!} \left\langle \left(\int_0^{\hbar\beta} d\tau\, V_{\rm int}(\mathbf{w}(\tau)) \right)^n \right\rangle_\Omega^{\mathbf{w}_0} . \tag{7.20}$$

This can be written in the exponential form

$$Z^{\mathbf{w}_0} = Z_\Omega^{\mathbf{w}_0} \exp\left\{ \sum_{n=1}^{\infty} \frac{(-1)^n}{\hbar^n n!} \left\langle \left(\int_0^{\hbar\beta} d\tau\, V_{\rm int}(\mathbf{w}(\tau)) \right)^n \right\rangle_{\Omega,c}^{\mathbf{w}_0} \right\}, \tag{7.21}$$

where the subscript c indicates as usual cumulants. The lowest cumulants are related to the full expectation values as follows:

$$\begin{aligned} \langle O_1(\mathbf{w}(\tau_1))\rangle_{\Omega,c}^{\mathbf{w}_0} &= \langle O_1(\mathbf{w}(\tau_1))\rangle_\Omega^{\mathbf{w}_0} , \\ \langle O_1(\mathbf{w}(\tau_1))O_2(\mathbf{w}(\tau_2))\rangle_{\Omega,c}^{\mathbf{w}_0} &= \langle O_1(\mathbf{w}(\tau_1))O_2(\mathbf{w}(\tau_2))\rangle_\Omega^{\mathbf{w}_0} - \langle O_1(\mathbf{w}(\tau_1))\rangle_\Omega^{\mathbf{w}_0} \langle O_2(\mathbf{w}(\tau_2))\rangle_\Omega^{\mathbf{w}_0} , \\ &\vdots \quad , \end{aligned} \tag{7.22}$$

where $O_i(\mathbf{w}(\tau_j))$ denotes any observable depending on position and momentum. Recalling the relations (7.12) between partition functions and effective classical Hamiltonians we obtain from (7.21) the effective classical Hamiltonian as a cumulant expansion:

$$H_{\rm eff}(\mathbf{w}_0) = -\frac{1}{\beta} \ln Z_\Omega^{\mathbf{w}_0} + \frac{1}{\beta} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{\hbar^n n!} \left\langle \left(\int_0^{\hbar\beta} d\tau\, V_{\rm int}(\mathbf{w}(\tau)) \right)^n \right\rangle_{\Omega,c}^{\mathbf{w}_0} . \tag{7.23}$$

Up to now, we did not make any approximation. The expansion on the right-hand side is an exact expression for the effective classical Hamiltonian for all components of Ω.

For systems with a nontrivial interaction, we are capable of calculating only some initial truncated part of the series (7.23), say up to the Nth order, leading to the approximate effective classical Hamiltonian

$$\mathcal{H}_\Omega^{(N)}(\mathbf{w}_0) = -\frac{1}{\beta} \ln Z_\Omega^{\mathbf{w}_0} + \frac{1}{\beta} \sum_{n=1}^{N} \frac{(-1)^{n+1}}{\hbar^n n!} \left\langle \left(\int_0^{\hbar\beta} d\tau\, V_{\rm int}(\mathbf{w}(\tau)) \right)^n \right\rangle_{\Omega,c}^{\mathbf{w}_0} . \tag{7.24}$$

This depends explicitly on the parameters Ω. Since the exact expression (7.23) is independent of Ω, the best approximation for $\mathcal{H}_\Omega^{(N)}(\mathbf{w}_0)$ should depend on Ω *minimally*. Thus the optimal solution will be found by determining the parameters from the $2d^2 + d$ conditions

$$\frac{\partial}{\partial \Omega_{ij}} \mathcal{H}_\Omega^{(N)}(\mathbf{w}_0) \stackrel{!}{=} 0. \tag{7.25}$$

Let us denote the optimal variational parameters to Nth order by $\Omega_{ij}^{(N)}(\mathbf{w}_0)$. Inserting these into Eq. (7.24) yields the optimal effective classical Hamiltonian $\mathcal{H}^{(N)}(\mathbf{w}_0)$.