Finite -Temperature Field Theory of Ultracold Gases

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Contents

Preface

Bosonic atoms cooled down to very low temperatures in the micro or nano Kelvin regime show features, which have fascinated experimental as well as theoretical physicists for decades. Matter wave coherence properties, vortices, effects of superfluid flow and collective excitations have been observed and theoretically studied. These macroscopic quantum phenomena occur below a critical temperature, where Bosons form a coherent quantum state called Bose-Einstein condensate (BEC).

This new state of matter has been predicted by Einstein in 1924 [1] for non-interacting gases, whose particles obey the Bose statistics [2]. Fourteen years later, London [3, 4] and Tisza [5] applied these ideas to the qualitative description of superfluid Helium. However, a quantitative agreement between experiment and theory failed because of the high density and strong interactions in Helium that prevent the formation of a real macroscopic condensate. That is why in Helium only 10 percent of the atoms reside in the coherent ground-state even at $T = 0$. This led to the search of weakly-interacting Bose gases with a higher condensate fraction. It took more than 70 years after their theoretical prediction until Bose-Einstein condensates were first realized experimentally in 1995 in dilute atomic gases for rubidium [6], sodium [7], and lithium [8, 9]. Based on advanced laser and evaporative cooling techniques research groups at MIT and JILA were able to produce condensates of more than 10^6 atoms. Their realization in the laboratory has enabled physicists to study fundamental quantum theory on large scales and was therefore rewarded with the Nobel price of physics in 2001.

Today Bose-Einstein physics has become a highly interdisciplinary field. The new area of quantum optics uses the coherence properties of the condensates to investigate the possibility of building matter wave lasers and components for quantum computers [10]. Even in nuclear and particle physics the long-range correlations of ultracold bosons have led to many applications in interferometry and heavy-ion reactions [11]. Bose condensates were also found in other systems. In condensed matter physics, superconductivity has been explained with the help of Bose condensed Cooper pairs [12] since the fifties of the last century. Bose-Einstein condensation of excitons [13] and magnons [14] has been predicted, however its experimental evidence is still pending.

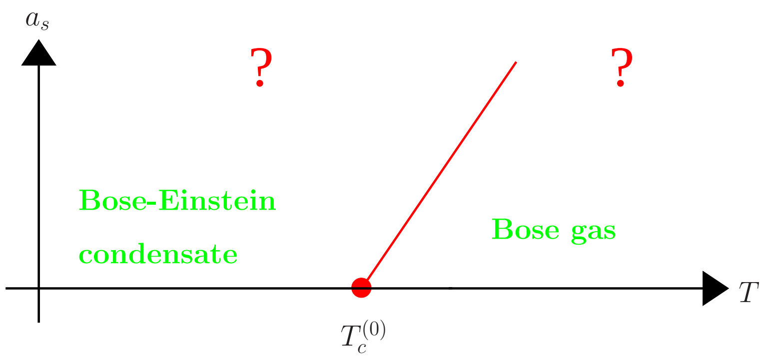


Figure 1: Finite temperature phase diagram in the a_s-T plane. The straight line indicates the prediction of classical field theory valid locally in the vicinity of $T_c^{(0)}$. The global structure of the whole phase diagram has not been investigated up to now.

Recently, another quantum state of matter has been discovered in which a boson gas is trapped near zero temperature in an optically generated lattice of standing laser beams [15]. Due to the tunnelling between adjoint potential wells and Bloch's theorem, the bosons lie in energy bands and behave similarly to free particles. Thus they form a superfluid phase which is delocalized over the lattice. As the wells deepen, a quantum phase transition occurs, localizing the atoms in the wells. The latter phase is analogous to a Mott insulator in electronic systems, and its properties were discussed theoretically in Refs. [16, 17]. With these experiments one enters a new field of physics with ultracold gases as one can bring a dilute gas of bosons into a strongly correlated regime where interaction induced correlations are dominant.

So far, most experimental work has dealt with BECs in magnetic traps and many theoretical investigations have been focused on such systems [18–20]. However, there are interesting unsolved theoretical problems also in homogeneous BECs with arbitrarily weak two-particle interactions. For instance, one important fundamental property of homogeneous BECs has been posing a long-time puzzle to field theorists: In which direction and by which amount does a repulsive interaction push the critical temperature? Although this problem appears to be very simple, it has been answered in many contradictory ways [21–43]. Most of these works are based on the classical limit of field theory, where only the zero Matsubara modes of the fields are included. With this approximation one was able to calculate the leading shift in the critical temperature which turned out to be linear in the s-wave scattering length a_s. In a finite temperature phase diagram of the $a_s - T$ plane, this corresponds to a linear curve starting at the critical temperature $T_c^{(0)}$ of a non-interacting gas where $a_s = 0$ as illustrated in Fig. 1. The next leading correction to this curve has been calculated recently by Arnold and co-workers

[31] by matching the full quantum field theory to the classical three dimensional theory. They obtained a second-order result in the shift of the critical temperature. However, their result is not satisfactory as it is valid only for small a_s and cannot reach the regime, where the Mott insulator transition occurs. Thus, up to now the full phase diagram (Fig. 1) is yet unknown.
The goal of this thesis is to fill this gap and to understand the critical properties of both, weakly interacting gases as well as strongly correlated optical boson lattices above and, especially, below the critical point. Our results will be obtained from an application of field-theoretical methods of many-body physics. In particular, we shall derive the full phase diagram in the $a_s - T$ plane.

In more detail we shall proceed as follows:

1. We shall calculate the temperature dependent diagrams for the vacuum and the self-energy in arbitrary dimensions d up to the second perturbative order. While for fermions this has been done a long time ago, there exists for weakly interacting bosons in the dilute limit only a calculation of the vacuum diagrams in exactly $d = 3$ dimensions by Huang et al. [44–46]. As a first application we want to investigate how nonzero Matsubara modes and therefore quantum effects influence the shift of the critical temperature and compare our results with that of the work of Arnold et al [31].

2. Next we shall investigate the entire phase diagram (Fig. 1). To this end we apply a systematic loop expansion, where the fluctuations of the bose fields around the condensate are taken into account order by order. This allows us to find the transition line in the whole temperature regime of the phase diagram [47, 48].

3. The same field-theoretical methods as mentioned above will then be applied to Bose-Einstein condensates trapped in optical lattices [47]. There the periodicity leads to a quasi-free behavior due to Bloch's theorem, which enables us to treat this system as effectively homogeneous. At $T = 0$, a quantum phase transition from the Mott insulator to the superfluid phase is found and compared with recent experimental data [15]. Furthermore, our calculations make theoretical predictions for the behavior of the system at finite temperatures that can be tested experimentally.

The work is organized as follows:

Part1: In Chapter 1 we review the properties of the ideal Bose gas at finite temperature and show how weak interactions can be included. Optical boson lattices are introduced as an experimental realization of the Bose-Hubbard model. In Chapter 2 the basic tools of thermal field theory such as Matsubara sum and effective action formalism are provided. We end this part by reviewing a new resummation technique called variational perturbation theory [49, 50] in Chapter 3. This powerful tool was developed in our group to turn weak-coupling divergent series into strong-coupling convergent ones and will be used in various contexts throughout this thesis (Chapter 7, Sections 9.2, 10.2).

Part2: Finite temperature perturbation theory up to the second order in the s-wave scattering length is carried out for temperatures above the critical point. According to the Feynman rules of many-body theory and Wick's theorem the Hugenholtz diagrams and their weights are obtained for the vacuum and self-energy in Chapter 4. In Chapters 5 and 6 we calculate these diagrams in dimensional regularization using the space-time representation of the free propagator. As a first application, we investigate in Chapter 7 the influence of non-zero Matsubara modes on the shift of the critical temperature in $d = 3$ dimensions.

Part3: A finite temperature loop expansion for the effective potential is performed in Chapter 8 with the help of the background method. We introduce the Popov approximation as a variationally resummed version of the Bogoliubov approximation for the effective potential in Chapter 9 and calculate the number of non-condensed atoms. We investigate the effective potential of dilute gases in the temperature regime below the critical point and compute the whole phase diagram with the help of variational perturbation theory (Chapter 10). Second, we calculate the phase diagram of optical boson lattices with the help of a hopping expansion. At $T = 0$ we compare our results with existing experimental values [15] and make theoretical predictions for the behavior at finite temperatures (Chapter 11).

Part I:

Physical and Mathematical Foundations

Chapter 1

Bose-Einstein Condensation

1.1 Ideal Bose Gas

In three dimensions, nature is made up of two different sorts of particles: fermions and bosons. Fermions obey the Pauli exclusion principle which states that two fermions cannot occupy the same quantum state. Bose particles in contrast, like to occupy the same quantum state, which can harbour an arbitrary number of them. In this section we review the ideal Bose gas at finite temperature in the grand-canonical ensemble. It is described by the fundamental Bose-Einstein distribution function:

$$\langle n(\mathbf{k})\rangle = \frac{1}{e^{\beta[\epsilon(\mathbf{k})-\mu]}-1} = \sum_{n=1}^{\infty} e^{-\beta[\epsilon(\mathbf{k})-\mu]n}\,, \tag{1.1}$$

where $\langle n(\mathbf{k})\rangle$ denotes the mean occupation number per single particle energy level $\epsilon(\mathbf{k})$, $\beta = 1/k_BT$ is the inverse temperature and μ the chemical potential. Because of the positivity of the mean occupation number, the chemical potential cannot exceed the ground-state energy $\epsilon(\mathbf{0})$ and is limited to values below $\epsilon(\mathbf{0})$).

Consider now N bosons in a finite box of volume V and impose periodic boundary conditions. The total particle number is obtained from (1.1) by summing over all possible quantum states:

$$N = \sum_{\mathbf{k}} \langle n(\mathbf{k})\rangle\,, \tag{1.2}$$

where we have assumed spin zero for the bosons. In the thermodynamic limit, where N and V tend to infinity while the particle density $n = N/V$ is kept fixed, the sum can be replaced by an integral over all continuous energy levels $\epsilon(\mathbf{k}) = \hbar^2\mathbf{k}^2/2m$:

$$\sum_{\mathbf{k}} \to \int_0^{\infty} g(\epsilon)d\epsilon\,, \tag{1.3}$$

where

$$g(\epsilon) = \frac{d\Sigma(\epsilon)}{d\epsilon} = \frac{2\pi V}{(2\pi\hbar)^3}\,(2m)^{3/2}\epsilon^{1/2} \tag{1.4}$$

is the density of states, which follows from the phase space volume Σ in three dimensions:

$$\Sigma(\epsilon) = \int_V d^3\mathbf{x} \int_{S_\epsilon} \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} = \frac{2\pi V}{(2\pi\hbar)^3}\,(2m)^{3/2} \int_0^\epsilon \sqrt{\epsilon'}\, d\epsilon' \,. \tag{1.5}$$

Consequently, the particle number (1.2) is given by the integral

$$N = \frac{2\pi V}{h^3}\,(2m)^{3/2} \int_0^\infty d\epsilon\, \frac{\sqrt{\epsilon}}{e^{\beta(\epsilon-\mu)} - 1} = \frac{V}{\lambda^3}\,\zeta_{3/2}(z) \,. \tag{1.6}$$

In the last step we have introduced the polylogarithmic function $\zeta_\nu(z)$ defined by

$$\zeta_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty d\epsilon\, \frac{\epsilon^{\nu-1}}{e^{\beta(\epsilon-\mu)} - 1} \stackrel{(1.1)}{=} \sum_{n=1}^{\infty} \frac{z^n}{n^\nu} \,, \tag{1.7}$$

the thermal wave length $\lambda = \sqrt{2\pi\hbar^2\beta/m}$ and the fugacity $z = e^{\beta\mu}$. For $z = 1$ the polylogarithmic function $\zeta_\nu(z)$ reaches its maximum value and reduces to Riemann's zeta function $\zeta_\nu(1)$.

The above semi-classical consideration neglects one important detail: Although for big volumes, the one-particle states are very dense, replacing the sum by an integral is not really justified. This approximation (1.3) is wrong in the limit $\epsilon \to 0$. For particles in a box with periodic boundary conditions, thus exists a ground-state described by the wave function $\phi_\mathbf{0} = 1/\sqrt{V}$, which does not contribute to the integral in (1.6) due to the vanishing of the density of states. The state $\mathbf{k} = \mathbf{0}$ plays an important role for the phenomenon of BEC. It must be treated separately, changing (1.6) to

$$N = N_{\text{ex}} + N_0 = \frac{V}{\lambda^3}\,\zeta_{3/2}(z) + \frac{z}{1-z} \,, \tag{1.8}$$

where N_{ex} is the number of particles in the excited states and N_0 is the number of particles residing in the ground state, obtained from (1.1) for the ground-state energy $\epsilon(\mathbf{0}) = 0$. This number diverges as soon as the chemical potential approaches the ground-state energy: $\mu = 0$. How can this be understood physically? As we work in the thermodynamic limit, we should better consider the particle density, which is a finite quantity:

$$n = n_{\text{ex}} + n_0 = \frac{1}{\lambda^3}\,\zeta_{3/2}(z) + \frac{N_0}{V} \,. \tag{1.9}$$

In the limit $z \to 1$, the polylogarithmic function and thus the density of excited particles reaches its maximum $n_{\rm ex}^{\rm max} = \zeta(3/2)/\lambda^3$, and $n_0 = N_0/V$ is a finite quantity given by $n_0 = n - n_{\rm ex}^{\rm max}$. If now particles are added to the system, they would immediately reside into the ground state, because $n_{\rm ex}$ has already reached its maximum. This macroscopic occupation of the ground-state level is called Bose-Einstein condensation (BEC) and n_0 is called the condensate density. The condition $n_0 = 0$ is equivalent to

$$n\lambda_c^3 = \zeta(3/2)\,, \tag{1.10}$$

and defines the critical temperature of BEC

$$T_c^{(0)} = \frac{2\pi\hbar^2}{mk_B}\left(\frac{n}{\zeta(3/2)}\right)^{2/3}\,, \tag{1.11}$$

with $\zeta(3/2) \approx 2.6124$. From the proportionality $n \sim \lambda^{-3}$ the relative part of the condensed atoms is given by

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c^{(0)}}\right)^{3/2}\,. \tag{1.12}$$

One of the most amazing features of BEC is that it occurs even in ideal gases just because of statistics, although we know from the theory of critical phenomena that long-range correlations are responsible for phase transitions. That is why one often refers to BEC as being driven by "statistical interactions". However, the above idealization is somewhat artificial and, of course, we have to include real interactions to see how the nature of Bose-Einstein condensation is affected.

1.2 Weak Interactions in Dilute Gases

Bosons interact with one another through binary collisions that are treated in the framework of scattering theory. In general, the interaction potential is very complicated and can only be computed in ab initio calculations. For an experimental realization of BEC it is important to circumvent three-particle collisions that would lead to a solidification of the gas. Therefore, the density of the gas is kept so low that the thermal wave length $\lambda \sim n^{-1/3}$ is much larger than the effective extension of the interaction potential. Thus, the true complicated interatomic potential can be replaced by an effective two-particle contact interaction [18]

$$V_{\rm int}(\mathbf{x},\mathbf{x}') = g\,\delta(\mathbf{x}-\mathbf{x}')\,, \tag{1.13}$$

where the coupling constant g is related to the the s-wave scattering length a_s via

$$g = \frac{4\pi\hbar^2 a_s}{m}\,. \tag{1.14}$$

This delta potential has to be interpreted for $a_s > 0$ as a repulsive hard-core potential that prevents mutual penetration of the atoms. In second quantization the most general many-body action describing bosons of a grand-canonical ensemble with a two-particle interaction $V_{\rm int}(\mathbf{x},\mathbf{x}')$ reads in imaginary-times (see Section 2.1):

$$\mathcal{A}[\psi(\mathbf{x},\tau),\psi^*(\mathbf{x},\tau)] = \int_0^{\hbar\beta} d\tau \int d^dx \, \{\psi^*(\mathbf{x},\tau)[\hbar\partial_\tau + h(\mathbf{x}) - \mu]\psi(\mathbf{x},\tau) \tag{1.15}$$
$$+\frac{1}{2}\int_0^{\hbar\beta} d\tau \int d^dx \int d^dx' \psi(\mathbf{x},\tau)\psi(\mathbf{x}',\tau)V_{\rm int}(\mathbf{x},\mathbf{x}')\psi^*(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau)\}\,,$$

where $h(\mathbf{x})$ denotes the one-particle Hamilton operator

$$h(\mathbf{x}) = -\frac{\hbar^2}{2m}\Delta + V_{\rm ext}(\mathbf{x}) \tag{1.16}$$

with an arbitrary external potential $V_{\rm ext}(\mathbf{x})$. Including the interaction term (1.13), we get

$$\mathcal{A}[\psi(\mathbf{x},\tau),\psi^*(\mathbf{x},\tau)] = \int_0^{\hbar\beta} d\tau \int d^dx \, \{\psi^*(\mathbf{x},\tau)[\hbar\partial_\tau + h(\mathbf{x}) - \mu]\psi(\mathbf{x},\tau)$$
$$+\frac{g}{2}\psi(\mathbf{x},\tau)^2\psi^*(\mathbf{x},\tau)^2\}\,. \tag{1.17}$$

In a typical BEC with a_s of the order of Å and particle distances of a few thousand Å, the gas parameter $a_s n^{1/3} \sim a_s\lambda$ is very small, which allows to describe the condensate as a weakly interacting gas. In this weak-coupling regime, where the ratio γ

$$\gamma = \frac{\epsilon_{\rm int}}{\epsilon_{\rm kin}} = 8\pi a_s n^{1/3} \tag{1.18}$$

between the interaction energy $\epsilon_{\rm int} = gn$ and the kinetic energy $\epsilon_{\rm kin} = \hbar^2 n^{2/3}/2m$ is small, we are able to treat the interaction term in (1.17) in the framework of perturbation theory (see Part 2). Note that this is based on the assumption $\lambda \sim n^{-1/3}$, which is in particular true near $T_c^{(0)}$. For the description of the condensate at lower temperatures the density and thus the gas parameter increases and we have to use a different approach (see Part 3). From (1.18) we see that there is another possibility to reach the strong-coupling regime, namely by increasing the scattering length a_s. This is indeed possible by using a so-called Feshbach resonance [51]. This has been realized recently in ^{85}Rb, where the scattering length a_s has been tuned over several orders of magnitude and a collapse of the condensate has been observed. In the next section we describe a third, entirely different approach for reaching the strong correlated regime.

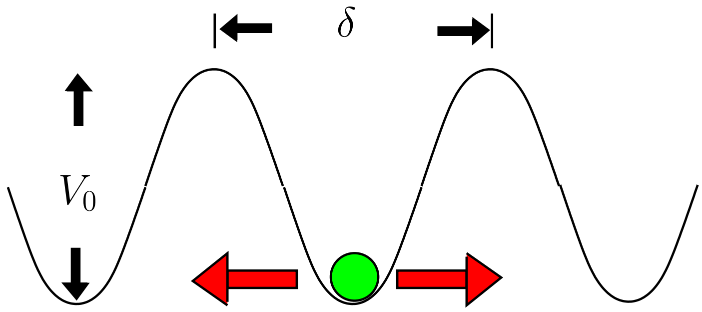


Figure 1.1: Potential landscape build up from crossing laser beams

1.3 Strong Correlations in Optical Boson Lattices

A fascinating field in the physics of BEC is the possibility to store single atoms in a periodic optical lattice potential of lattice spacing δ:

$$V_{\rm lat}(\mathbf{x}) = V_0 \sum_{i=1}^{d} \sin(q_i x_i)^2 \,, \quad q_i = \pi/\delta \,. \tag{1.19}$$

Such a potential landscape is created by using a standing wave interference pattern of two counter propagating laser beams where the lattice spacing δ equals half of the laser wave length $\lambda = 2\delta$. There, neutral atoms are stored due to interactions between the light field of a laser beam and the induced dipole moment of the atoms. The wave vector $\mathbf{q}$ defines the recoil energy $E_r = \hbar^2\mathbf{q}^2/2m$. The Hamiltonian for interacting bosonic particles (1.13) in such an external trapping potential reads

$$H = \int d^3x \left\{ \psi^\dagger(\mathbf{x},t) \left[-\frac{\hbar^2}{2m}\Delta + V_{\rm lat}(\mathbf{x}) - \mu \right] \psi(\mathbf{x},t) + \frac{g}{2}\, \psi(\mathbf{x},t)^2 \psi^\dagger(\mathbf{x},t)^2 \right\} \,, \tag{1.20}$$

where $\psi(\mathbf{x},t), \psi^\dagger(\mathbf{x},t)$ are the boson field operators. Characteristic for particles in an optical lattice is the emergence of a band structure. The wave function of a single particle in a periodic lattice potential is best described by so-called Wannier functions [52]. They constitute an orthogonal and normalized set of wave functions that are maximally localized at individual lattice sites.

1.3.1 Bose-Hubbard Hamiltonian

For low temperatures it is justified to assume that all particles move only in the lowest band, so that the field operators $\psi(\mathbf{x},t)$ can be expanded in the basis of Wannier functions $w(\mathbf{x}-\mathbf{x}_i)$ of the lowest band:

$$\psi(\mathbf{x},t) = \sum_i a_i(t) w(\mathbf{x}-\mathbf{x}_i) \,, \tag{1.21}$$

where $a_i(t)$ is the particle annihilation operator acting on the ith lattice site in the Heisenberg picture. For $\psi^*(\mathbf{x},t)$ the corresponding expansion coefficient is the creation operator $a_i^*(t)$. Both operators obey the canonical equal time commutation relation for bosons $[a_i(t), a_j^*(t)] = \delta_{ij}$. With this expansion the Hamilton operator (1.20) reduces to the famous Bose-Hubbard Hamiltonian [16]:

$$H = -J \sum_{<i,j>} a_i^*(t) a_j(t) - \mu \sum_i n_i(t) + \frac{U}{2} \sum_i n_i(t)(n_i(t)-1)\,, \tag{1.22}$$

where the particle operator $n_i(t) = a_i^*(t)a_i(t)$ counts the number of bosons on the ith site. The first term describes the kinetic energy that delocalizes each atom over the lattice through tunnelling. Here the corresponding sum includes only tunnelling between neighboring lattice sites. It's strength is given by the tunnelling matrix element

$$J = -\int d^3x\, w(\mathbf{x}-\mathbf{x}_i) \left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{lat}}(\mathbf{x}) \right) w(\mathbf{x}-\mathbf{x}_j)\,. \tag{1.23}$$

The second term with the chemical potential μ just acts as a Lagrangian multiplier to fix the mean number of particles in the grand-canonical potential. The last term of (1.22) describes the interaction between two atoms on a single lattice site with the interaction strength

$$U = g \int |w(\mathbf{x}-\mathbf{x}_i)|^4\, d^3x\,. \tag{1.24}$$

For $a_s > 0$ the interaction is repulsive and tends to localize the atoms to their lattice sites. Thus the first and last term in (1.22) compete with each other. In the experiment both parameters can be changed by varying the potential depth V_0 of the optical lattice potential (1.19). If the potential depth V_0 is increased the tunnelling barrier between neighboring lattice sites is raised and thus J decreases. At the same time the on-site interaction U increases, because of the tighter confinement of the wave function on a lattice site. In analogy to condensed matter physics a state where the potential (1.19) is so high that all atoms are localized at individual lattice sites is called Mott insulator. In the opposite limit when the tunnelling matrix element dominates the Bose-Hubbard Hamiltonian (1.22) the atoms are in the superfluid phase and are delocalized over the whole lattice.

1.3.2 Tight Binding Approximation

If the individual potential wells are deep, i.e., $V_0 \gg E_r$, the single particle Wannier functions $w(\mathbf{x}-\mathbf{x}_i)$ in the nearly harmonic wells are given by oscillator ground-state wave functions at the lattice sites with size $a_0 = \sqrt{\hbar/M\omega_0}$ and energy $\hbar\omega_0 \approx 2E_r\,(V_0/E_r)^{1/2}$.

Due to the low temperatures we can restrict our calculations to the lowest energy band arising from Bloch's theorem, which reads, up to a trivial additive constant,

$$\epsilon(\mathbf{k}) = 2J \sum_{i=1}^{3} [1 - \cos(k_i \delta)] \,. \tag{1.25}$$

This standard textbook result is valid for an arbitrary shaped periodic potential and follows from simple perturbative calculations. The tight-binding approximation shows that the width of the band $4J$ depends on the tunnelling strength (1.23), which can be calculated from the exact result for the width of the lowest band [52]:

$$J = \frac{4}{\sqrt{\pi}} E_r \left(\frac{V_0}{E_r}\right)^{3/4} \exp\left[-2\left(\frac{V_0}{E_r}\right)^{1/2}\right] . \tag{1.26}$$

The interaction strength U can be obtained from (1.24) by taking $w(\mathbf{x})$ as the Gaussian ground state in the nearly harmonic oscillator potentials [17, 52]:

$$U = \frac{a_s}{a_0} \frac{2\hbar\omega_0}{\sqrt{2\pi}} = \frac{2\pi a_s}{\lambda} \sqrt{\frac{8}{\pi}} E_r \left(\frac{V_0}{E_r}\right)^{3/4} . \tag{1.27}$$

1.3.3 Superfluid-Mott Insulator Transition

Researchers from the Max Planck institute for quantum optics in Garching, Germany were able to transform a dilute gas of cold atoms from a superfluid to a Mott insulator and back again simply by varying the intensity of the laser beam.The experimental optical lattice of Ref. [15] is made of laser beams with wavelength $\lambda = 2\delta$=852 nm and contains about 2×10^5 atoms ^{87}Rb with $a_s \approx 4.76$ nm [18]. Its energy scale is $E_r \approx \hbar \times 20\,\text{kHz}$ $\approx k_B \times 150$ nK and V_0/E_r is raised from 12 to 22. In this range, J/E_r drops from 0.014 to 0.002, U/E_r increases from 0.36 to 0.57, $\hbar\omega_0/E_r$ increases from 0.36 to 0.57.

Expanding the small-$\mathbf{k}$ behavior of the band energy (1.25) as $\hbar^2\mathbf{k}^2/2M_{\text{eff}} + \ldots$, the band width $4J$ defines an effective mass M_{eff} of the particles $M_{\text{eff}} = \hbar^2/2J\delta n^2$. We already mentioned in the last section that in a typical BEC the gas parameter $a_s n^{1/3}$ is very small. For the particles tightly bound in an optical lattice, however, $a_{\text{eff}}\, n^{1/3} = \gamma/8\pi$ can be made quite large. In the experiment [15] for temperatures near zero we have $\gamma = U/J = 0.0248 \exp(2\sqrt{V_0/E_r})$, so that the increase of the potential depth V_0/E_r from 12 to 22 raises $a_{\text{eff}} n^{1/3}$ from 1 to 11.7. The phase transition between the two states occured around $V_0 \approx 13E_r$. To find out which phase is present they released the atoms from the trap and looked for the interference pattern which is present in the superfluid phase and absent in the Mott insulator regime.

Above the quantum phase transition, they observed a gap in the excitation energies of the bosons, which pins the atoms to their potential wells. Expressed differently, the Goldstone modes of translations have become massive and the associated phase fluctuations decoherent, in accordance with the criterion found in Ref. [53]. For increasing temperatures, we expect the critical $a_{\text{eff}}n^{1/3}$ to decrease until it hits zero as T reaches roughly the free BEC critical temperature (1.11). In the above experiment where V_0/E_r is raised from 12 to 22, the temperature $T_c^{(0)}$ drops from 14.2 nK to 1.93 nK, implying that $T_c^{(0)}/E_r$ drops from 0.094 to 0.013. Hence J, and k_BT are much smaller than $\hbar\omega_0$, so that we can ignore all higher bands and the tight-binding approximation is justified.

Chapter 2

Thermal Field Theory

This chapter provides the basic field-theoretic methods of many-body theory that are used extensively throughout the thesis. In fact, there are two different approaches to field theory, the operator formalism and the functional integral formalism. All thermodynamic properties at finite temperature and non-zero chemical potential follow from the grand-canonical partition function, which is defined by a functional integral. As a first example we calculate the grand-canonical potential and the Green function of a free Bose gas for temperatures above the critical point of BEC in Section 2.1. Afterwards we introduce in Section 2.2 the effective action as a thermodynamic potential that describes the behavior of many-body systems below the phase transition.

2.1 Imaginary Time Formalism

In many-body theory [54] the problem is to evaluate the grand-canonical partition function

$$\mathcal{Z} \;=\; \oint \mathcal{D}\psi \oint \mathcal{D}\psi^* \exp\left\{-\frac{1}{\hbar}\mathcal{A}[\psi^*,\psi]\right\} , \tag{2.1}$$

where $\mathcal{A}[\psi^*,\psi]$ is the euclidian action (1.17) for bosons. Here the circle of the integral indicates that the integration has to be performed over all periodic fields

$$\psi(\mathbf{x},0) = \psi(\mathbf{x},\hbar\beta) , \qquad \psi^*(\mathbf{x},0) = \psi^*(\mathbf{x},\hbar\beta) \tag{2.2}$$

in the imaginary time $\tau \in [0,\hbar\beta]$. Note that for fermions the fields are anti-periodic in the imaginary time τ.

2.1.1 Free Partition Function

We now consider the quantum statistical partition function

$$\mathcal{Z}^{(0)} = \oint \mathcal{D}\psi \oint \mathcal{D}\psi^* e^{-\frac{1}{\hbar}\mathcal{A}^{(0)}[\psi,\psi^*]} \tag{2.3}$$

for an interaction-free Bose gas, which is described by the euclidian action (1.17) for $g = 0$:

$$\mathcal{A}^{(0)}[\psi^*(\mathbf{x},\tau),\psi(\mathbf{x},\tau)] = \int_0^{\hbar\beta} d\tau \int d^d x\, \psi^*(\mathbf{x},\tau)\, [\hbar\partial_\tau + h(\mathbf{x}) - \mu]\, \psi(\mathbf{x},\tau)\,. \tag{2.4}$$

A common way to compute such a functional integral is to expand the bosonic fields with respect to one-particle wave functions $\psi_{\mathbf{k}}(\mathbf{x})$ which are chosen to be eigenfunctions of the one-particle Hamilton operator (1.16):

$$h(\mathbf{x})\psi_{\mathbf{k}}(\mathbf{x}) = \epsilon(\mathbf{k})\psi_{\mathbf{k}}(\mathbf{x})\,. \tag{2.5}$$

Because of the periodicity of the bosonic fields with respect to the imaginary times τ in (2.2) we also perform a so-called Matsubara decomposition with respect to τ:

$$\psi(\mathbf{x},\tau) = \sum_{\mathbf{k}}\sum_m c_{\mathbf{k}m}\psi_{\mathbf{k}}(\mathbf{x})e^{-i\omega_m\tau}\,, \qquad \psi^*(\mathbf{x},\tau) = \sum_{\mathbf{k}}\sum_m c^*_{\mathbf{k}m}\psi^*_{\mathbf{k}}(\mathbf{x})e^{i\omega_m\tau}\,. \tag{2.6}$$

The expansion coefficients $c_{\mathbf{k}m}$ and $c^*_{\mathbf{k}m}$ are complex numbers. The periodicity of the fields (2.2) leads to the condition $\exp(-i\hbar\beta\omega_m) = 1$, which can be full-filled with the choice

$$\omega_m = \frac{2\pi m}{\hbar\beta}\,, \qquad m = \pm 0, 1, 2, \ldots\,. \tag{2.7}$$

These frequencies are called Matsubara frequencies. Inserting (2.6) into (2.4), we take into account (2.5) and use the orthogonality relations

$$\int_0^{\hbar\beta} e^{i(\omega_m-\omega_{m'})\tau} = \hbar\beta\,\delta_{m,m'}\,, \qquad \int d^d x\, \psi^*_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}'}(\mathbf{x}) = \delta_{\mathbf{k},\mathbf{k}'} \tag{2.8}$$

to obtain for the euclidian action:

$$\mathcal{A}^{(0)}[\psi^*(\mathbf{x},\tau),\psi(\mathbf{x},\tau)] = \sum_{\mathbf{k}}\sum_m c^*_{\mathbf{k}m}c_{\mathbf{k}m}\left[-i\hbar\omega_m + \epsilon(\mathbf{k}) - \mu\right]\,. \tag{2.9}$$

A summation over all periodic fields $\psi(\mathbf{x},\tau)$ and $\psi^*(\mathbf{x},\tau)$ corresponds to a summation over all expansion coefficients in (2.6), thus the functional measure becomes a product of simple integrals over $c_{\mathbf{k}m}$ and $c^*_{\mathbf{k}m}$:

$$\oint \mathcal{D}\psi(\mathbf{x},\tau)\mathcal{D}\psi^*(\mathbf{x},\tau) \quad\longrightarrow\quad \prod_{\mathbf{k}}\prod_{m=-\infty}^{\infty}\int dc^*_{\mathbf{k}m}\int dc_{\mathbf{k}m}N_{\mathbf{k}m} \tag{2.10}$$

with the normalization constant $N_{\mathbf{k}m} = \beta/2\pi$ [49]. Thus the partition function (2.3) is given by

$$\mathcal{Z}^{(0)} = \prod_{\mathbf{k}}\prod_{m=-\infty}^{\infty}\frac{\beta}{2\pi}\int dc^*_{\mathbf{k}m}\int dc_{\mathbf{k}m}e^{-\beta c^*_{\mathbf{k}m}c_{\mathbf{k}m}[-i\hbar\omega_m+\epsilon(\mathbf{k})-\mu]}\,. \tag{2.11}$$

We decompose the complex expansion coefficients $c_{\mathbf{k}m}, c^*_{\mathbf{k}m}$ into their real and imaginary parts

$$c_{\mathbf{k}m} = \mathrm{Re}\, c_{\mathbf{k}m} + i\mathrm{Im}\, c_{\mathbf{k}m}\,, \qquad c^*_{\mathbf{k}m} = \mathrm{Re}\, c_{\mathbf{k}m} - i\mathrm{Im}\, c_{\mathbf{k}m}\,, \tag{2.12}$$

and apply the rules for a two-dimensional coordinate transformation

$$\int dc^*_{\mathbf{k}m} \int dc_{\mathbf{k}m} = 2 \int d\mathrm{Re}\, c^*_{\mathbf{k}m} \int d\mathrm{Im}\, c_{\mathbf{k}m} \tag{2.13}$$

to perform the complex Gaussian integrals in (2.11), yielding

$$\mathcal{Z}^{(0)} = \prod_{\mathbf{k}} \prod_{m=-\infty}^{\infty} \frac{1}{-i\hbar\omega_m + \epsilon(\mathbf{k}) - \mu}\,. \tag{2.14}$$

From this we obtain the grand-canonical potential of thermodynamics

$$\Omega^{(0)} = -\frac{1}{\beta} \ln \mathcal{Z}^{(0)} = \frac{1}{\beta} \sum_{\mathbf{k}} \sum_{m=-\infty}^{\infty} \ln[-i\hbar\omega_m + \epsilon(\mathbf{k}) - \mu]\,. \tag{2.15}$$

Now we calculate the sum over the Matsubara frequencies by applying the bosonic Poisson formula (A.15).

At first, we rewrite the Matsubara sum in (2.15) in a more convenient way:

$$M = 2 \sum_{m=-\infty}^{\infty} \ln[-i\hbar\omega_m + \epsilon(\mathbf{k}) - \mu] = \sum_{m=-\infty}^{\infty} \ln\left[\hbar^2\omega_m^2 + E(\mathbf{k})^2\right]\,, \tag{2.16}$$

where we introduced the short-hand notation $E(\mathbf{k}) = \epsilon(\mathbf{k}) - \mu$. Second, we apply the Poisson formula (A.15) to obtain

$$M = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dx \ln\left[\frac{4\pi^2 x^2}{\beta^2} + E(\mathbf{k})^2\right] e^{-2\pi i m x} \tag{2.17}$$

and replace the logarithm via identity (B.5) to arrive at

$$\begin{aligned} M &= \sum_{m=-\infty}^{\infty} \left(-\frac{\partial}{\partial z}\right) \left\{ \frac{1}{\Gamma(z)} \int_0^{\infty} d\tau \tau^{z-1} e^{-E(\mathbf{k})^2\tau} \right. \\ &\quad \left. \times \int_{-\infty}^{\infty} dx \exp\left(\frac{4\pi^2\tau x^2}{\beta^2} - 2\pi i m x\right) \right\}\Bigg|_{z=0}\,. \end{aligned} \tag{2.18}$$

The x integral can be calculated via quadratic completion, yielding:

$$M = \frac{\beta}{2\sqrt{\pi}} \sum_{m=-\infty}^{\infty} \left(-\frac{\partial}{\partial z}\right) \left\{ \frac{1}{\Gamma(z)} \int_0^{\infty} d\tau \tau^{z-\frac{3}{2}} \exp\left[-E(\mathbf{k})^2\tau - \frac{\beta^2 m^2}{4\tau}\right] \right\}\Bigg|_{z=0}. \tag{2.19}$$

At $z = 0$ the Laurent expansion of the Gamma function $\Gamma(z)$ reads [55]

$$\Gamma(z) = \frac{1}{z} + O(z^0)\,. \tag{2.20}$$

Thus we obtain the relationship

$$\left(-\frac{\partial}{\partial z}\right)\frac{f(z)}{\Gamma(z)}\bigg|_{z=0} = \left(-\frac{\partial}{\partial z}\right)\{z\,[f(0)+f(0)z+\ldots]\}\bigg|_{z=0} = -f(0)\,, \tag{2.21}$$

which is valid for functions $f(z)$ that are analytic at $z = 0$. So we obtain for the sum in (2.19):

$$M \;=\; \frac{-\beta}{2\sqrt{\pi}}\sum_{m=-\infty}^{\infty}\int_0^\infty d\tau\tau^{-\frac{3}{2}}\exp\left[-E(\mathbf{k})^2\tau - \frac{\beta^2 m^2}{4\tau}\right]\,. \tag{2.22}$$

Now we split the sum as follows:

$$M \;=\; I_0 + I_m \tag{2.23}$$

with

$$I_0 = -\frac{\beta}{2\sqrt{\pi}}\int_0^\infty d\tau\tau^{-\frac{3}{2}}e^{-E(\mathbf{k})^2\tau} \tag{2.24}$$

and

$$I_m = -2\sum_{m=1}^{\infty}\frac{\beta}{2\sqrt{\pi}}\int_0^\infty d\tau\tau^{-\frac{3}{2}}\exp\left[-E(\mathbf{k})^2\tau - \frac{\beta^2 m^2}{4\tau}\right]\,. \tag{2.25}$$

The contribution I_0 gives directly

$$I_0 \;=\; \frac{-\beta}{2\sqrt{\pi}}\int_0^\infty d\tau\tau^{-\frac{3}{2}}e^{-E(\mathbf{k})^2\tau} = \beta E(\mathbf{k})\,. \tag{2.26}$$

The remaining τ-integral in I_m can be found in [55], yielding

$$I_m \;=\; -\frac{2\sqrt{2\beta E(\mathbf{k})}}{\sqrt{\pi}}\sum_{m=1}^{\infty}\frac{1}{\sqrt{m}}K_{-\frac{1}{2}}(\beta m E(\mathbf{k})) = -2\sum_{m=1}^{\infty}\frac{e^{-\beta E(\mathbf{k})m}}{m}\,, \tag{2.27}$$

where we used the fact that the Bessel function $K_{-1/2}(z)$ can be related to the exponential function [55] via

$$K_{-1/2}(z) = \sqrt{\frac{\pi}{2z}}\,e^{-z}\,. \tag{2.28}$$

If we consider the geometric sum

$$f'(x) := \sum_{m=1}^{\infty} x^{m-1} = \sum_{m=0}^{\infty} x^m = \frac{1}{1-x}\,, \tag{2.29}$$

an integration with respect to x yields together with $f(0) = 0$

$$f(x) \quad = \quad \sum_{m=1}^{\infty} \frac{x^m}{m} = -\ln(1-x)\,. \tag{2.30}$$

Applying this result to (2.27) gives us the contribution I_m:

$$I_m = 2\ln[1 - e^{-\beta E(\mathbf{k})}]\,. \tag{2.31}$$

So the final result for the Matsubara sum reads:

$$M = \beta E(\mathbf{k}) + 2\ln[1 - e^{-\beta E(\mathbf{k})}]\,. \tag{2.32}$$

Inserting this result in (2.15) yields for the grand-canonical potential

$$\Omega^{(0)} = \frac{1}{2}\sum_{\mathbf{k}} [\epsilon(\mathbf{k}) - \mu] + \frac{1}{\beta}\sum_{\mathbf{k}} \ln\left\{1 - e^{-\beta[\epsilon(\mathbf{k}]-\mu)}\right\}\,. \tag{2.33}$$

The first part of this equation, the so-called vacuum contribution, does not depend on the temperature and diverges as soon as we sum over all possible wave vectors. However, we can ignore that contribution at the moment, because for $T > T_c$ this can be absorbed in the renormalization of the energy. Therefore we consider

$$\Omega^{(0)} = \frac{1}{\beta}\sum_{\mathbf{k}} \ln\left\{1 - e^{-\beta[\epsilon(\mathbf{k})-\mu]}\right\} \tag{2.34}$$

and differentiate this result with respect to the chemical potential to obtain the particle number

$$N = -\frac{\partial\Omega^{(0)}}{\partial\mu} = \sum_{\mathbf{k}} \frac{1}{e^{\beta[\epsilon(\mathbf{k})-\mu]} - 1}\,. \tag{2.35}$$

The sum goes over all possible states $\mathbf{k}$. Therefore we read off the average number of particles in the state $\mathbf{k}$:

$$\langle n(\mathbf{k})\rangle = \frac{1}{e^{\beta[\epsilon(\mathbf{k})-\mu]} - 1}\,, \tag{2.36}$$

which is nothing else but the famous Bose-Einstein distribution function (1.1). In Section 1.1 the equation (2.36) was the starting point for a thermodynamic discussion of a homogeneous BEC, where one replaces the sum over the wave vectors $\mathbf{k}$ by a continuous integral (1.3). For the grand-canonical potential (2.34) this results together with (1.7) in d dimensions to

$$\Omega^{(0)} = \frac{V}{\beta\lambda^d}\zeta_{d/2+1}(z) \tag{2.37}$$

The corresponding result for the particle density (1.6) has already been calculated in Section 1.1 in $d = 3$ dimensions.

2.1.2 Free Propagator

One of the most important quantities in nonrelativistic quantum field theory is the Green function defined as the ensemble average of the free, time-ordered product of field operators

$$G(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) = \langle T\left[\psi(\mathbf{x}_1, \tau_1)\psi^\dagger(\mathbf{x}_2, \tau_2)\right]\rangle\,, \tag{2.38}$$

where the ensemble average of an arbitrary function of the field operators is defined by

$$\langle f\left[\psi(\mathbf{x}_1, \tau_1)\psi^\dagger(\mathbf{x}_2, \tau_2)\right]\rangle = \frac{\mathrm{Tr}\, f\left[\psi(\mathbf{x}_1, \tau_1)\psi^\dagger(\mathbf{x}_2, \tau_2)\right] e^{-\beta(H-\mu N)}}{\mathrm{Tr}\, e^{-\beta(H-\mu N)}}\,. \tag{2.39}$$

Here H is the second-quantized Hamilton operator of the free system, N is the second quantized particle number operator and T the time-ordering operator, which is defined by

$$\begin{aligned} T\left[\psi(\mathbf{x}_1, \tau_1)\psi^\dagger(\mathbf{x}_2, \tau_2)\right] &= \Theta(\tau_1 - \tau_2)\psi(\mathbf{x}_1, \tau_1)\psi^\dagger(\mathbf{x}_2, \tau_2) \\ &\quad + \Theta(\tau_2 - \tau_1)\psi^\dagger(\mathbf{x}_2, \tau_2)\psi(\mathbf{x}_1, \tau_1)\,. \end{aligned} \tag{2.40}$$

A short calculation shows that the Green function (2.38) fulfills the inhomogeneous Schrödinger equation in imaginary times

$$\left[\hbar\partial_\tau + h(\mathbf{x}) - \mu\right] G(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) = \hbar\delta(\tau_1 - \tau_2)\delta^{(d)}(\mathbf{x}_1 - \mathbf{x}_2)\,, \tag{2.41}$$

where the first quantized one-particle Hamilton operator $h(\mathbf{x})$ is shifted by the chemical potential μ. One could consider this as a starting point for calculating the Green function, but we choose another approach as we want to get familiar with functional integrals. In the framework of functional integral quantization the definition of the Green function (2.38) is equivalent to

$$\begin{aligned} G(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) &= \langle \psi(\mathbf{x}_1, \tau_1)\psi^*(\mathbf{x}_2, \tau_2)\rangle \\ &= \frac{1}{\mathcal{Z}^{(0)}} \oint \mathcal{D}\psi(\mathbf{x}, \tau) \oint \mathcal{D}\psi^*(\mathbf{x}, \tau)\psi(\mathbf{x}_1, \tau_1)\psi^*(\mathbf{x}_2, \tau_2) e^{-\frac{1}{\hbar}\mathcal{A}^{(0)}[\psi, \psi^*]}\,, \end{aligned} \tag{2.42}$$

which is also referred to as the two-point correlation function. Now we use the Matsubara decomposition of the Bose fields (2.6) to get for the Green function:

$$G(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = \frac{1}{\mathcal{Z}^{(0)}}\prod_{\mathbf{k}}\prod_{m=-\infty}^{\infty}\frac{\beta}{2\pi}\sum_{\mathbf{k}'}\sum_{m'=-\infty}^{\infty}\sum_{\mathbf{k}''}\sum_{m''=-\infty}^{\infty}\psi_{\mathbf{k}'}(\mathbf{x}_1)\psi^*_{\mathbf{k}''}(\mathbf{x}_2) \tag{2.43}$$
$$\times e^{-i\omega_{m'}\tau_1}e^{i\omega_{m''}\tau_2}\int dc^*_{\mathbf{k}m}\int dc_{\mathbf{k}m}c^*_{\mathbf{k}''m''}c_{\mathbf{k}'m'}\exp\left\{-\beta c^*_{\mathbf{k}m}c_{\mathbf{k}m}\left[-i\hbar\omega_m+\epsilon(\mathbf{k})-\mu\right]\right\}\,.$$

For $(\mathbf{k}'m') \neq (\mathbf{k}''m'')$ the above integrals are odd in $c_{\mathbf{k}m}, c^*_{\mathbf{k}m}$ so that only diagonal integrals with $(\mathbf{k}'m') = (\mathbf{k}''m'')$ are nonzero:

$$G(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = \frac{1}{\mathcal{Z}^{(0)}}\sum_{\mathbf{k}'}\psi_{\mathbf{k}'}(\mathbf{x}_1)\psi^*_{\mathbf{k}'}(\mathbf{x}_2)\sum_{m'=-\infty}^{\infty}e^{i\omega_{m'}(\tau_2-\tau_1)}$$
$$\times\frac{\beta}{2\pi}\int dc^*_{\mathbf{k}'m'}\int dc_{\mathbf{k}'m'}c^*_{\mathbf{k}'m'}c_{\mathbf{k}'m'}\exp\left\{-\beta c^*_{\mathbf{k}'m'}c_{\mathbf{k}'m'}[-i\hbar\omega_{m'}+\epsilon(\mathbf{k}')-\mu]\right\}$$
$$\times\prod_{\mathbf{k}\neq\mathbf{k}'}\prod_{\substack{m=-\infty\\ m\neq m'}}^{\infty}\frac{\beta}{2\pi}\int dc^*_{\mathbf{k}m}\int dc_{\mathbf{k}m}\exp\left\{-\beta c^*_{\mathbf{k}m}c_{\mathbf{k}m}[-i\hbar\omega_m+\epsilon(\mathbf{k})-\mu]\right\}\,. \tag{2.44}$$

With help of the decomposition (2.12) and the transformation (2.13), we can solve the integrals to arrive at

$$G(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = \frac{1}{\mathcal{Z}^{(0)}}\sum_{\mathbf{k}'}\psi_{\mathbf{k}'}(\mathbf{x}_1)\psi^*_{\mathbf{k}'}(\mathbf{x}_2)\sum_{m'=-\infty}^{\infty}\frac{e^{-i\omega_{m'}(\tau_1-\tau_2)}}{\beta[-i\hbar\omega_{m'}+\epsilon(\mathbf{k})-\mu]^2}$$
$$\times\prod_{\mathbf{k}\neq\mathbf{k}'}\prod_{\substack{m=-\infty\\ m\neq m'}}^{\infty}\frac{1}{-i\hbar\omega_m+\epsilon(\mathbf{k})-\mu}\,. \tag{2.45}$$

If we now insert the result (2.14) we obtain

$$G(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = \frac{1}{\beta}\sum_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{x}_1)\psi^*_{\mathbf{k}}(\mathbf{x}_2)\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m(\tau_1-\tau_2)}}{-i\hbar\omega_m+\epsilon(\mathbf{k})-\mu}\,. \tag{2.46}$$

Of course, this expression shows nothing else than the Matsubara decomposition of the Green function

$$G(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = \frac{1}{\hbar\beta}\sum_{\mathbf{k}}\sum_{m=-\infty}^{\infty}G(\mathbf{k},m)\psi_{\mathbf{k}}(\mathbf{x}_1)\psi^*_{\mathbf{k}}(\mathbf{x}_2)e^{-i\omega_m(\tau_1-\tau_2)} \tag{2.47}$$

with the expansion coefficient:

$$G(\mathbf{k},m) = \frac{\hbar}{-i\hbar\omega_m+\epsilon(\mathbf{k})-\mu}\,. \tag{2.48}$$

It remains to calculate the Matsubara sum

$$S_{\mathbf{k}}\left(\tau_1-\tau_2\right)=\frac{1}{\beta}\sum_{m=-\infty}^{\infty}\frac{e^{-i\omega_m(\tau_1-\tau_2)}}{-i\hbar\omega_m+E(\mathbf{k})}\,. \tag{2.49}$$

This must be done by applying Poisson's formula (A.15), leading to

$$S_{\mathbf{k}}\left(\tau_1-\tau_2\right) \;=\; \frac{i}{2\pi}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}dx\frac{e^{-2\pi i(\tau_1-\tau_2+\hbar\beta n)/\hbar\beta}}{x+i\beta E(\mathbf{k})/2\pi}e^{-2\pi inx}\,. \tag{2.50}$$

The fundamental integral on the right hand side

$$I_{a,b}=\frac{i}{2\pi}\int_{-\infty}^{\infty}dx\frac{e^{-iax}}{x+ib}\,,\quad b>0 \tag{2.51}$$

is trivially evaluated. The denominator of the integrand has a singularity at $x=-ib$. For $a>0$, the integration contour on the real axis of the complex plane can be closed by a semicircle in the lower half plane and the residue theorem yields

$$I_{a,b}=\underset{x\,=\,-ib}{\mathrm{Res}}\;\frac{e^{-iax}}{x+ib}=e^{-ab}\,. \tag{2.52}$$

For $a<0$ the contour has to be closed in the upper half of the complex plane. As the integrand has no singularity there, the integral I_{ab} vanishes. Thus we find for all values of a and $b>0$:

$$I_{a,b}=\Theta(a)e^{-ab}\,. \tag{2.53}$$

Inserting this result in (2.49), the sum reads

$$S_{\mathbf{k}}(\tau_1-\tau_2)=\sum_{n=-\infty}^{\infty}\Theta(\tau_1-\tau_2+\hbar\beta n)e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1-\tau_2+\hbar\beta n)}\,. \tag{2.54}$$

For $(\tau_1-\tau_2)\in(0,\hbar\beta)$, the Heaviside function forces the sum to run only over positive n, so that we deal with a geometric series

$$S_{\mathbf{k}}(\tau_1-\tau_2)^+ \;=\; e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1-\tau_2)}\sum_{n=0}^{\infty}e^{-\beta E(\mathbf{k})n}=\frac{e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1-\tau_2-\hbar\beta/2)}}{2\sinh\beta E(\mathbf{k})/2}\,. \tag{2.55}$$

For $\tau_1-\tau_2\in(0,-\hbar\beta)$ a similar calculation leads to:

$$S_{\mathbf{k}}(\tau_1-\tau_2)^- \;=\; e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1-\tau_2)}\sum_{n=-1}^{\infty}e^{-\beta E(\mathbf{k})n}=\frac{e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1-\tau_2+\hbar\beta/2)}}{2\sinh\beta E(\mathbf{k})/2} \tag{2.56}$$

So for $(\tau_1 - \tau_2) \in (-\hbar\beta, +\hbar\beta)$ we get the final result

$$\begin{aligned} S_{\mathbf{k}}(\tau_1 - \tau_2) &= \Theta(\tau_1 - \tau_2)\, S_{\mathbf{k}}(\tau_1 - \tau_2)^+ + \Theta(\tau_2 - \tau_1) S_{\mathbf{k}}(\tau_1 - \tau_2)^- \\ &= \frac{\Theta(\tau_1 - \tau_2)\, e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1 - \tau_2 - \hbar\beta/2)} + \Theta(\tau_2 - \tau_1) e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1 - \tau_2 + \hbar\beta/2)}}{2\sinh \beta E(\mathbf{k})/2}\,, \end{aligned} \tag{2.57}$$

which leads to the Green function

$$\begin{aligned} G(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) &= \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{x}_1) \psi_{\mathbf{k}}^*(\mathbf{x}_2) \\ &\times \frac{\Theta(\tau_1 - \tau_2)\, e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1 - \tau_2 - \hbar\beta/2)} + \Theta(\tau_2 - \tau_1) e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1 - \tau_2 + \hbar\beta/2)}}{2\sinh \beta E(\mathbf{k})/2}\,. \end{aligned} \tag{2.58}$$

It is worth noting that the Green function is homogeneous with respect to the imaginary time.

So far we considered systems with an arbitrary one-particle Hamilton operator (1.16),where $V_{\rm ext}(\mathbf{x})$ is an arbitrary external potential. Now we restrict ourself to the free case $V_{\rm ext}(\mathbf{x}) = 0$, where the Green function (2.58) becomes also homogeneous in space, because the one-particle wave functions $\psi_{\mathbf{k}}(\mathbf{x}), \psi_{\mathbf{k}}^*(\mathbf{x})$ solving (2.5) represent plane waves

$$\psi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{x}}\,, \qquad \psi_{\mathbf{k}}^*(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{-i\mathbf{k}\mathbf{x}} \tag{2.59}$$

and the one-particle spectrum becomes $\epsilon(\mathbf{k}) = \hbar^2 \mathbf{k}^2/2m$. In this limit, we can replace the sum in (2.58) by an integral analogous to (1.3):

$$\begin{aligned} G(\mathbf{x}_1 - \mathbf{x}_2, \tau_1 - \tau_2) &= \int \frac{d^d\mathbf{k}}{(2\pi)^d}\, e^{i\mathbf{k}(\mathbf{x}_1 - \mathbf{x}_2)} \\ \times &\frac{\Theta(\tau_1 - \tau_2)\, e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1 - \tau_2 - \hbar\beta/2)} + \Theta(\tau_2 - \tau_1) e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau_1 - \tau_2 + \hbar\beta/2)}}{2\sinh \beta E(\mathbf{k})/2}\,. \end{aligned} \tag{2.60}$$

We end this section by specializing (2.60) to two important cases.

Special Case 1: Equal Arguments For equal arguments (2.60) simplifies to

$$G(\mathbf{0}, 0) = \int \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{e^{\beta E(\mathbf{k})/2}}{2\sinh \beta E(\mathbf{k})/2} = \int \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{e^{\beta E(\mathbf{k})} - 1}\,, \tag{2.61}$$

which is nothing else but the particle number (1.2), yielding with (1.6) in $d = 3$ dimensions:

$$G(\mathbf{0}, 0) = \frac{V}{\lambda^3}\, \zeta_{3/2}(z)\,, \tag{2.62}$$

where $z = e^{\beta\mu}$ denotes the fugacity.

Special Case 2: High Temperature Limit Consider the Matsubara sum in (2.46). For high temperatures $T \to \infty$, i.e. $\beta \to 0$, all Matsubara frequencies (2.7), except the zero mode $m = 0$, become infinite and thus give no contribution. As only the zero mode survives, we get from (2.46):

$$G(\mathbf{x}_1 - \mathbf{x}_2, 0) = \frac{2m}{\beta} \int \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{e^{i\mathbf{k}(\mathbf{x}_1 - \mathbf{x}_2)}}{(\hbar\mathbf{k})^2 - 2m\mu}\,, \qquad \beta \to 0\,. \tag{2.63}$$

2.2 Effective Action Formalism

In Section 2.1 we have calculated the grand-canonical potential of a free Bose gas above the critical temperature of BEC. Now we develop a formalism that allows to calculate thermodynamic quantities below T_c. In that case the condensation of bosons into their ground state means that the grand-canonical ensemble averages of the fields $\psi(\mathbf{x}, \tau)$, $\psi^*(\mathbf{x}, \tau)$ do not vanish. To describe such a nonzero ensemble average we have to couple the fields linearly to artificial current fields $j(\mathbf{x}, \tau)$, $j^*(\mathbf{x}, \tau)$. Thus we consider the action

$$\mathcal{A}[\psi, \psi^*; j, j^*] = \mathcal{A}[\psi, \psi^*] - \int_0^{\hbar\beta} \int d^dx \, [j^*(\mathbf{x}, \tau)\psi(\mathbf{x}, \tau) + \psi^*(\mathbf{x}, \tau) j(\mathbf{x}, \tau)] \tag{2.64}$$

and the resulting partition function

$$\mathcal{Z}[j^*, j] = \oint \mathcal{D}\psi \oint \mathcal{D}\psi^* e^{-\frac{1}{\hbar}\mathcal{A}[\psi,\psi^*;j,j^*]}\,. \tag{2.65}$$

The logarithm of this partition function yields the negative grand-canonical potential

$$W[j, j^*] = \ln \mathcal{Z}[j^*, j]\,. \tag{2.66}$$

From that we can calculate the ensemble averages of the fields

$$\Psi_j(\mathbf{x}_1, \tau_1) \equiv \Psi(\mathbf{x}_1, \tau_1)[j, j^*] = \frac{1}{\mathcal{Z}[j^*, j]} \oint \mathcal{D}\psi \oint \mathcal{D}\psi^* \psi(\mathbf{x}_1, \tau_1) e^{-\frac{1}{\hbar}\mathcal{A}[\psi,\psi^*;j,j^*]} \tag{2.67}$$

and

$$\Psi_j^*(\mathbf{x}_1, \tau_1) \equiv \Psi^*(\mathbf{x}_1, \tau_1)[j, j^*] = \frac{1}{\mathcal{Z}[j^*, j]} \oint \mathcal{D}\psi \oint \mathcal{D}\psi^* \psi^*(\mathbf{x}_1, \tau_1) e^{-\frac{1}{\hbar}\mathcal{A}[\psi,\psi^*;j,j^*]} \tag{2.68}$$

as functional derivatives of $W[j, j^*]$ with respect to the currents fields

$$\Psi_j(\mathbf{x}_1, \tau_1) = \hbar \frac{\delta W[j, j^*]}{\delta j^*(\mathbf{x}_1, \tau_1)}\,, \qquad \Psi_j^*(\mathbf{x}_1, \tau_1) = \hbar \frac{\delta W[j, j^*]}{\delta j(\mathbf{x}_1, \tau_1)}\,. \tag{2.69}$$

The index j of the fields indicates that these averages are of course functionals of the current fields and by inversion one could, in principle, get the currents back as functionals of the fields. We use (2.69) as a motivation to define the effective action $\Gamma[\Psi_j, \Psi_j^*]$ as a functional Legendre transformed of (2.66) with respect to the currents:

$$\Gamma[\Psi_j, \Psi_j^*] = W[j, j^*] - \frac{1}{\hbar}\int_0^{\hbar\beta}\int d^dx \left[j^*(\mathbf{x},\tau)\Psi_j(\mathbf{x},\tau) + \Psi_j^*(\mathbf{x},\tau)j(\mathbf{x},\tau)\right] . \tag{2.70}$$

The functional derivative of the effective action with respect to the fields yields the following Legendre identity:

$$\begin{aligned}\frac{\delta\Gamma[\Psi_j,\Psi_j^*]}{\delta\Psi_j^*(\mathbf{x}_1,\tau_1)} &= \int_0^{\hbar\beta}\int d^dx \left[\frac{\delta W[j,j^*]}{\delta j^*(\mathbf{x},\tau)}\frac{\delta j^*(\mathbf{x},\tau)}{\delta\psi_j^*(\mathbf{x}_1,\tau_1)} + \frac{\delta W[j,j^*]}{\delta j(\mathbf{x},\tau)}\frac{\delta j(\mathbf{x},\tau)}{\delta\psi_j^*(\mathbf{x}_1,\tau_1)}\right] \\ &\quad -\frac{1}{\hbar}\int_0^{\hbar\beta}\int d^dx \left[\frac{\delta j^*(\mathbf{x},\tau)}{\delta\Psi_j^*(\mathbf{x}_1,\tau_1)}\Psi_j(\mathbf{x},\tau) + \frac{\delta j(\mathbf{x},\tau)}{\delta\Psi_j^*(\mathbf{x}_1,\tau_1)}\Psi_j^*(\mathbf{x},\tau)\right] - \frac{1}{\hbar}j(\mathbf{x}_1,\tau_1) .\end{aligned} \tag{2.71}$$

Inserting the relationship (2.69) and doing the same calculation of (2.71) for the complex conjugated field shows that the currents can be obtained by functional derivatives of the effective action:

$$\frac{\delta\Gamma[\Psi_j,\Psi_j^*]}{\delta\Psi_j^*(\mathbf{x}_1,\tau_1)} = -\frac{1}{\hbar}j(\mathbf{x}_1,\tau_1) , \qquad \frac{\delta\Gamma[\Psi_j,\Psi_j^*]}{\delta\Psi_j(\mathbf{x}_1,\tau_1)} = -\frac{1}{\hbar}j^*(\mathbf{x}_1,\tau_1) . \tag{2.72}$$

Let us consider the physical limit in which the artificially introduced current fields vanish, i.e. $j(\mathbf{x}_1,\tau_1) \to 0$ and $j^*(\mathbf{x}_1,\tau_1) \to 0$. In this limit the effective action (2.70) coincides with the negative grand-canonical potential (2.66):

$$\Gamma[\Psi_0, \Psi_0^*] = W[0,0] = \ln \mathcal{Z} . \tag{2.73}$$

At the same time the ensemble averages (2.69) tend towards those physical fields Ψ_0 and Ψ_0^* that extremize the effective action

$$\left.\frac{\delta\Gamma[\Psi_j,\Psi_j^*]}{\delta\Psi_j^*(\mathbf{x}_1,\tau_1)}\right|_{\Psi_0,\Psi_0^*} = \left.\frac{\delta\Gamma[\Psi_j,\Psi_j^*]}{\delta\Psi_j(\mathbf{x}_1,\tau_1)}\right|_{\Psi_0,\Psi_0^*} = 0 . \tag{2.74}$$

This important observation enables us to formulate a general scheme for the description of our system below T_c:

- Compute the negative grand-canonical potential (2.66) from the partition function $\mathcal{Z}[j^*, j]$
- Perform a functional Legendre transform with respect to the currents to obtain the effective action (2.70) as a functional of the field averages.
- Extremize the effective action according to (2.74) to yield the grand-canonical potential $\Omega(T,\mu,V) = -\Gamma[\Psi_0,\Psi_0^*]/\beta$, which is now valid above and below T_c. From that follow all thermodynamic quantities above and below the critical point.

It is important to note that there exists a more efficient way to obtain the effective action, the so-called background method. This method will be elaborated in Part 3 of this thesis in the context of the finite temperature loop expansion.

Chapter 3

Variational Perturbation Theory

3.1 Motivation

Useful approximate information of real physical systems is gained, for instance, via perturbation expansions. They are based on the fact that quite often a physical quantity f can be exactly calculated for a special value g_0 of a coupling constant g. The whole function $f(g)$ is then determined perturbatively in the deviation $g - g_0$ from this special value g_0. For the following discussion we assume without loss of generality that $g_0 = 0$ and that the respective weak-coupling coefficients a_n are known up to some order N:

$$f_N(g) = \sum_{n=0}^{N} a_n g^n \, . \tag{3.1}$$

A prominent example for such a weak-coupling series is the anomalous magnetic moment of the electron $g_{\rm e}$ which is expanded in powers of the Sommerfeld feinstructure constant α. Theoretical calculations have been performed up to the order $N = 3$ [56] and yield a numerical value which coincides with the experimental value $g_{\rm e} = 2.0023193043(74)$ [57] up to 9 digits. It is this impressive agreement which has established quantum electrodynamics as the prototype for relativistic quantum field theories.

However, already in 1952, Freeman Dyson pointed out that the quality of this agreement depends crucially on the smallness of the Sommerfeld feinstructure constant $\alpha \approx 0.0073$ [58]. He discovered that physical quantities in quantum electrodynamics have a vanishing convergence radius with respect to the Sommerfeld feinstructure constant α. Thus an expansion in powers of α can never converge for any positive value of α however small it may be. In fact it turns out that the expansion of the anomalous magnetic moment of the electron $g_{\rm e}$ in powers of the Sommerfeld feinstructure constant α is not an example for a convergent but for an asymptotic series (see Fig. 3.1). Whereas a convergent series is expanded around a regular point $g_0 = 0$ in the complex g-plane and has a finite convergence radius, an asymptotic series is expanded around a singular point $g_0 = 0$. In the latter case, typically the negative Re g-axis does not belong to the convergence region. Convergence occurs only in the sector of a circle, so the convergence radius vanishes per definition. For practical purposes, both convergent and asymptotic series have in common that they lead to good approximations as long as they are evaluated for small coupling constants g. The difference between a convergent and an asymptotic series reveals itself, if one investigates their properties for an increase of the order N. For a fixed value of the coupling constant g, an increase in N leads to an improved approximation for a convergent series as its weak-coupling coefficients a_n tend to zero in the limit $n \to \infty$. For an asymptotic series one observes the phenomenon that the approximation is improved as long as N is smaller than a critical value N_c. If N exceeds N_c it turns out that the approximation diverges. The reason for this is the large-order behavior of the weak-coupling coefficients a_n. They turn out not to decrease but to increase factorially with n.

Thus asymptotic series have to be resummed in order to extract from them reasonable physical results. The crudest method to approximate a function $f(g)$ with an asymptotic series employ Padé approximants [59]. These are rational functions with the same power series expansions as $f(g)$. A better approximation can be found by using in addition the large-order behavior of the weak-coupling coefficients a_n. By means of Borel transformations the factorial growth of a_n can be eliminated [60], and a successive Padé approximation is applied. The resulting Padé-Borel method approximates the left-hand cut of the function $f(g)$ in the complex g-plane by a string of poles. This procedure can be improved further by a conformal mapping technique in which the complex g-plane is mapped into a unit circle which contains the original left-hand cut on its circumference [61].

Another powerful tool for extracting physical results from asymptotic series is provided by variational methods which were initially invented by many research groups in quantum mechanics and then applied to quantum field theory. For instance, the so-called δ-expansion amounts to a resummation of perturbation series (see, for instance, Refs. [62–70]) which is performed by introducing artificially an effective harmonic oscillator and by optimizing the trial frequency according to the principle of minimal sensitivity [71]. It turns out that the δ-expansion procedure corresponds to a systematic extension of a variational approach in quantum statistics [72–75] to arbitrary orders [49, 76, 77] and is now called variational perturbation theory. It allows to evaluate the asymptotic series (3.1) for all values of the coupling constant g. As a special case it also converts the weak-coupling series (3.1) into its strong-coupling limit which typically reads

$$f(g) = g^{p/q} \sum_{m=0}^{\infty} b^{(m)} g^{-2m/q} \,. \tag{3.2}$$

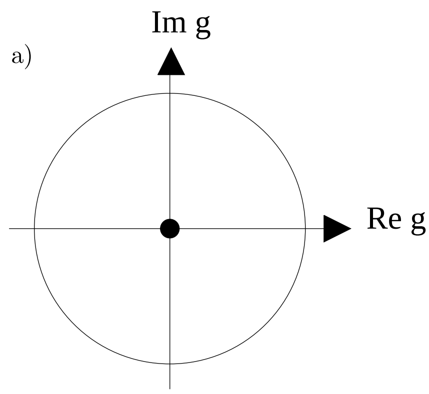


Figure 3.1: Comparing schematically analytic properties of convergent a) and asymptotic b) series.

Here p and q denote real numbers which determine the strong-coupling behavior and $b^{(m)}$ represent the strong-coupling coefficients. For the ground-state energy of the anharmonic oscillator with $p = 1$ and $q = 3$, the convergence was shown to be exponentially fast even for infinite coupling strength [78–80].

In recent years, variational perturbation theory has been extended in a way, which also allows for the resummation of divergent perturbation expansions which arise from renormalizing the ϕ^4-theory of critical phenomena [77, 81–83]. The corresponding perturbation coefficients are available up to six and partly to seven loops in $d = 3$ [84, 85] and up to five loops in $d = 4 - \epsilon$ dimensions [86]. The most important new feature of this field-theoretic variational perturbation theory is that it accounts for the anomalous power approach to the strong-coupling limit which the δ-expansion cannot do. According to (3.2) this approach is governed by an irrational critical exponent $\omega = 2/q$ as was first shown by Wegner [87] in the context of critical phenomena. In contrast to the δ-expansion, the field-theoretic variational perturbation expansions cannot be derived from adding and subtracting a harmonic term. Instead, a self-consistent procedure is set up to determine this irrational critical Wegner exponent. The theoretical results of the field-theoretic variational perturbation theory are in excellent agreement with the only experimental value measured so far with a challenging accuracy, the critical exponent α governing the behavior of the specific heat near the superfluid phase transition of ^{4}He. The high accuracy was reached by performing a microgravity experiment in a satellite orbiting around the earth [88, 89].

3.2 General Procedure

In this section we follow Refs. [49, 83] and outline the general procedure for resumming an asymptotic perturbation series with the help of variational perturbation theory. In order to estimate the quality of the resummation we emphasize, in particular, how to convert given weak-coupling expansions into their strong-coupling limit.

3.2.1 Arbitrary Coupling Constant

Consider the weak-coupling series (3.1) of a physical quantity f as a function of a coupling constant g which is truncated at order N. Rewrite this weak-coupling expansion by introducing an auxiliary parameter κ which rescales the quantity f and the coupling constant g by a factor κ^p and κ^q, respectively, and set afterwards $\kappa = 1$:

$$f_N(g) = \kappa^p \sum_{n=0}^{N} a_n \left(\frac{g}{\kappa^q}\right)^n \Big|_{\kappa=1} . \tag{3.3}$$

Here p and q denote parameters which will determine the strong-coupling behavior as we will see below. Now we introduce the variational parameter K according to Kleinert's square-root trick

$$\kappa = K\sqrt{1+gr}\,, \tag{3.4}$$

and define the abbreviation

$$r = \frac{1}{g}\left(\frac{\kappa^2}{K^2} - 1\right) . \tag{3.5}$$

Substituting (3.4) into the truncated weak-coupling series (3.3), we obtain

$$f_N(g) = \sum_{n=0}^{N} a_n K^{p-nq} (1+gr)^{(p-nq)/2} g^n . \tag{3.6}$$

Then the factor $(1+gr)^\alpha$ with $\alpha \equiv (p-nq)/2$ is expanded by means of generalized binomials, i.e.

$$(1+gr)^\alpha = \sum_{k=0}^{N-n} \binom{\alpha}{k} \left(\frac{1}{K^2} - 1\right)^k g^n + \mathcal{O}\left(g^{N-n}\right) , \tag{3.7}$$

with the binomial being defined as

$$\binom{\alpha}{k} \equiv \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)} . \tag{3.8}$$

Furthermore, in deriving (3.7) we have used (3.5) and have set $\kappa \equiv 1$. Thus the function $f_N(g)$ becomes K-dependent and reduces to

$$f_N(g,K) = \sum_{n=0}^{N} \left[\sum_{k=0}^{N-n} \binom{(p-nq)/2}{k} \left(\frac{1}{K^2}-1\right)^k K^{p-nq} \right] a_n g^n \,. \tag{3.9}$$

According to the principle of minimal sensitivity [71], we minimize the influence of K on $f_N(g,K)$ by searching for local extrema, i.e., from the condition

$$\left. \frac{\partial f_N(g,K)}{\partial K} \right|_{K=K_N(g)} = 0 \,. \tag{3.10}$$

It may happen that this condition is not solvable. In this case, in accordance with the principle of minimal sensitivity [71], we look for turning points instead, i.e., we determine the variational parameter $K_N(g)$ by solving

$$\left. \frac{\partial^2 f_N(g,K)}{\partial K^2} \right|_{K=K_N(g)} = 0 \,. \tag{3.11}$$

The solutions of Eqs. (3.10) or (3.11) then yield the variational result $f_N(g,K_N(g))$ which turns out to be a good approximation for the function $f(g)$ for all values of the coupling constant g. The quality of this approximation can be estimated by investigating the strong-coupling limit as a special case.

3.2.2 Strong-Coupling Limit

A careful analysis of the conditions (3.10) and (3.11) for the function (3.9) shows that the variational parameter $K_N(g)$ turns out to have the strong-coupling behavior

$$K_N(g) = g^{1/q} \left(K_N^{(0)} + K_N^{(1)} g^{-2/q} + ... \right) \,. \tag{3.12}$$

Thus the approximation $f_N(g,K_N(g))$ of $f(g)$ behaves in the strong-coupling limit as

$$f_N(g,K_N(g)) = g^{p/q} \left[b_N^{(0)}(K_N^{(0)}) + b_N^{(1)}(K_N^{(0)},K_N^{(1)}) g^{-2/q} + ... \right] \,. \tag{3.13}$$

We see that the fraction p/q tells us the leading power behavior in g and $2/q$ indicates the approach to scaling. The leading strong-coupling coefficient $b_N^{(0)}(K_N^{(0)})$ turns out to be given by

$$b_N^{(0)}(K_N^{(0)}) = \sum_{n=0}^{N} \sum_{k=0}^{N-n} \binom{(p-nq)/2}{k} (-1)^k a_n (K_N^{(0)})^{p-nq} \,, \tag{3.14}$$

where the inner sum can be further simplified, using [55, Eq. (0.151)]

$$\sum_{k=0}^{m}(-1)^k\binom{\alpha}{k}=(-1)^m\binom{\alpha-1}{m}\,. \tag{3.15}$$

Thus the strong-coupling coefficient (3.14) reduces to

$$b_N^{(0)}(K_N^{(0)})=\sum_{n=0}^{N}(-1)^{N-n}\binom{(p-nq)/2-1}{N-n}a_n(K_N^{(0)})^{p-nq}\,. \tag{3.16}$$

In order to optimize the variational parameter $K_N^{(0)}$, we look again for an extremum

$$\frac{\partial b_N^{(0)}(K_N^{(0)})}{\partial K_N^{(0)}}=0 \tag{3.17}$$

or for a saddle point

$$\frac{\partial^2 b_N^{(0)}(K_N^{(0)})}{\partial K_N^{(0)2}}=0\,. \tag{3.18}$$

Inserting the optimized $K_N^{(0)}$ in (3.16) then leads to the approximation $b_N^{(0)}(K_N^{(0)})$ of the strong-coupling coefficient.

Part II:

Finite-Temperature

Perturbation Theory

Chapter 4

Second-Order Perturbation Theory

4.1 Grand-Canonical Potential

In this section we treat the weak two-particle interaction (1.13) in the framework of finite temperature perturbation theory. The starting point of our considerations is the functional integral for the partition function

$$\mathcal{Z} = \oint \mathcal{D}\psi \oint \mathcal{D}\psi^* e^{-\left\{\mathcal{A}^{(0)}[\psi,\psi^*]+\mathcal{A}^{(\rm int)}[\psi,\psi^*]\right\}/\hbar}, \tag{4.1}$$

where $\mathcal{A}^{(0)}$ denotes the free part (2.4) of the euclidian action in (4.1)

$$\mathcal{A}^{(0)}[\psi(\mathbf{x},\tau),\psi^*(\mathbf{x},\tau)] = \int_0^{\hbar\beta} d\tau \int d^dx\, \psi^*(\mathbf{x},\tau)[\hbar\partial_\tau + h(\mathbf{x}) - \mu]\psi(\mathbf{x},\tau) \tag{4.2}$$

and $\mathcal{A}^{(\rm int)}$ includes the two-particle delta interaction (1.13) which is valid for dilute Bose gases:

$$\mathcal{A}^{(\rm int)}[\psi(\mathbf{x},\tau),\psi^*(\mathbf{x},\tau)] = \frac{g}{2}\int_0^{\hbar\beta} d\tau \int d^dx\, \psi(\mathbf{x},\tau)^2\psi^*(\mathbf{x},\tau)^2 \,. \tag{4.3}$$

Here the coupling constant g is assumed to be a small quantity. Thus we are allowed to evaluate the exponential function $\exp(-\mathcal{A}^{(\rm int)}/\hbar)$ into a Taylor series up to the order $\mathcal{O}(g^3)$:

$$e^{-\mathcal{A}^{(\rm int)}[\psi,\psi^*]/\hbar} = 1 - \frac{g}{2\hbar}\int_1 \psi_1^{*2}\psi_1^2 + \frac{g^2}{8\hbar^2}\int_1\int_2 \psi_1^{*2}\psi_2^{*2}\psi_1^2\psi_2^2 + \mathcal{O}(g^3)\,. \tag{4.4}$$

Here we have introduced a short-hand notation for the space and imaginary time integrals

$$\int_0^{\hbar\beta} d\tau_i \int d^dx_i \equiv \int_i \quad , \tag{4.5}$$

and the Bose fields:

$$\psi(\mathbf{x}_i,\tau_i) \equiv \psi_i\,, \quad \psi^*(\mathbf{x}_i,\tau_i) \equiv \psi_i^*\,. \tag{4.6}$$

Inserting the expansion (4.4) into (4.1) and defining the ensemble average for an arbitrary function F of the Bose fields ψ, ψ^* as

$$\langle F(\psi(\mathbf{x},\tau),\psi^*(\mathbf{x},\tau))\rangle = \frac{1}{\mathcal{Z}^{(0)}}\oint \mathcal{D}\psi \oint \mathcal{D}\psi^* F(\psi(\mathbf{x},\tau),\psi^*(\mathbf{x},\tau))\, e^{-\frac{1}{\hbar}\mathcal{A}^{(0)}[\psi,\psi^*]}\,, \tag{4.7}$$

yields the partition function evaluated up to the second order in the coupling constant g:

$$\mathcal{Z} \;=\; \mathcal{Z}^{(0)}\left\{1 - \frac{g}{2\hbar}\int_1 \langle \psi_1^{*2}\psi_1^2\rangle + \frac{g^2}{8\hbar^2}\int_1\int_2 \langle \psi_1^{*2}\psi_2^{*2}\psi_1^2\psi_2^2\rangle\right\}\,, \tag{4.8}$$

where $\mathcal{Z}^{(0)}$ was defined by (2.3).

One of the most important statements of quantum field theory is encountered through Wick's theorem. It states that an unperturbed average of a n fold product of fields can be reduced by a contraction to a $(n-2)$ fold product:

$$\langle \psi_1\psi_2\dots\psi_n\rangle = \langle\psi_1\psi_2\rangle\,\langle\psi_3\psi_4\dots\psi_n\rangle + \langle\psi_1\psi_3\rangle\,\langle\psi_2\psi_4\dots\psi_n\rangle + \langle\psi_1\psi_n\rangle\,\langle\psi_2\psi_3\dots\psi_{n-1}\rangle \tag{4.9}$$

Through its iteration, a n fold product can be therefore represented through summation over all possible contractions. Consequently, the averages in (4.8) can be represented through two-point correlation functions according to

$$\langle \psi_1^{*2}\psi_1^2\rangle = 2\langle\psi_1^*\psi_1\rangle \tag{4.10}$$

and

$$\begin{aligned}\langle \psi_1^{*2}\psi_2^{*2}\psi_1^2\psi_2^2\rangle \;&=\; 4\langle\psi_1^*\psi_1\rangle^2\,\langle\psi_2^*\psi_2\rangle^2 + 16\langle\psi_1^*\psi_1\rangle\,\langle\psi_1^*\psi_2\rangle\,\langle\psi_2^*\psi_1\rangle\langle\psi_2^*\psi_2\rangle\\ &\quad +4\langle\psi_1^*\psi_2\rangle^2\,\langle\psi_2^*\psi_1\rangle^2\,.\end{aligned} \tag{4.11}$$

Note that the remaining two-point correlation or Green function

$$\langle\psi_i^*\psi_j\rangle = G(\mathbf{x}_i,\tau_i;\mathbf{x}_j,\tau_j) \equiv G_{ij}\,. \tag{4.12}$$

has already been calculated (2.58). Thus the partition function (4.8) is given by

$$\mathcal{Z} \;=\; \mathcal{Z}^{(0)}\left\{1 - \frac{g}{\hbar}\int_1 G_{11} + \frac{g^2}{2\hbar^2}\int_1\int_2 \Big[G_{11}G_{22} + 4G_{11}G_{22}G_{12}G_{21} + G_{12}^2G_{21}^2\Big]\right\} \tag{4.13}$$

The connection to thermodynamics is established by the grand-canonical potential:

$$\Omega = -\frac{1}{\beta} \ln \mathcal{Z} \, . \tag{4.14}$$

After a Taylor expansion of the logarithm we obtain the grand-canonical potential up to second order in perturbation theory:

$$\Omega = -\frac{1}{\beta} \ln \mathcal{Z}^{(0)} + \frac{g}{\hbar\beta} \int_1 G_{11}^2 - \frac{g^2}{2\beta\hbar^2} \int_1 \int_2 \left[4 G_{11} G_{22} G_{12} G_{21} + G_{12}^2 G_{21}^2 \right] + \mathcal{O}(g^3) \, . \tag{4.15}$$

This perturbative result can be represented through diagrams according to the following Feynman rules of our theory. A straight line with an arrow stands for the interaction-free Green function (2.60)

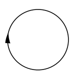
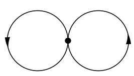
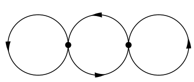
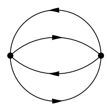
1 2

$$\equiv \; G_{12} = \int \frac{d^d p}{(2\pi\hbar)^d} \frac{e^{\frac{i}{\hbar}\mathbf{p}(\mathbf{x}_1 - \mathbf{x}_2)}}{2 \sinh \frac{\beta}{2} \left(\frac{\mathbf{p}^2}{2M} - \mu \right)}$$
$$\times \left[\Theta(\tau_1 - \tau_2) \, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{p}^2}{2M} - \mu\right)\left(\tau_1 - \tau_2 - \frac{\hbar\beta}{2}\right)} + \Theta(\tau_2 - \tau_1) \, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{p}^2}{2M} - \mu\right)\left(\tau_1 - \tau_2 + \frac{\hbar\beta}{2}\right)} \right] , \tag{4.16}$$

and a vertex represents the ψ^4 interaction

$$= -\frac{4\pi\hbar a_s}{M} \int d^3 x \int_0^{\hbar\beta} d\tau \; . \tag{4.17}$$

Thus the diagrammatic representation of (4.15) reads

$$\Omega(V,T,\mu) = -\frac{1}{\beta} \ln \mathcal{Z} =$$  $+$  $+\,2$  $+\,\frac{1}{2}$  .

Note that it is possible to set up a graphical recursive construction method for the Hugenholtz diagrams [90] contributing to the grand-canonical potential [91].

4.2 Self-Energy

We introduce the Green function for the interacting system as

$$G^{\mathrm{c}}(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) \equiv G_{12}^{\mathrm{c}} = \frac{1}{\mathcal{Z}} \oint \mathcal{D}\psi \oint \mathcal{D}\psi^* \psi_1 \psi_2^* \, e^{-\frac{1}{\hbar}\left(\mathcal{A}^{(0)}[\psi,\psi^*] + \mathcal{A}^{\mathrm{int}}[\psi,\psi^*]\right)} , \tag{4.18}$$

and denote the corrections to the free Green function G_{12} due to interactions as self-energy Σ_{12}:

$$\Sigma(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) \equiv \Sigma_{12} = G_{12}^{-1} - G_{12}^{\mathrm{c}-1}\,. \tag{4.19}$$

Multiplying Eq. (4.19) with the free and the interacting Green function and integrating over space and imaginary time yields the Dyson equation

$$G_{12}^{\mathrm{c}} = G_{12} + \int_3\int_4 G_{13}\Sigma_{34}G_{42}^{\mathrm{c}}\,. \tag{4.20}$$

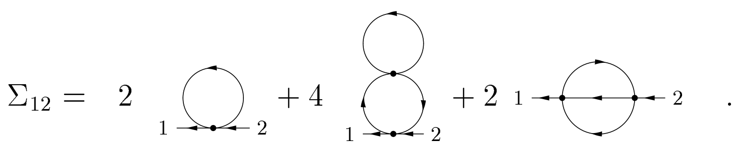
In analogy to the previous section we perform a Taylor expansion of the interaction part (4.4) in (4.18) and obtain with help of the definitions (4.5)-(4.7) a second order result for the Green function of the weakly interacting Bose gas:

$$\begin{aligned} G_{12}^{\mathrm{c}} &= G_{12} - \frac{2g}{\hbar}\int_3 G_{13}G_{33}G_{32} + \frac{2g^2}{\hbar^2}\int_3\int_4 [2G_{13}G_{34}G_{43}G_{44}G_{32} \\ &\quad + 2G_{13}G_{34}G_{44}G_{33}G_{42} + G_{13}G_{34}^2G_{43}^2] + \mathcal{O}(g^3)\,. \end{aligned} \tag{4.21}$$

Inserting this result into the Dyson equation (4.20) we read off the corresponding expansion for the self energy:

$$\Sigma_{12} = -\frac{2g}{\hbar}\,\delta_{12}G_{11} + \frac{4g^2}{\hbar^2}G_{12}G_{21}G_{22} + \frac{2g^2}{\hbar^2}G_{12}^2G_{21} + \mathcal{O}(g^3)\,. \tag{4.22}$$

In analogy to (4.18) the self energy (4.22) can be represented diagramatically



Let us briefly discuss some characteristic properties of the self-energy. In case of homogeneous BEC's, where the external potential is zero, the free Green function possesses translational invariance in space and imaginary time (2.60), which transfers itself because of Wick's theorem to the interacting Green function (4.18)

$$G^{\mathrm{c}}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = G^{\mathrm{c}}(\mathbf{x}_1-\mathbf{x}_2;\tau_1-\tau_2) \tag{4.23}$$

and also to the self energy (4.19)

$$\Sigma(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = \Sigma(\mathbf{x}_1-\mathbf{x}_2;\tau_1-\tau_2) \tag{4.24}$$

evaluated up to arbitrary orders in the coupling constant g. Because of this symmetry, (4.22) simplifies to

$$\begin{aligned} \Sigma(\mathbf{x},\tau) &= -\frac{2g}{\hbar}\,\delta(\mathbf{x})\delta(\tau)G(\mathbf{0},0) + \frac{4g^2}{\hbar^2}G(\mathbf{0},0)G(\mathbf{x},\tau)G(-\mathbf{x},-\tau) \\ &\quad + \frac{2g^2}{\hbar^2}G(\mathbf{x},\tau)^2G(-\mathbf{x},-\tau)\,. \end{aligned} \tag{4.25}$$

Furthermore, we perform a Matsubara decomposition of the self-energy

$$\Sigma(\mathbf{x},\tau) = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty} e^{-i\omega_m\tau}\int \frac{d^dp}{(2\pi\hbar^2)^d}\, e^{i\mathbf{px}/\hbar}\,\Sigma(\mathbf{p},\omega_m)\,, \tag{4.26}$$

where the expansion coefficients are given by

$$\Sigma(\mathbf{p},\omega_m) = \int_0^{\hbar\beta} d\tau\, e^{i\omega_m\tau}\int d^dx\, e^{-i\mathbf{px}/\hbar}\Sigma(\mathbf{x},\tau)\,. \tag{4.27}$$

The mathematical structure of the coefficient (4.27) can be restricted through a further symmetry consideration. As the Green function (4.18) is rotational invariant, the self-energy possesses the same property:

$$\Sigma(R\mathbf{x}_1,\tau_1;R\mathbf{x}_2,\tau_2) = \Sigma(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2)\,, \tag{4.28}$$

which is valid for every unitary matrix with $RR^{\mathrm{T}} = 1$. Because of

$$\begin{aligned}
\Sigma(R\mathbf{p},\omega_m) &\overset{(4.27)}{=} \int_0^{\hbar\beta} d\tau\, e^{i\omega_m\tau}\int d^dx\, e^{-i\mathbf{p}(R^T\mathbf{x})/\hbar}\Sigma(\mathbf{x},\tau)\\
&\overset{\mathbf{x}'=R^T\mathbf{x}}{=} \int_0^{\hbar\beta} d\tau\, e^{i\omega_m\tau}\int d^dx'\, e^{-i\mathbf{px}'/\hbar}\Sigma(R\mathbf{x}',\tau)\\
&\overset{(4.28)}{=} \int_0^{\hbar\beta} d\tau\, e^{i\omega_m\tau}\int d^dx\, e^{-i\mathbf{px}'/\hbar}\Sigma(\mathbf{x},\tau)\\
&\overset{(4.27)}{=} \Sigma(\mathbf{p},\omega_m)
\end{aligned} \tag{4.29}$$

the rotational invariance of the self energy implies the same property for its Fourier- and Matsubara coefficient $\Sigma(\mathbf{p},\omega_m)$. Therefore $\Sigma(\mathbf{p},\omega_m)$ has the following expansion for small momenta:

$$\Sigma(\mathbf{p},\omega_m) = \Sigma_0(\mathbf{0},\omega_m) + \Sigma_2(\mathbf{0},\omega_m)\mathbf{p}^2 + \mathcal{O}(\mathbf{p}^4)\,. \tag{4.30}$$

4.3 Renormalization

In the last section we observed that also the Green function (4.18) possesses translational invariance. Thus it can be decomposed in analogy to (4.26). Of course the relationship (4.19) holds also for the expansion coefficients of such a decomposition:

$$G^{\mathrm{c}\,-1}(\mathbf{p},\omega_m) = G^{-1}(\mathbf{p},\omega_m) - \Sigma(\mathbf{p},\omega_m)\,. \tag{4.31}$$

With the result (2.48) we get for the Fourier- and Matsubara coefficient of the Green function

$$G^{\mathrm{c}}(\mathbf{p},\omega_m) = \frac{1}{G^{\mathrm{c}\,-1}(\mathbf{p},\omega_m)} = \frac{\hbar}{-i\hbar\omega_m + \mathbf{p}^2/2m - \mu - \hbar\Sigma(\mathbf{p},\omega_m)}\,. \tag{4.32}$$

By means of this equation we want to discuss the physical meaning of the self energy. For the free Bose gas, where $\Sigma = 0$ and $G^{\mathrm{c}} = G$, the chemical potential μ as well as the physical mass m can be obtained from the inverse of the Fourier-Matsubara coefficient (2.48):

$$\mu = -\hbar G^{-1}(\mathbf{0}, 0) \tag{4.33}$$

and

$$\frac{1}{m} = 2\hbar \left.\frac{\partial G^{-1}(\mathbf{p}, 0)}{\partial \mathbf{p}^2}\right|_{\mathbf{p}=\mathbf{0}} . \tag{4.34}$$

Eq. (4.33) shows an important physical fact: For the free Bose gas the phase transition can be defined by the vanishing of the bare chemical potential μ. This implies that the two-point correlation function and therefore the corresponding correlation length diverges at the critical point, which indicates that the phase transition is directly related to long-range correlations.

Now we consider the case where the interaction is included and thus the self energy does not vanish. Inserting (4.30) into (4.32) yields

$$G^{\mathrm{c}\,-1}(\mathbf{p}, \omega_m) = -i\omega_m - \frac{1}{\hbar}\left[\mu - \hbar\Sigma_0(\mathbf{0}, \omega_m)\right] + \frac{1}{2\hbar}\left[\frac{1}{m} - 2\hbar\Sigma_2(\mathbf{0}, \omega_m)\right]\mathbf{p}^2 + \mathcal{O}(\mathbf{p}^4)\,. \tag{4.35}$$

We see that in the interacting case the role of the bare chemical potential and the bare physical mass is played by its renormalized quantities defined by

$$\mu_r = -\hbar G^{\mathrm{c}\,-1}(\mathbf{0}, 0) = \mu + \hbar\Sigma(\mathbf{0}, 0) \tag{4.36}$$

and

$$\frac{1}{m_r} = \frac{1}{m} - 2\hbar \left.\frac{\partial \Sigma(\mathbf{p}, 0)}{\partial \mathbf{p}^2}\right|_{\mathbf{p}=\mathbf{0}} . \tag{4.37}$$

We define now the phases transition through the requirement that (4.32) diverges at the critical point and thus shows long-range correlations. Consequently, the critical point is reached as soon as the renormalized chemical pontential μ_r is zero:

$$\mu_r \overset{T=T_c}{=} 0\,. \tag{4.38}$$

Finally, we state the perturbation expansion for the renormalized chemical potential, which can be obtained from (4.25), (4.27) and (4.36):

$$\begin{aligned}
\mu_r &= \mu + \int_0^{\hbar\beta} d\tau \int d^d x \Sigma(\mathbf{x}, \tau) = \mu - \frac{2g}{\hbar} G(\mathbf{0}, 0) \\
&\quad + \frac{4g^2}{\hbar^2} G(\mathbf{0}, 0) \int_0^{\hbar\beta} d\tau \int d^d x\, G(\mathbf{x}, \tau) G(-\mathbf{x}, -\tau) \\
&\quad + \frac{2g^2}{\hbar^2} \int_0^{\hbar\beta} d\tau \int d^d x\, G(\mathbf{x}, \tau)^2 G(-\mathbf{x}, -\tau)\,.
\end{aligned} \tag{4.39}$$

Chapter 5

Calculation of Vacuum Diagrams

The goal of this chapter is to calculate the second-order contributions to the grand-canonical potential (4.15) of a dilute weakly interacting Bose gas, which can be decomposed as follows

$$\Omega = \Omega^{(0)} + \Omega^{(1)} + \Omega^{(2)} \, . \tag{5.1}$$

The zeroth order term $\Omega^{(0)}$ has already been calculated in (2.37):

$$\Omega^{(0)} = -\frac{1}{\beta} \ln \mathcal{Z}^{(0)} = \frac{V}{\beta \lambda^d} \zeta_{d/2+1}(z) \, . \tag{5.2}$$

The first order contribution $\Omega^{(1)}$ follows from the translational invariance of the free Green function and the result (2.62):

$$\Omega^{(1)} = \frac{g}{\hbar \beta} \int_1 G_{11}^2 = g V G(\mathbf{0}, 0)^2 = \frac{2V}{\beta \lambda^d} \left(\frac{a_s}{\lambda} \right) \zeta_{d/2}(z)^2 \, . \tag{5.3}$$

The second order contribution $\Omega^{(2)}$ consists of two diagrams

$$\Omega^{(2)} = -\frac{2}{\beta} T - \frac{1}{2\beta} B = -\frac{2}{\beta} \frac{g^2}{\hbar^2} \int_1 \int_2 G_{11} G_{22} G_{12} G_{21} - \frac{1}{2\beta} \frac{g^2}{\hbar^2} \int_1 \int_2 G_{12}^2 G_{21}^2 \, , \tag{5.4}$$

where T denotes the so-called triple chain and B the basketball diagram. Both diagrams are more involved and are therefore calculated in the next two sections.

5.1 Triple Chain

The triple chain diagram is given by (5.4):

$$T = \left(-\frac{g}{\hbar} \right)^2 G(\mathbf{0}; 0)^2 \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int d^d x_1 \int d^d x_2 G(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) G(\mathbf{x}_2, \tau_2; \mathbf{x}_1, \tau_1) \, , \tag{5.5}$$

where $G(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2)$ is the many-body Green function for bosons (2.58):

$$\begin{aligned} T &= \frac{1}{\lambda^{2d}} \left(-\frac{g}{\hbar}\right)^2 \zeta_{d/2}(z)^2 \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int d^d x_1 \int d^d x_2 \int \frac{d^d p}{(2\pi\hbar)^d} \int \frac{d^d q}{(2\pi\hbar)^d} \\ &\quad \times \frac{1}{2} e^{\frac{i}{\hbar}\mathbf{p}(\mathbf{x}_1 - \mathbf{x}_2)} \frac{\theta(\tau_1 - \tau_2)\, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{p}^2}{2m} - \mu\right)\left(\tau_1 - \tau_2 - \frac{\hbar\beta}{2}\right)} + (1 \Longleftrightarrow 2)}{\sinh \frac{\beta}{2}\left(\frac{\mathbf{p}^2}{2m} - \mu\right)} \\ &\quad \times \frac{1}{2} e^{\frac{i}{\hbar}\mathbf{q}(\mathbf{x}_1 - \mathbf{x}_2)} \frac{\theta(\tau_1 - \tau_2)\, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{q}^2}{2m} - \mu\right)\left(\tau_1 - \tau_2 - \frac{\hbar\beta}{2}\right)} + (1 \Longleftrightarrow 2)}{\sinh \frac{\beta}{2}\left(\frac{\mathbf{q}^2}{2m} - \mu\right)} . \end{aligned} \tag{5.6}$$

At first, we calculate the spatial integrals

$$\int d^d x_1 \int d^d x_2 \, e^{\frac{i}{\hbar}(\mathbf{x}_1 - \mathbf{x}_2)(\mathbf{p} - \mathbf{q})} = V (2\pi\hbar)^d \delta^{(d)}(\mathbf{p} - \mathbf{q}) . \tag{5.7}$$

If we insert this delta function, one of the momentum integrals in (5.6) breaks down. At the same time we can simplify the fractions by using the definition of the Heaviside function θ to arrive at:

$$T = \frac{V}{4} \left(-\frac{g}{\hbar}\right)^2 \frac{\zeta_{d/2}(z)^2}{\lambda^{2d}} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int \frac{d^d p}{(2\pi\hbar)^d} \frac{\theta(\tau_1 - \tau_2) + \theta(\tau_2 - \tau_1)}{\sinh \frac{\beta}{2}\left(\frac{\mathbf{p}^2}{2m} - \mu\right)^2} . \tag{5.8}$$

The remaining integrals with respect to the imaginary time just give a dimensionless constant

$$\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \left[\theta(\tau_1 - \tau_2) + \theta(\tau_2 - \tau_1)\right] = \hbar\beta . \tag{5.9}$$

Finally, we are left with one momentum integral:

$$T = \frac{\hbar\beta V}{4} \left(-\frac{g}{\hbar}\right)^2 \frac{\zeta_{d/2}(z)^2}{\lambda^{2d}} \int \frac{d^d p}{(2\pi\hbar)^d} \frac{1}{\sinh \frac{\beta}{2}\left(\frac{\mathbf{p}^2}{2m} - \mu\right)^2} . \tag{5.10}$$

Partial integration yields together with (1.7):

$$T = \frac{\hbar\beta V}{\lambda^{2d}} \left(-\frac{g}{\hbar}\right)^2 \zeta_{d/2}(z)^2 \zeta_{d/2-1}(z) . \tag{5.11}$$

Finally replacing the coupling constant g in favor of the s-wave scattering length via (1.14) results in

$$T = \frac{4V}{\lambda^d} \left(\frac{a_s}{\lambda}\right)^2 \zeta_{d/2}(z)^2 \zeta_{d/2-1}(z) . \tag{5.12}$$

5.2 Basketball

The definition of the basketball diagram (5.4) reads:

$$B = \left(-\frac{g}{\hbar}\right)^2 \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int d^d x_1 \int d^d x_2 \, G(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2)^2 G(\mathbf{x}_2, \tau_2; \mathbf{x}_1, \tau_1)^2 . \quad (5.13)$$

We insert (2.58)

$$\begin{aligned} B \;=\; & \left(-\frac{g}{\hbar}\right)^2 \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int d^d x_1 \int d^d x_2 \int \frac{d^d p}{(2\pi\hbar)^d} \int \frac{d^d q}{(2\pi\hbar)^d} \int \frac{d^d k}{(2\pi\hbar)^d} \int \frac{d^d l}{(2\pi\hbar)^d} \\ & \times \frac{1}{2} e^{\frac{i}{\hbar}\mathbf{p}(\mathbf{x}_1-\mathbf{x}_2)} \frac{\theta(\tau_1-\tau_2)\, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{p}^2}{2m}-\mu\right)\left(\tau_1-\tau_2-\frac{\hbar\beta}{2}\right)} + (1 \Longleftrightarrow 2)}{\sinh\frac{\beta}{2}\left(\frac{\mathbf{p}^2}{2m}-\mu\right)} \\ & \times \frac{1}{2} e^{\frac{i}{\hbar}\mathbf{q}(\mathbf{x}_1-\mathbf{x}_2)} \frac{\theta(\tau_1-\tau_2)\, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{q}^2}{2m}-\mu\right)\left(\tau_1-\tau_2-\frac{\hbar\beta}{2}\right)} + (1 \Longleftrightarrow 2)}{\sinh\frac{\beta}{2}\left(\frac{\mathbf{q}^2}{2m}-\mu\right)} \\ & \times \frac{1}{2} e^{\frac{i}{\hbar}\mathbf{k}(\mathbf{x}_2-\mathbf{x}_1)} \frac{\theta(\tau_2-\tau_1)\, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{k}^2}{2m}-\mu\right)\left(\tau_2-\tau_1-\frac{\hbar\beta}{2}\right)} + (1 \Longleftrightarrow 2)}{\sinh\frac{\beta}{2}\left(\frac{\mathbf{k}^2}{2m}-\mu\right)} \\ & \times \frac{1}{2} e^{\frac{i}{\hbar}\mathbf{l}(\mathbf{x}_2-\mathbf{x}_1)} \frac{\theta(\tau_2-\tau_1)\, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{l}^2}{2m}-\mu\right)\left(\tau_2-\tau_1-\frac{\hbar\beta}{2}\right)} + (1 \Longleftrightarrow 2)}{\sinh\frac{\beta}{2}\left(\frac{\mathbf{l}^2}{2m}-\mu\right)} , \end{aligned} \quad (5.14)$$

and follow the same steps as in the previous section. At first we calculate the spatial integrals

$$\int d^d x_1 \int d^d x_2 \, e^{\frac{i}{\hbar}(\mathbf{x}_1-\mathbf{x}_2)(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l})} = V\,(2\pi\hbar)^d\, \delta^{(d)}(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l}) \, . \quad (5.15)$$

Then we simplify the fractions by using the definition of the Heaviside function θ to arrive at

$$\begin{aligned} B \;=\; & \frac{1}{16}\left(-\frac{g}{\hbar}\right)^2 V \int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}}\int_{\mathbf{l}} (2\pi\hbar)^d\, \delta^{(d)}(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l}) \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \\ & \times \frac{\theta(\tau_1-\tau_2)\, e^{\gamma\left(\tau_1-\tau_2-\frac{\hbar\beta}{2}\right)} + (1 \Longleftrightarrow 2)}{\sinh\left(\frac{\beta}{2}E_{\mathbf{p}}\right)\sinh\left(\frac{\beta}{2}E_{\mathbf{q}}\right)\sinh\left(\frac{\beta}{2}E_{\mathbf{k}}\right)\sinh\left(\frac{\beta}{2}E_{\mathbf{l}}\right)} , \end{aligned} \quad (5.16)$$

where we have introduced the short-hand notation

$$E_{\mathbf{p}} = \mathbf{p}^2/2m - \mu \quad (5.17)$$

and

$$\gamma = -\left(E_{\mathbf{p}} + E_{\mathbf{q}} - E_{\mathbf{k}} - E_{\mathbf{l}}\right)/\hbar\,. \tag{5.18}$$

Now we compute the integrals with respect to the imaginary times:

$$\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \left[\theta\left(\tau_1-\tau_2\right) e^{\gamma\left(\tau_1-\tau_2-\frac{\hbar\beta}{2}\right)} + \theta\left(\tau_1-\tau_2\right) e^{\gamma\left(\tau_1-\tau_2+\frac{\hbar\beta}{2}\right)}\right] = \frac{2\hbar\beta}{\gamma}\sinh\frac{\hbar\beta\gamma}{2}\,. \tag{5.19}$$

Inserting this result in (5.16) yields

$$B = \frac{g^2\beta V}{8}\int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}}\int_{\mathbf{l}} \frac{(2\pi\hbar)^d\,\delta^{(d)}\left(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l}\right)}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}}\frac{\sinh\frac{\beta}{2}\left(E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}\right)}{\sinh\frac{\beta E_{\mathbf{p}}}{2}\sinh\frac{\beta E_{\mathbf{q}}}{2}\sinh\frac{\beta E_{\mathbf{k}}}{2}\sinh\frac{\beta E_{\mathbf{l}}}{2}}. \tag{5.20}$$

We make contact with the Bose distribution, which can be expressed through the hyperbolic sine function:

$$n(E) = \frac{1}{e^{\beta E}-1} = \frac{e^{-\frac{\beta E}{2}}}{e^{\frac{\beta E}{2}} - e^{-\frac{\beta E}{2}}} = \frac{e^{-\frac{\beta E}{2}}}{2\sinh\frac{\beta E}{2}}\,. \tag{5.21}$$

So the basketball (5.20) becomes:

$$\begin{aligned} B &= g^2\beta V\int_{\mathbf{p}}\int_{\mathbf{q}}\int_{k}(2\pi\hbar)^d\,\delta^{(d)}\left(\mathbf{p}+\mathbf{q}-k-l\right)\frac{n(E_{\mathbf{p}})n(E_{\mathbf{q}})n(E_{\mathbf{k}})n(E_{\mathbf{l}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}} \\ &\quad\times\left[e^{\beta(E_{\mathbf{k}}+E_{\mathbf{l}})} - e^{\beta(E_{\mathbf{p}}+E_{\mathbf{q}})}\right]. \end{aligned} \tag{5.22}$$

The Bose distribution (5.21) has the interesting property

$$n(E)e^{\beta E} = n(E) + 1\,, \tag{5.23}$$

which, at first, complicates (5.22):

$$\begin{aligned} B &= g^2\beta V\int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}}\int_{l}(2\pi\hbar)^d\,\delta^{(d)}\left(\mathbf{p}+\mathbf{q}-\mathbf{k}-l\right) \\ &\quad\times\left[\frac{n(E_{\mathbf{p}})n(E_{\mathbf{q}})n(E_{\mathbf{k}}) + n(E_{\mathbf{p}})n(E_{\mathbf{q}})n(E_{\mathbf{l}}) + n(E_{\mathbf{p}})n(E_{\mathbf{q}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}}\right. \\ &\quad\left.-\frac{n(E_{\mathbf{p}})n(E_{\mathbf{k}})n(E_{\mathbf{l}}) + n(E_{\mathbf{q}})n(E_{\mathbf{k}})n(E_{\mathbf{l}}) + n(E_{\mathbf{k}})n(E_{\mathbf{l}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}}\right]. \end{aligned} \tag{5.24}$$

But by permuting the integration variables, one can show

$$n(E_{\mathbf{p}})n(E_{\mathbf{q}})n(E_{\mathbf{k}}) \hat{=} n(E_{\mathbf{p}})n(E_{\mathbf{q}})n(E_{\mathbf{l}}) \hat{=} -n(E_{\mathbf{p}})n(E_{\mathbf{k}})n(E_{\mathbf{l}}) \hat{=} -n(E_{\mathbf{q}})n(E_{\mathbf{k}})n(E_{\mathbf{l}}) \tag{5.25}$$

and

$$n(E_{\mathbf{p}})n(E_{\mathbf{q}}) \;\hat{=}\; -n(E_{\mathbf{k}})n(E_{\mathbf{l}})\,, \tag{5.26}$$

which finally simplifies the basketball (5.24):

$$B = 2g^2\beta V \int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}}\int_{\mathbf{l}} (2\pi\hbar)^d\,\delta^{(d)}\left(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l}\right)\frac{2n(E_{\mathbf{p}})n(E_{\mathbf{q}})n(E_{\mathbf{k}})+n(E_{\mathbf{p}})n(E_{\mathbf{q}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}} \tag{5.27}$$

Let us first consider the term in (5.27) containing three Bose distributions:

$$I_1 = \int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}}\int_{\mathbf{l}} (2\pi\hbar)^d\,\delta^{(d)}\left(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l}\right)\frac{n(E_{\mathbf{p}})n(E_{\mathbf{q}})n(E_{\mathbf{k}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}}\,. \tag{5.28}$$

With the help of

- the Fourier representation of the delta function:

$$(2\pi\hbar)^d\,\delta^{(d)}(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l}) \;=\; \int d^dx\, e^{i(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l})/\hbar}\,, \tag{5.29}$$

- the modified Schwinger trick (B.3)

$$\frac{1}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}} \;=\; \mathrm{Re}\lim_{\epsilon\downarrow 0}\int_0^{i\infty} d\lambda e^{-(E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}-i\epsilon)\lambda}\,, \tag{5.30}$$

- and the series representation of the Bose distribution function (1.1)

$$n(E_{\mathbf{p}})n(E_{\mathbf{q}})n(E_{\mathbf{k}}) \;=\; \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty} e^{-\beta(E_{\mathbf{p}}a+E_{\mathbf{q}}b+E_{\mathbf{k}}c)}\,, \tag{5.31}$$

we rewrite the momentum integrals in (5.28):

$$\begin{aligned} I_1 \;=\; & \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty} z^{a+b+c}\,\mathrm{Re}\lim_{\epsilon\downarrow 0}\int_0^{i\infty} d\lambda e^{-i\epsilon\lambda}\int d^dx\int_{\mathbf{p}} e^{-\frac{\mathbf{p}^2}{2m}(\beta a+\lambda)+\frac{i}{\hbar}\mathbf{x}\mathbf{p}} \\ & \times\int_{\mathbf{q}} e^{-\frac{\mathbf{q}^2}{2m}(\beta b+\lambda)+\frac{i}{\hbar}\mathbf{x}\mathbf{q}}\int_{\mathbf{k}} e^{-\frac{\mathbf{k}^2}{2m}(\beta c-\lambda)-\frac{i}{\hbar}\mathbf{x}\mathbf{k}}\int_{\mathbf{l}} e^{-\frac{\mathbf{l}^2}{2m}\lambda-\frac{i}{\hbar}\mathbf{x}\mathbf{l}}\,, \end{aligned} \tag{5.32}$$

which are simple Fresnel integrals [55], yielding :

$$\int_{\mathbf{l}} e^{-\frac{\mathbf{l}^2}{2m}\lambda+\frac{i}{\hbar}\mathbf{x}\mathbf{l}} = \int_{\mathbf{q}} e^{-\frac{\mathbf{l}^2}{2m}\lambda+\frac{i}{\hbar}\mathbf{x}\mathbf{l}} \;=\; \left(\frac{m}{2\pi}\right)^{d/2}\frac{e^{-\frac{m\mathbf{x}^2}{2\hbar^2\lambda}}}{\hbar^d\lambda^{d/2}} \tag{5.33}$$

$$\int_{\mathbf{p}} e^{-\frac{\mathbf{p}^2}{2m}(\beta a-\lambda)-\frac{i}{\hbar}\mathbf{x}\mathbf{p}} \;=\; \left(\frac{m}{2\pi}\right)^{d/2}\frac{e^{-\frac{m\mathbf{x}^2}{2\hbar^2(\beta a-\lambda)}}}{\hbar^d\left(\beta a-\lambda\right)^{d/2}}\,. \tag{5.34}$$

Hence, the integral (5.32) becomes

$$I_1 = \left(\frac{m}{2\pi}\right)^{2d}\frac{1}{\hbar^{4d}}\sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty}z^{a+b+c}\mathrm{Re}\lim_{\epsilon\downarrow 0}\int_0^{i\infty}d\lambda\frac{e^{-i\epsilon\lambda}}{\left[\lambda\left(\beta a-\lambda\right)\left(\beta b-\lambda\right)\left(\beta c+\lambda\right)\right]^{d/2}}$$
$$\times\int d^dx\exp\left\{-\frac{m\mathbf{x}^2}{2\hbar^2}\left(\frac{1}{\lambda}+\frac{1}{\beta a-\lambda}+\frac{1}{\beta b-\lambda}+\frac{1}{\beta c+\lambda}\right)\right\}. \quad (5.35)$$

Evaluating the spatial integral, we obtain

$$I_1 = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3d/2}\beta\sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty}z^{a+b+c}\mathrm{Re}\int_0^{i\infty}d\lambda\frac{1}{\left[abc+2ab\lambda-\left(a+b+c\right)\lambda^2\right]^{d/2}}. \quad (5.36)$$

In the same way one gets for the second integral in (5.27):

$$I_2 = \int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}}\int_{\mathbf{l}}(2\pi\hbar)^d\,\delta^{(d)}\left(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l}\right)\frac{n(E_{\mathbf{p}})n(E_{\mathbf{q}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}-E_{\mathbf{l}}} \quad (5.37)$$

$$= \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3d/2}\beta\sum_{a=1}^{\infty}\sum_{b=1}^{\infty}z^{a+b}\mathrm{Re}\int_0^{i\infty}d\lambda\frac{1}{\left[2ab-\left(a+b\right)\lambda\right]^{d/2}\lambda^{d/2}}. \quad (5.38)$$

Thus the preliminary result for the basketball diagam (5.13) reads:

$$B = 2g^2\beta^2V\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3d/2}\left(2B_1+B_2\right) = 8\frac{a^2V}{\lambda^{3d-4}}\left(2B_1+B_2\right), \quad (5.39)$$

where:

$$B_1 = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty}z^{a+b+c}\mathrm{Re}\int_0^{i\infty}d\lambda\frac{1}{\left[abc-2ab\lambda-\left(a+b+c\right)\lambda^2\right]^{d/2}}, \quad (5.40)$$

$$B_2 = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}z^{a+b}\mathrm{Re}\int_0^{i\infty}d\lambda\frac{1}{\left[-2ab-\left(a+b\right)\lambda\right]^{d/2}\lambda^{d/2}}. \quad (5.41)$$

Calculation of $\mathbf{B_2}$ At first we consider (5.41) as it easier to calculate than (5.40). The denominator in (5.41) is treated with the Schwinger trick (B.1) yielding:

$$B_2 = \frac{1}{\Gamma(d/2)}\sum_{a=1}^{\infty}\sum_{b=1}^{\infty}z^{a+b}\,\mathrm{Re}\,i\int_0^{\infty}dx\,x^{d/2-1}e^{2iabx}\int_0^{\infty}d\lambda\,\lambda^{-d/2}e^{-(a+b)x\lambda} \quad (5.42)$$

The remaining integrals are simple Gamma functions [55] and thus we obtain:

$$B_2 = -\frac{2^{1-d}}{\Gamma(d/2)}\Gamma(1-d/2)\Gamma(d-1)\cos(\pi d/2)\sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\frac{z^{a+b}}{(ab)^{d-1}(a+b)^{1-d/2}}. \quad (5.43)$$

We replace the term $1/(a+b)^{1-d/2}$ in (5.43) according to the Schwinger trick (B.1) to make contact with polylogarithmic functions (A.1):

$$B_2 = -\frac{2^{1-d}\,\Gamma(d-1)\cos\frac{\pi d}{2}}{\Gamma(d/2)}\int_0^\infty dx\, x^{-d/2}\zeta_{d-1}\left(e^{\beta\mu - x}\right)^2 . \tag{5.44}$$

If we now apply Robinson's formula (A.4) we have to calculate integrals of the general form

$$\int_0^\infty dx x^{-d/2}\left(-\beta\mu + x\right)^\alpha = \frac{\Gamma(d/2-\alpha-1)\Gamma(1-d/2)}{\Gamma(-\alpha)} . \tag{5.45}$$

Note that the argument of the Gamma function in the denominator would be always a negative integer so that it diverges and the whole expression tends to zero. However there are two terms of the Robinson expansion that survive for $d = 3$:

$$\begin{aligned} B_2 &= -\frac{2^{1-d}\,\Gamma(d-1)\cos\frac{\pi d}{2}}{\Gamma(d/2)}\int_0^\infty dx\, x^{-d/2}\Big[\Gamma(2-d)^2\left(-\beta\mu+x\right)^{2d-4} \\ &\quad -2\zeta(d-2)\Gamma(2-d)\left(-\beta\mu+x\right)^{d-1}\Big] . \end{aligned} \tag{5.46}$$

The integration produces compensating divergent Gamma functions, yielding

$$\begin{aligned} B_2 &= -\frac{2^{1-d}\,\Gamma(d-1)\Gamma(1-d/2)\cos\frac{\pi d}{2}}{\Gamma(d/2)}\Bigg[\left(-\beta\mu\right)^{3d/2-3}\frac{\Gamma(2-d)^2\Gamma(3-3d/2)}{\Gamma(4-2d)} \\ &\quad -2\left(-\beta\mu\right)^{d/2}\zeta(d-2)\frac{\Gamma(2-d)\Gamma(-d/2)}{\Gamma(1-d)}\Bigg] . \end{aligned} \tag{5.47}$$

According to the rules of dimensional regularization (see Appendix B) we evaluate (5.47) in $d = 3-2\epsilon$ dimension into a power series with respect to the deviation ϵ and realize that B_2 is zero in the physical limit $\epsilon \to 0$:

$$B_2 \overset{3-2\epsilon}{=} \mathcal{O}\left(\epsilon\right) . \tag{5.48}$$

Thus we conclude that B_2 does not contribute to the basketball diagram in three dimensions.

Calculation of $\mathbf{B_1}$ As before we first apply (B.1) to (5.40)

$$\begin{aligned} B_1 &= \frac{1}{\Gamma(d/2)}\sum_{a=1}^\infty\sum_{b=1}^\infty\sum_{c=1}^\infty z^{a+b+c}\,\mathrm{Re}\, i\int_0^\infty dx\, x^{d/2-1}e^{-abcx} \\ &\quad \times\int_0^\infty d\lambda\exp\left\{2iabx\lambda - (a+b+c)\,x\lambda^2\right\} . \end{aligned} \tag{5.49}$$

With the help of the standard integrals [55]

$$\int_0^\infty d\lambda\, \lambda^{\nu-1} e^{-\beta\lambda^2-\gamma\lambda} = (2\beta)^{-\nu/2}\,\Gamma(\nu) e^{\gamma^2/\nu\beta} D_{-\nu}\left(\frac{\gamma}{\sqrt{2\beta}}\right) \tag{5.50}$$

$$\int_0^\infty dt\, e^{-tz} t^{-1+\beta/2} D_{-\nu}\left(2\sqrt{kt}\right) = \frac{\sqrt{\pi}\,\Gamma\left(\beta\right)\left(z+k\right)^{-\beta/2}}{2^{\beta+\nu/2-1}\Gamma\left((\nu+\beta+1)/2\right)}\, {}_2F_1\left(\frac{\nu}{2},\frac{\beta}{2},\frac{\nu+\beta+1}{2},\frac{z-k}{z+k}\right), \tag{5.51}$$

where $D_\nu(z)$ are parabolic cylinder functions, we get:

$$B_1 = \frac{2^{1-d}\sqrt{\pi}\,\Gamma(d-1)}{\Gamma(d/2)\Gamma(\frac{d+1}{2})}\sum_{a=1}^\infty\sum_{b=1}^\infty\sum_{c=1}^\infty \frac{z^{a+b+c}}{(abc)^{\frac{d-1}{2}}\sqrt{a+b+c}} \times \mathrm{Re}\, i\, {}_2F_1\left(\frac{1}{2},\frac{d-1}{2},\frac{d+1}{2},1+\frac{ab}{c\,(a+b+c)}\right). \tag{5.52}$$

The above hypergeometric function is still a complex one as one can see with help of its integral representation [55]

$${}_2F_1\left(\alpha,\beta,\gamma,z\right) = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma-\beta)}\int_0^1 dt\, t^{\beta-1}\left(1-t\right)^{\gamma-\beta-1}\left(1-tz\right)^{-\alpha} \tag{5.53}$$

But by transforming the argument [55] according to

$$\begin{aligned} {}_2F_1\left(\alpha,\beta,\gamma,z\right) &= \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)}\, {}_2F_1\left(\alpha,\beta,\alpha+\beta-\gamma+1,1-z\right) \\ &+ \left(1-z\right)^{\gamma-\alpha-\beta}\frac{\Gamma(\gamma)\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\Gamma(\beta)}\, {}_2F_1\left(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1,1-z\right), \end{aligned} \tag{5.54}$$

we can separate out its imaginary part:

$$\begin{aligned} &\mathrm{Im}\, {}_2F_1\left(\frac{1}{2},\frac{d-1}{2},\frac{d+1}{2},1+\frac{ab}{c\,(a+b+c)}\right) \\ &= -\frac{2\Gamma(\frac{d+1}{2})}{\Gamma(\frac{d-1}{2})}\left(\frac{ab}{c\,(a+b+c)}\right)^{\frac{1}{2}}\, {}_2F_1\left(d/2,1,\frac{3}{2},-\frac{ab}{c\,(a+b+c)}\right). \end{aligned} \tag{5.55}$$

to arrive at

$$B_1 = \frac{2^{2-d}\sqrt{\pi}\,\Gamma(d-1)}{\Gamma(d/2)\Gamma(\frac{d-1}{2})}\sum_{a=1}^\infty\sum_{b=1}^\infty\sum_{c=1}^\infty \frac{z^{a+b+c}}{(ab)^{d/2-1}\, c^{d/2}\,(a+b+c)}\, {}_2F_1\left(d/2,1,\frac{3}{2},-\frac{ab}{c\,(a+b+c)}\right) \tag{5.56}$$

After simplifying the Gamma functions [55], we state the preliminary result for B_1:

$$B_1 = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty} \frac{z^{a+b+c}}{(ab)^{d/2-1}\, c^{d/2}\,(a+b+c)}\, {}_2F_1\left(d/2, 1, \frac{3}{2}, -\frac{ab}{c\,(a+b+c)}\right) . \tag{5.57}$$

It is useful to transform the argument of the hypergeometric function yielding

$$B_1 = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty} \frac{z^{a+b+c}}{(abc)^{d/2-1}\,(a+c)(b+c)}\, {}_2F_1\left(1, \frac{3-d}{2}, \frac{3}{2}, \frac{ab}{(a+c)(b+c)}\right) . \tag{5.58}$$

If we would now set $d=3$, we were left with the famous sum of Huang et al. [44–46]:

$$B_1 \overset{d=3}{=} \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty} \frac{z^{a+b+c}}{\sqrt{abc}(a+c)(b+c)} . \tag{5.59}$$

However, we are interested in the phase transition (4.38) and thus in an expansion in powers of the chemical potential μ. This is connected with the appearance of UV divergencies characterized by ϵ poles for $d = 3 - 2\epsilon$. To separate out these poles we need the above generalization (5.58) of the Huang result for arbitrary dimension d.

As we are not really interested in the basketball itself, but in its contribution to the particle number we differentiate (5.58) with respect to the chemical potential μ:

$$\frac{1}{\beta}\frac{\partial B_1}{\partial \mu} = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty} \frac{(a+b+c)z^{a+b+c}}{(abc)^{d/2-1}\,(a+c)(b+c)}\, {}_2F_1\left(1, \frac{3-d}{2}, \frac{3}{2}, \frac{ab}{(a+c)(b+c)}\right) \tag{5.60}$$

Because of the symmetry of the sums, (5.60) is equivalent to

$$\frac{1}{\beta}\frac{\partial B_1}{\partial \mu} = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty} \frac{(2a+c)z^{2a+c}}{(abc)^{d/2-1}\,(a+c)(b+c)}\, {}_2F_1\left(1, \frac{3-d}{2}, \frac{3}{2}, \frac{ab}{(a+c)(b+c)}\right) \tag{5.61}$$

To get the desired expansion for small chemical potential μ, we take the series representation of the hypergeometric function [55]

$${}_2F_1\left(\alpha, \beta, \gamma, z\right) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)} \sum_{q=0}^{\infty} \frac{\Gamma(q+\alpha)\Gamma(q+\beta)}{q!\Gamma(q+\gamma)} \tag{5.62}$$

yielding

$$\frac{1}{\beta}\frac{\partial B_1}{\partial \mu} = \frac{\sqrt{\pi}}{2\Gamma(\frac{3-d}{2})} \sum_{q=0}^{\infty} \frac{\Gamma(\frac{3-d}{2}+q)}{\Gamma(\frac{3}{2}+q)} \sum_{a=1}^{\infty}\sum_{b=1}^{\infty}\sum_{c=1}^{\infty} \frac{(2a+c)z^{a+b+c}}{(ab)^{d/2-1-q}\, c^{d/2-1}(a+c)^{q+1}(b+c)^{q+1}} . \tag{5.63}$$

For the denominator in $1/(a+b)^{q+1}$ we apply (B.1) to make contact with polylogarithmic functions (A.1):

$$\begin{aligned}\frac{1}{\beta}\frac{\partial B_1}{\partial \mu} &= \frac{\sqrt{\pi}}{2\Gamma(\frac{3-d}{2})}\sum_{q=0}^{\infty}\frac{\Gamma(\frac{3-d}{2}+q)}{\Gamma(q+1)^2\Gamma(\frac{3}{2}+q)}\int_0^{\infty}dx\,x^q\int_0^{\infty}dy\,y^q \\ &\quad\times\Big[2\zeta_{d/2-2-q}(ze^{-x})\zeta_{d/2-1-q}(ze^{-y})\zeta_{d/2-1}(ze^{-x-y}) \\ &\qquad+\zeta_{d/2-1-q}(ze^{-x})\zeta_{d/2-1-q}(ze^{-y})\zeta_{d/2-2}(ze^{-x-y})\Big]\,. \end{aligned} \tag{5.64}$$

Now we have expressed the basketball contribution to the particle density through polylogarithmic functions in arbitrary dimensions. This is a very nice result, because we can now use the Robinson expansion (A.4) to calculate all contributions for a small chemical potential μ.

Singular pieces At first we calculate only the singular terms of the Robinson expansion. To do so, it is more convenient to start at (5.60) and to write with (B.1):

$$a+b+c=\frac{1}{(a+b+c)^{-1}}=\frac{1}{\Gamma(-1)}\int_0^{\infty}dz\,z^{-2}e^{-(a+b+c)z}\,, \tag{5.65}$$

yielding

$$\frac{1}{\beta}\frac{\partial B_1}{\partial \mu} = \frac{\sqrt{\pi}}{2\Gamma(\frac{3-d}{2})}\sum_{q=0}^{\infty}\frac{\Gamma(\frac{3-d}{2}+q)}{\Gamma(q+1)^2\Gamma(\frac{3}{2}+q)}\,I(q)\,, \tag{5.66}$$

where

$$\begin{aligned} I(q) &= \frac{1}{\Gamma(-1)}\int_0^{\infty}\frac{dz}{z^2}\int_0^{\infty}dx\,x^q\int_0^{\infty}dy\,y^q \\ &\quad\times\zeta_{d/2-1-q}(ze^{-x-z})\zeta_{d/2-1-q}(ze^{-y-z})\zeta_{d/2-1}(ze^{-x-y-z})\,. \end{aligned} \tag{5.67}$$

The singular terms of the Robinson formula (A.4) are

$$\zeta_{\nu}^{\rm sing}(e^x)=\Gamma(1-\nu)(-x)^{\nu-1}\,. \tag{5.68}$$

Thus we obtain from (5.67) the singular term

$$\begin{aligned} I^{\rm sing}(q) &= (-\beta\mu)^{3d/2-5}\frac{\Gamma(2+q-d/2)\Gamma(2-d/2)}{\Gamma(-1)}\int_0^{\infty}dz\,z^{-2}(1+z)^{3d/2-4} \\ &\quad\times\int_0^{\infty}dx\,x^q(1+x)^{d/2-2-q}\int_0^{\infty}dy\,y^q(1+y)^{d/2-2-q}(1+x+y)^{d/2-2}\,. \end{aligned} \tag{5.69}$$

The first integral can be done immediately. The last integral is one of the integral representations of the hypergeometric function [55]. So we are left with a standard integral over Gauss hypergeometric function

$$
\begin{aligned}
I^{\rm sing}(q) &= (-\beta\mu)^{3d/2-5}\frac{\Gamma(2+q-d/2)^2\Gamma(2-d/2)\Gamma(3-d)\Gamma(1+q)\Gamma(5-3d/2)}{\Gamma(4-d+q)\Gamma(4-3d/2)} \\
&\times\int_0^\infty dx\, x^q(1+x)^{d/2-2-q}\,{}_2F_1\left(2-d/2,3-d,4-d+q,-x\right)\,, \qquad (5.70)
\end{aligned}
$$

which gives once more a hypergeometric one [55]:

$$
\begin{aligned}
&\int_0^\infty dx\, x^q(1+x)^{d/2-2-q}\,{}_2F_1\left(2-d/2,3-d,4-d+q,-x\right) = \\
&\frac{\Gamma(1+q)\Gamma(1-d/2)}{\Gamma(2+q-d/2)}\,{}_3F_2\left(2-d/2,3-d,q+1,4-d+q,d/2\right) \\
&+\frac{\Gamma(4-d+q)\Gamma(4-3d/2)\Gamma(d/2-1)}{\Gamma(2-d/2)\Gamma(5+q-3d/2)} \\
&\times\,{}_3F_2\left(3-d,4-3d/2,2+q-d/2,5+q-3d/2,2-d/2,1\right)\,. \qquad (5.71)
\end{aligned}
$$

Because of the argument $3-d=2\epsilon$ in both hypergeometric functions, we can now evaluate them up to $\mathcal{O}(\epsilon)$:

$$
{}_3F_2\left(2-d/2,3-d,q+1,4-d+q,d/2,1\right) = 1+(4-4\ln 2)\,\epsilon+\mathcal{O}(\epsilon^2)\,, \qquad (5.72)
$$

and

$$
{}_3F_2\left(3-d,4-3d/2,2+q-d/2,5+q-3d/2,2-d/2,1\right) = 1-4\ln 2\,\epsilon+\mathcal{O}(\epsilon^2)\,. \qquad (5.73)
$$

The remaining sums can be simply calculated:

$$
\begin{aligned}
\sum_{q=0}^{\infty}\frac{\Gamma(\frac{3-d}{2}+q)\Gamma(2+q-d/2)^2}{q!\Gamma(\frac{3}{2}+q)\Gamma(5+q-3d/2)} &= 2\frac{\Gamma(\frac{3-d}{2})\Gamma(2-d/2)^2}{\sqrt{\pi}\Gamma(5-3d/2)}\left[1+(2-\ln 4)\epsilon\right]=\frac{2}{\epsilon}+4+\mathcal{O}(\epsilon)\,, \\
\sum_{q=0}^{\infty}\frac{\Gamma(\frac{3-d}{2}+q)\Gamma(2+q-d/2)}{\Gamma(\frac{3}{2}+q)\Gamma(4-d+q)} &= 4\frac{1-2^{d-2}}{(d-2)(d-3)}=\frac{2}{\epsilon}-8\ln 2+4+\mathcal{O}(\epsilon)\,. \qquad (5.74)
\end{aligned}
$$

Putting all together and evaluating all terms up to the order $\mathcal{O}(\epsilon)$ gives us the singular contribution of B_1 to the particle number:

$$
\frac{1}{\beta}\frac{\partial B_1^{\rm sing}}{\partial\mu} \overset{d=3-2\epsilon}{=} \frac{\pi^{3/2}}{\sqrt{-\beta\mu}}\left[\frac{1}{\epsilon}+2-10\ln 2-3\gamma-3\ln(-\beta\mu)\right]+\mathcal{O}(\epsilon)\,. \qquad (5.75)
$$

So the overall contribution of the basketball diagram to the particle number, which comes only from the zero matsubara modes, reads:

$$
\frac{1}{\beta}\frac{\partial B^{\rm sing}}{\partial\mu} \overset{d=3-2\epsilon}{=} 16\frac{a^2V}{\lambda^5}\frac{\pi^{3/2}}{\sqrt{-\beta\mu}}\left[\frac{1}{\epsilon}+2-10\ln 2-3\gamma-3\ln(-\beta\mu)+6\ln\lambda\right]\,. \qquad (5.76)
$$

Comparison with High Temperature Limit Integrating the result above we arrive at

$$B^{\rm sing} = -32\frac{a^2V\pi^{\frac{3}{2}}}{\lambda^5}\sqrt{-\beta\mu}\left(\frac{1}{\epsilon}+8-3\gamma-10\ln 2-3\ln x+6\ln\lambda\right). \tag{5.77}$$

This is the most singular contribution to the fully temperature dependent basketball. It was calculated by only considering the singular Robinson terms which corresponds to zero Matsubara modes. To compare this result with the classical limit of ϕ^4 theory we multiply $B^{\rm sing}$ with the commonly used MS scale $\left(\frac{e^\gamma s^2}{4\pi}\right)^{3\epsilon}$:

$$B^{\rm sing}_{MS} = -32\frac{a^2V\pi^{3/2}}{\lambda^5}\sqrt{-\beta\mu}\left[\frac{1}{\epsilon}+8-4\ln 2+6\ln\left(\frac{s}{2M}\right)\right], \tag{5.78}$$

where $M=\sqrt{-2m\mu}$. Indeed, this expression coincides exactly with the high temperature or classical limit of the basketball diagram in ϕ^4 field theory [92].

Regular pieces In the vicinity of the phase transition the renormalized chemical potential vanishes. Therefore, we only need to expand physical quantities, for instance, the particle number up to $\mathcal{O}(\mu^0)$, if we want to calculate its critical properties. To get these constant contributions which stem from regular Robinson terms we start at (5.64). There we can neglect all $q>0$ terms, which are either of order $\mathcal{O}(\mu)$ or of order $\mathcal{O}(\epsilon)$.

$$\begin{aligned}\frac{1}{\beta}\frac{\partial B_1^{\rm q=0}}{\partial\mu} &= \int_0^\infty dx\int_0^\infty dy\,\Big[2\zeta_{d/2-2}(ze^{-x})\zeta_{d/2-1}(ze^{-y})\zeta_{d/2-1}(ze^{-x-y})\\ &\quad+\zeta_{d/2-1}(ze^{-x})\zeta_{d/2-1}(ze^{-y})\zeta_{d/2-2}(ze^{-x-y})\Big]. \end{aligned}\tag{5.79}$$

Using

$$\frac{d}{dx}\zeta_\nu(ze^{-x}) = -\zeta_{\nu-1}(ze^{-x}), \tag{5.80}$$

integration by parts yields

$$\int_0^\infty dx\zeta_{-1/2}(ze^{-x})\zeta_{1/2}(ze^{-x-y}) = \zeta_{1/2}(z)\zeta_{1/2}(ze^{-y}) - \int_0^\infty dx\zeta_{1/2}(ze^{-x})\zeta_{-1/2}(ze^{-x-y}). \tag{5.81}$$

Inserting (5.81) into (5.79) yields

$$\frac{1}{\beta}\frac{\partial B_1^{q=0}}{\partial\mu} = I_1 - I_2, \tag{5.82}$$

where

$$I_1 = 2\zeta_{1/2}(z) \int_0^\infty dx \zeta_{1/2}(ze^{-x})^2 \tag{5.83}$$

and

$$I_2 = \int_0^\infty dx \int_0^\infty dy \zeta_{1/2}(ze^{-x})\zeta_{1/2}(ze^{-y})\zeta_{-1/2}(ze^{-x-y}) \,. \tag{5.84}$$

This is the starting point for an expansion with respect to small chemical potential μ. We substract in (5.83) the singular pieces of the Robinson formula (A.4) and set $d = 3$ and $\mu = 0$ in the rest

$$\begin{aligned} I_1 &= 2\zeta_{d/2-1}(z)\Gamma(2-d/2) \int_0^\infty \Big[\Gamma(2-d/2)\left(-\beta\mu + x\right)^{d-4} \\ &\quad + 2\zeta(d/2-1)\left(-\beta\mu + x\right)^{d/2-2}\Big] + 4\pi C_1 \,, \end{aligned} \tag{5.85}$$

where C_1 is a constant, which is given by:

$$C_1 = \lim_{\mu\to 0} \frac{1}{4\pi} \int_0^\infty dx \left[\zeta_{1/2}(e^{\beta\mu - x})^2 - \frac{\pi}{-\beta\mu + x}\right] . \tag{5.86}$$

A numerical evaluation leads to

$$C_1 \approx -0.57 \,. \tag{5.87}$$

We calculate the integrals and evaluate the remaining polylogarithmic function in (5.85) to obtain

$$\begin{aligned} I_1 &= I_1^{\text{sing}} - \frac{2\zeta(d/2-1)\Gamma(2-d/2)^2(-\beta\mu)^{d-3}}{d-3} - \frac{8\Gamma(2-d/2)^2\zeta(d/2-1)(-\beta\mu)^{d-3}}{d-2} \\ &\quad + 8\pi C_1 \zeta(d/2-1) + \mathcal{O}[(-\beta\mu)^{d/2-1}] \,. \end{aligned} \tag{5.88}$$

Here I_1^{sing} is the contribution in (5.83) corresponding only to singular Robinson terms, which has been already calculated and is included in B^{sing} (5.77):

$$I_1^{\text{sing}} = -\frac{2\Gamma(2-d/2)^3(-\beta\mu)^{3d/2-5}}{d-3} + 8\pi C_1 \Gamma(2-d/2)(-\beta\mu)^{d/2-2} \tag{5.89}$$

$$\overset{d=3-2\epsilon}{=} \frac{\pi^{3/2}}{\sqrt{-\beta\mu}} \left[\frac{1}{\epsilon} - 3\ln(-\beta\mu) - 3\gamma - 6\ln 2 + 8C_1\right] . \tag{5.90}$$

The whole integral gives in $d = 3 - 2\epsilon$:

$$\begin{aligned} I_1 &= \frac{\pi^{3/2}}{\sqrt{-\beta\mu}} \left[\frac{1}{\epsilon} - 3\ln(-\beta\mu) - 3\gamma - 6\ln 2 + 8C_1\right] \\ &\quad + \pi\zeta(\tfrac{1}{2}) \left[\frac{1}{\epsilon} - 2\ln(-\beta\mu) - \frac{5}{2}\gamma - \frac{11}{2}\ln 2 - \frac{1}{2}\ln\pi - \frac{\pi}{4} + 8C_1 - 8\right] + \mathcal{O}(\sqrt{-\beta\mu}) \,. \end{aligned} \tag{5.91}$$

The second integral is a little bit more elaborate:

$$
\begin{aligned}
I_2 &= \Gamma(3-d/2)\,(-\beta\mu)^{3d/2-5}\,\Gamma(2-d/2)^2\int_0^\infty dx\int_0^\infty dy \\
&\quad\times\left[(1+x)^{d/2-2}\,(1+y)^{d/2-2}\,(1+x+y)^{d/2-3}\right] \\
&\quad+2\Gamma(2-d/2)\Gamma(3-d/2\zeta(d/2-1)\,(-\beta\mu)^{d-3}\int_0^\infty dx\int_0^\infty dy \\
&\quad\times\left[(1+x)^{d/2-2}\,(1+x+y)^{d/2-3}\right] \\
&\quad+4\pi C_2+\mathcal{O}\left(\sqrt{-\beta\mu}\right) \qquad (5.92)
\end{aligned}
$$

The constant C_2 is given by substracting the above singular pieces from the polylogarithmic functions and setting $d=3$ in the rest:

$$
\begin{aligned}
C_2 &= \lim_{\mu\to 0}\int_0^\infty dx\int_0^\infty dy\,\Big[\zeta_{1/2}(ze^{-x})\zeta_{1/2}(ze^{-y})\zeta_{d/2-2}(ze^{-x-y}) \qquad (5.93)\\
&\quad-\frac{\pi^{3/2}}{2(-\beta\mu+x)^{1/2}(-\beta\mu+y)^{1/2}(-\beta\mu+x+y)^{3/2}}-\frac{\pi\zeta(1/2)}{(-\beta\mu+x)^{1/2}(-\beta\mu+x+y)^{3/2}}\Big]\,.
\end{aligned}
$$

A numerical evaluation leads to

$$
C_2 \approx 0.26\,. \qquad (5.94)
$$

The first integral includes once more the singular pieces, which are already included in $B^{\rm sing}$. We can calculate them with the same method used there, yielding:

$$
\begin{aligned}
I_2^{\rm sing} &= \Gamma(3-d/2)\,(-\beta\mu)^{3d/2-5}\,\Gamma(2-d/2)^2\int_0^\infty dx\int_0^\infty dy \\
&\quad\times(1+x)^{d/2-2}\,(1+y)^{d/2-2}\,(1+x+y)^{d/2-3} \\
&\overset{d=3-2\epsilon}{=} \frac{2\pi^{3/2}\ln 2}{\sqrt{-\beta\mu}}\,. \qquad (5.95)
\end{aligned}
$$

The second integral is standard [55], yielding:

$$
\begin{aligned}
&\int_0^\infty dx\int_0^\infty dy\,(1+x)^{d/2-2}\,(1+x+y)^{d/2-3} \\
&=\int_0^\infty dx\,(1+x)^{d-4}\int_0^\infty dy\,(1+y)^{d/2-3}=\frac{2}{(d-3)(d-4)}\,. \qquad (5.96)
\end{aligned}
$$

So the result for the second integral reads:

$$
\begin{aligned}
I_2 &= I_2^{\rm sing}+\frac{4\Gamma(2-d/2)\Gamma(3-d/2)\zeta(d/2-1)\,(-\beta\mu)^{d-3}}{(d-3)(d-4)}+4\pi C_2+\mathcal{O}(\sqrt{-\beta\mu}) \\
&\overset{d=3-2\epsilon}{=} \frac{2\pi^{3/2}\ln 2}{\sqrt{-\beta\mu}}+\pi\zeta(1/2)\left[\frac{1}{\epsilon}-2\ln(-\beta\mu)-\frac{5}{2}\gamma-\frac{11}{2}\ln 2-\frac{1}{2}\ln\pi-\frac{\pi}{4}\right] \\
&\quad+4\pi C_2+\mathcal{O}(\sqrt{-\beta\mu})\,. \qquad (5.97)
\end{aligned}
$$

So the result for the $q=0$ contribution to the particle number, which includes all regular terms up to $\mathcal{O}(\sqrt{\mu})$ is:

$$\begin{aligned}\frac{1}{\beta}\frac{\partial B_1^{q=0}}{\partial\mu} &= \frac{\pi^{3/2}}{\sqrt{-\beta\mu}}\left[\frac{1}{\epsilon}-3\ln(-\beta\mu)-3\gamma-8\ln 2+8C_1\right] \\ &\quad -8\pi\zeta(1/2)+8\pi\zeta(\frac{1}{2})C_1-4\pi C_2\mathcal{O}(\sqrt{\mu})\,. \qquad (5.98)\end{aligned}$$

Final Result The contribution of the whole basketball diagram to the particle number, expanded up to $\mathcal{O}(\sqrt{-\beta\mu})$, reads:

$$\begin{aligned}\frac{1}{\beta}\frac{\partial B}{\partial\mu} &= \frac{16a^2V}{\lambda^5}\left\{\frac{\pi^{3/2}}{\sqrt{-\beta\mu}}\left[\frac{1}{\epsilon}-3\ln(-\beta\mu)+6\ln\lambda-3\gamma-10\ln 2+2+8C_1\right]\right. \\ &\quad \left. -8\pi\zeta(1/2)+8\pi\zeta(1/2)C_1-4\pi C_2\right\}+\mathcal{O}(\sqrt{\mu})\,, \qquad (5.99)\end{aligned}$$

where the constants c_1 and c_2 are given by (5.87) and (5.94) respectively. We have already mentioned that the terms of the first line in (5.99) correspond to the results of classical field theory [92]. On the other hand, the finite temperature contribution

$$K_{\mathrm{B}}=-8\pi\zeta(1/2)+8\pi\zeta(1/2)C_1-4\pi C_2\approx 54.4 \qquad (5.100)$$

agrees well with the result of Arnold et al. in [31, (5.30)] obtained from a matching calculation.

Chapter 6

Calculation of Self-Energy Diagrams

We consider all contributions of the self-energy (4.19) which are necessary to determine the renormalized chemical potential μ_r. According to (4.39) they are contained in

$$\Sigma(\mathbf{0}, \omega_m = 0) = \Sigma^{(1)}(\mathbf{0}, 0) + \Sigma^{(2)}(\mathbf{0}, 0) \,, \tag{6.1}$$

where the first order term yields (2.62)

$$\Sigma^{(1)}(\mathbf{0}, = 0) = -\frac{2g}{\hbar} G(\mathbf{0}, 0) = -\frac{4a_s}{\hbar\beta\lambda} \zeta_{d/2}(e^{\beta\mu}) \tag{6.2}$$

and the second order contribution

$$\begin{aligned} \Sigma^{(2)}(\mathbf{0}, 0) = 4D + 2S \;\; = \;\; & \frac{4g^2}{\hbar^2} G(\mathbf{0}, 0) \int_0^{\hbar\beta} d\tau \int d^d x \, G(\mathbf{x}, \tau) G(-\mathbf{x}, -\tau) \\ & + \frac{2g^2}{\hbar^2} \int_0^{\hbar\beta} d\tau \int d^d x \, G(\mathbf{x}, \tau)^2 G(-\mathbf{x}, -\tau) \end{aligned} \tag{6.3}$$

will be calculated in the next two sections. Here D denotes the double chain and S the sunset diagram in (6.3).

6.1 Double Chain

The integrals in the double chain diagram

$$D \;\; = \;\; \frac{g^2}{\hbar^2} G(\mathbf{0}, 0) \int_0^{\hbar\beta} d\tau \int d^d x \, G(\mathbf{x}, \tau) G(-\mathbf{x}, -\tau) \tag{6.4}$$

have already been computed in Section 5.1, yielding

$$D \;\; = \;\; 4V \left(\frac{a}{\lambda}\right)^2 \zeta_{d/2}(z) \zeta_{d/2-1}(z) \,. \tag{6.5}$$

6.2 Sunset

The sunset diagram is defined by

$$S = \frac{g^2}{\hbar^2} \int_0^{\hbar\beta} d\tau \int d^d x \, G(\mathbf{x},\tau)^2 G(-\mathbf{x},-\tau) \,. \tag{6.6}$$

Inserting (2.60) yields

$$\begin{aligned} S = & \left(-\frac{g}{\hbar}\right)^2 \int_0^{\hbar\beta} d\tau \int d^d x \int \frac{d^d p}{(2\pi\hbar)^d} \int \frac{d^d q}{(2\pi\hbar)^d} \int \frac{d^d k}{(2\pi\hbar)^d} \\ & \times \frac{1}{2} e^{\frac{i}{\hbar}\mathbf{p}\mathbf{x}} \frac{\theta(\tau) \, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{p}^2}{2m}-\mu\right)\left(\tau - \frac{\hbar\beta}{2}\right)} + (\tau \Longleftrightarrow -\tau)}{\sinh \frac{\beta}{2}\left(\frac{\mathbf{p}^2}{2m}-\mu\right)} \\ & \times \frac{1}{2} e^{\frac{i}{\hbar}\mathbf{q}\mathbf{x}} \frac{\theta(\tau) \, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{q}^2}{2m}-\mu\right)\left(\tau - \frac{\hbar\beta}{2}\right)} + (\tau \Longleftrightarrow -\tau)}{\sinh \frac{\beta}{2}\left(\frac{\mathbf{q}^2}{2m}-\mu\right)} \\ & \times \frac{1}{2} e^{-\frac{i}{\hbar}\mathbf{k}\mathbf{x}} \frac{\theta(\tau) \, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{k}^2}{2m}-\mu\right)\left(-\tau - \frac{\hbar\beta}{2}\right)} + (\tau \Longleftrightarrow -\tau)}{\sinh \frac{\beta}{2}\left(\frac{\mathbf{k}^2}{2m}-\mu\right)} \,. \end{aligned} \tag{6.7}$$

Now we repeat the same steps, that were necessary to calculate the basketball diagram:

- performing the space integrations,
- simplifying the fractions by using the definition of the Heaviside function,
- and working out the τ-integrals.

This yields the intermediate result:

$$S = \frac{g^2 \beta V}{4} \int_{\mathbf{p}} \int_{\mathbf{q}} \int_{\mathbf{k}} \frac{(2\pi\hbar)^d \, \delta^{(d)}(\mathbf{p}+\mathbf{q}-\mathbf{k})}{E_{\mathbf{p}} + E_{\mathbf{q}} - E_{\mathbf{k}}} \frac{\sinh \frac{\beta}{2}(E_{\mathbf{p}} + E_{\mathbf{q}} - E_{\mathbf{k}})}{\sinh \frac{\beta E_{\mathbf{p}}}{2} \sinh \frac{\beta E_{\mathbf{q}}}{2} \sinh \frac{\beta E_{\mathbf{k}}}{2}} \,. \tag{6.8}$$

Furthermore we

- make contact with the Bose distribution function

$$\sinh \frac{\beta E}{2} = 2n(E) e^{\frac{\beta E}{2}} \,, \tag{6.9}$$

- use its property

$$n(E) e^{\beta E} = n(E) + 1 \,, \tag{6.10}$$

- and permutate the indices using

$$n(E_{\mathbf{p}})n(E_{\mathbf{k}}) \hat{=} n(E_{\mathbf{q}})n(E_{\mathbf{k}}) \tag{6.11}$$

to arrive at

$$S = g^2\beta V \int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}} (2\pi\hbar)^d \, \delta^{(d)}(\mathbf{p}+\mathbf{q}-\mathbf{k}) \frac{2n(E_{\mathbf{p}})n(E_{\mathbf{k}}) - n(E_{\mathbf{p}})n(E_{\mathbf{q}}) + n(E_{\mathbf{k}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}} . \tag{6.12}$$

Now we consider the easiest piece, which contains only one Bose distribution:

$$I_3 = \int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}} (2\pi\hbar)^d \, \delta^{(d)}(\mathbf{p}+\mathbf{q}-\mathbf{k}) \frac{n(E_{\mathbf{k}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}} , \tag{6.13}$$

and calculate it by using the well known tricks (5.29)-(5.31) to obtain

$$I_3 = \sum_{a=1}^{\infty} \mathrm{Re} \lim_{\epsilon\downarrow 0} \int_0^{i\infty} d\lambda e^{(\mu-i\epsilon)\lambda} \int d^d x \int_{\mathbf{p}} e^{-\frac{\mathbf{p}^2}{2m}\lambda + \frac{i}{\hbar}\mathbf{x}\mathbf{p}} \int_{\mathbf{q}} e^{-\frac{\mathbf{p}^2}{2m}\lambda + \frac{i}{\hbar}\mathbf{x}\mathbf{q}} \int_{\mathbf{k}} e^{-\frac{\mathbf{p}^2}{2m}(\beta a-\lambda) - \frac{i}{\hbar}\mathbf{x}\mathbf{k}} . \tag{6.14}$$

The momentum integrals contained in I_3 are standard Fresnel integrals (5.33) and (5.34), yielding

$$\begin{aligned} I_3 &= \left(\frac{m}{2\pi}\right)^{3d/2} \frac{1}{\hbar^{3d}} \sum_{a=1}^{\infty} e^{\beta\mu a} \mathrm{Re} \lim_{\epsilon\downarrow 0} \int_0^{i\infty} d\lambda \frac{e^{(\mu-i\epsilon)\lambda}}{\lambda^d (\beta a-\lambda)^{d/2}} \\ &\quad \times \int d^d x \exp\left\{ -\frac{m\mathbf{x}^2}{2\hbar^2}\left(\frac{2}{\lambda}+\frac{1}{\beta a-\lambda}\right)\right\} . \end{aligned} \tag{6.15}$$

The remaining space integral in I_3 is Gaussian and is calculated immediately. Finally, we are left with a one dimensional integral

$$I_3 = \left(\frac{m}{2\pi\hbar}\right)^d \beta^{1-d} \sum_{a=1}^{\infty} e^{\beta\mu a} \mathrm{Re} \int_0^{i\infty} d\lambda \frac{e^{\beta\mu\lambda}}{(2a\lambda-\lambda^2)^{d/2}} . \tag{6.16}$$

The other integrals can be calculated in exactly the same manner, yielding:

$$\begin{aligned} I_1 &= 2\int_{\mathbf{p}}\int_{q}\int_{\mathbf{k}} (2\pi\hbar)^d \, \delta^{(d)}(\mathbf{p}+\mathbf{q}-\mathbf{k}) \frac{n(E_{\mathbf{p}})n(E_{\mathbf{k}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}} \\ &= 2\left(\frac{m}{2\pi\hbar}\right)^d \beta^{1-d} \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} e^{\beta\mu(a+b)} \mathrm{Re} \int_0^{i\infty} d\lambda \frac{e^{\beta\mu\lambda}}{(2b\lambda+ab-\lambda^2)^{d/2}} \end{aligned} \tag{6.17}$$

and

$$\begin{aligned} I_2 &= -\int_{\mathbf{p}}\int_{\mathbf{q}}\int_{\mathbf{k}} (2\pi\hbar)^d \, \delta^{(d)}\left(\mathbf{p}+\mathbf{q}-\mathbf{k}\right) \frac{n(E_{\mathbf{p}})n(E_{\mathbf{q}})}{E_{\mathbf{p}}+E_{\mathbf{q}}-E_{\mathbf{k}}} \\ &= -\left(\frac{m}{2\pi\hbar}\right)^d \beta^{1-d} \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} e^{\beta\mu(a+b)} \mathrm{Re} \int_0^{i\infty} d\lambda \frac{e^{\beta\mu\lambda}}{\left(ab-\lambda^2\right)^{d/2}} \,. \end{aligned} \tag{6.18}$$

Inserting (6.16)-(6.18) in (6.12) yields:

$$S = \frac{4a^2 V}{\lambda^{2d-4}} \left(2S_3 - S_2 + S_1\right) \,, \tag{6.19}$$

where

$$S_1 = \sum_{a=1}^{\infty} e^{\beta\mu a} \, \mathrm{Re} \, i \int_0^{\infty} dx \, \frac{e^{i\beta\mu x}}{\left(2iax + x^2\right)^{d/2}} \,, \tag{6.20}$$

$$S_2 = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} e^{\beta\mu(a+b)} \, \mathrm{Re} \, i \int_0^{\infty} dx \, \frac{e^{i\beta\mu x}}{\left(ab + x^2\right)^{d/2}} \,, \tag{6.21}$$

$$S_3 = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} e^{\beta\mu(a+b)} \, \mathrm{Re} \, i \int_0^{\infty} dx \frac{e^{i\beta\mu x}}{\left(2ixb + ab + x^2\right)^{d/2}} \,. \tag{6.22}$$

Our aim is now an expansion of the above sunset sums up to $O(\sqrt{-\beta\mu})$.

Calculation of S_1 Substituting the sums in S_1 by integrals like in Section A.2.2 yields the most singular contribution corresponding to the singular Robinson terms:

$$S_1^{\text{sing}} = \int_0^{\infty} da \, e^{\beta\mu a} \, \mathrm{Re} \, i \int_0^{\infty} dx \, \frac{e^{i\beta\mu x}}{\left(2iax + x^2\right)^{d/2}} \,. \tag{6.23}$$

We can separate out the dependence of this integral from the chemical potential:

$$S_1^{\text{sing}} = (-\beta\mu)^{d-2} \int_0^{\infty} da \, e^{-a} \, \mathrm{Re} \, i \int_0^{\infty} dx \, \frac{e^{-ix}}{\left(2iax + x^2\right)^{d/2}} \,. \tag{6.24}$$

This means that I_1 is of order $\mathcal{O}(-\beta\mu)$ in three dimension.

The same result can be obtained from a Taylor expansion of the exponential function in (6.20):

$$S_1 = \sum_{k=0}^{\infty} \frac{(\beta\mu)^k}{k!} \, \mathrm{Re} \, i^{k+1} \sum_{a=1}^{\infty} e^{\beta\mu a} \underbrace{\int_0^{\infty} dx \, \frac{x^k}{\left(2iax + x^2\right)^{d/2}}}_{:=I_1} \,. \tag{6.25}$$

The integral I_1 can be calculated with the Schwinger trick (B.1):

$$I_1 = \frac{1}{\Gamma(d/2)} \int_0^\infty dx\, x^{k-d/2} \int_0^\infty dy\, y^{d/2-1} e^{-(2ia+x)y} \tag{6.26}$$

yielding

$$I_1 = (2ia)^{1-d+k} \frac{\Gamma(1+k-d/2)\Gamma(d-1-k)}{\Gamma(d/2)} . \tag{6.27}$$

Inserting (6.27) in (6.25) yields:

$$S_1 = \frac{\cos\frac{\pi}{2}(2-d)}{2^{d-1}\Gamma(d/2)} \sum_{k=0}^\infty \frac{2^k \left(-\beta\mu\right)^k \Gamma(1+k-d/2)\Gamma(d-1-k)}{k!} \sum_{a=1}^\infty \frac{e^{\beta\mu a}}{a^{d-k-1}} . \tag{6.28}$$

The sum running over index a can be identified as a polylogarithmic function (A.1):

$$S_1 = \frac{\cos\frac{\pi}{2}(2-d)}{2^{d-1}\Gamma(d/2)} \sum_{k=0}^\infty \frac{2^k \left(-\beta\mu\right)^k \Gamma(1+k-d/2)\Gamma(d-1-k)}{k!} \zeta_{d-k-1}\left(e^{\beta\mu}\right) . \tag{6.29}$$

This expression is the starting point for an analysis of the sunset part S_1 for small $\beta\mu$. For this purpose we expand the polylogarithmic function according to Robinson formula (A.4).

$$\zeta_{d-k-1}\left(e^{\beta\mu}\right) = \Gamma(2+k-d)\left(-\beta\mu\right)^{d-k-2} + \zeta(d-k-1) + O(\beta\mu) . \tag{6.30}$$

We see immediately that the singular Robinson term gives a contribution of $O(\beta\mu)$ and thus has not to be considered in our analysis. The second term also vanishes because the cosine in the above sum gives zero and we have no compensating singularity for $k = 0$. Thus we obtain

$$S_1 = O(-\beta\mu) . \tag{6.31}$$

Calculation of S_2 From (6.21) we get for the singular piece of S_2:

$$S_2^{\text{sing}} = \left(-\beta\mu\right)^{d-3} \int_0^\infty da \int_0^\infty db\, e^{-(a+b)}\, \mathrm{Re}\, i \int_0^\infty dx\, \frac{e^{-ix}}{\left(ab+x^2\right)^{d/2}} . \tag{6.32}$$

The remaining integral can be calculated numerically, if we set $d = 3$:

$$S_2^{\text{sing}} \stackrel{d=3}{=} \int_0^\infty da \int_0^\infty db\, e^{-(a+b)} \int_0^\infty dx\, \frac{\sin x}{\left(ab+x^2\right)^{3/2}} = 2.5476 . \tag{6.33}$$

However, we are able to calculate S_2^{sing} exactly. To this end we introduce polar coordinates $a = r\cos\phi$ and $b = r\sin\phi$:

$$S_2^{\text{sing}} = \int_0^\infty dr\, r \int_0^{\pi/2} d\phi\, e^{-r(\cos\phi+\sin\phi)} \int_0^\infty dx\, \frac{\sin x}{(r^2\sin\phi\cos\phi + x^2)^{3/2}}\,. \quad (6.34)$$

Transforming the angle

$$u(\phi) = \frac{1}{1+\tan\phi} \quad (6.35)$$

and the radial variable

$$R(r) = r\frac{1+\tan\phi}{\sqrt{1+\tan^2\phi}} \quad (6.36)$$

results in

$$S_2^{\text{sing}} = \int_0^\infty dR\, R\, e^{-R} \int_0^1 du \int_0^\infty dx\, \frac{\sin x}{(R^2u - R^2u^2 + x^2)^{3/2}}\,. \quad (6.37)$$

Computing the u-integral yields

$$S_2^{\text{sing}} = 4\int_0^\infty dR\, R\, e^{-R} \int_0^\infty dx\, \frac{\sin x}{x(R^2+4x^2)}\,. \quad (6.38)$$

We decompose the denominator

$$S_2^{\text{sing}} = 4\int_0^\infty dR\, \frac{e^{-R}}{R} \int_0^\infty dx\, \sin x \left(\frac{1}{x} - \frac{4x}{R^2+4x^2}\right) \quad (6.39)$$

and calculate both x-integrals with the help of basic residue theory yielding:

$$\int_0^\infty dx\, \frac{\sin x}{x} = \frac{\pi}{2} \quad (6.40)$$

and

$$\int_0^\infty dx \frac{x\sin x}{R^2/4 + x^2} = -\frac{\pi}{2} e^{-R/2}\,. \quad (6.41)$$

The remaining integral over the radial component is straightforward

$$S_2^{\text{sing}} = 2\pi\left(\int_0^\infty \frac{dR}{R}\, e^{-R} - \int_0^\infty \frac{dR}{R}\, e^{-3R/2}\right) = 2\pi \ln\frac{3}{2}\,. \quad (6.42)$$

This coincides exactly with the numerical value (6.33)

To get the regular contribution of order $\mathcal{O}(\sqrt{-\beta\mu})$, we make a Taylor expansion

$$S_2 = \sum_{k=0}^{\infty} \frac{(\beta\mu)^k}{k!} \operatorname{Re} i^{k+1} \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} e^{\beta\mu(a+b)} \underbrace{\int_0^{\infty} dx \, \frac{x^k}{(ab+x^2)^{d/2}}}_{:=I_2} . \tag{6.43}$$

The following analysis is similar to the calculation of I_1. Therefore we only state the results:

$$I_2 \;=\; (ab)^{\frac{1-d+k}{2}} \frac{\Gamma(\frac{k+1}{2})\Gamma(\frac{d-k-1}{2})}{2\Gamma(d/2)} . \tag{6.44}$$

Inserting (6.44) into (6.43) yields

$$S_2 \;=\; \sum_{k=0}^{\infty} \frac{(\beta\mu)^k \cos\frac{\pi}{2}(k+1)\Gamma(\frac{k+1}{2})\Gamma(\frac{d-k-1}{2})}{2\Gamma(k+1)\Gamma(d/2)} \zeta_{\frac{d-k-1}{2}} \left(e^{\beta\mu}\right)^2 . \tag{6.45}$$

Because of the cosine, every second term of the sum is zero. Inserting the Robinson expansion for the polylogarithmic function

$$\zeta_{d/2-k}\left(e^{\beta\mu}\right) = \Gamma(1+k-d/2)\,(-\beta\mu)^{d/2-k-1} + \zeta\,(d/2-k) + O(\beta\mu)\,, \tag{6.46}$$

gives a square root contribution for $k=1$ and $d=3$ coming from mixing the singular term and the zeta function by the square of the polylogarithmic function:

$$S_2^{\text{reg}} \;=\; \frac{\Gamma(\frac{d-2}{2})\Gamma(\frac{4-d}{2})}{\Gamma(d/2)} \zeta\left(\frac{d-2}{2}\right)(-\beta\mu)^{\frac{d-2}{2}} + O(\beta\mu) \overset{d=3}{=} 2\sqrt{\pi}\,\zeta(1/2)\sqrt{-\beta\mu} + O(\beta\mu)\,. \tag{6.47}$$

So the final result for S_2 reads:

$$S_2 = 2\pi \ln\frac{3}{2} + 2\sqrt{\pi}\zeta(1/2)\sqrt{-\beta\mu} + O(\beta\mu) \tag{6.48}$$

Calculation of S_3 The part S_3 is the most complicate one. We are not able to calculate its singular terms as straightforward as for S_2. Thus, we expand the exponential function in a Taylor series

$$S_3 \;=\; \sum_{k=0}^{\infty} \frac{(\beta\mu)^k}{k!} \operatorname{Re} i^{k+1} \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} e^{\beta\mu(a+b)} \int_0^{\infty} dx \frac{x^k}{(2ixb+ab+x^2)^{d/2}} . \tag{6.49}$$

In analogy to (5.50) we treat the denominator with the Schwinger trick (B.1) and make use of (5.51) to obtain

$$\begin{aligned} S_3 &= \frac{2^{1-d}\sqrt{\pi}}{\Gamma(d/2)\,\Gamma\left(\frac{d+1}{2}\right)} \sum_{k=0}^{\infty} (\beta\mu)^k\, \Gamma(d-k-1)\,\mathrm{Re}\, i^{k+1} \\ &\quad \times \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} \frac{e^{\beta\mu(a+b)}}{(ab)^{\frac{d-k-1}{2}}}\, {}_2F_1\left(\frac{k+1}{2}, \frac{d-k-1}{2}, \frac{d+1}{2}, 1+\frac{b}{a}\right). \end{aligned} \tag{6.50}$$

The above hypergeometric function is still a complex one, as one can see with its integral representation (5.53). It can be transformed to real hypergeometric functions with the identity (5.54). Consequently, S_3 consists of two major parts

$$S_3 = S_{31} + S_{32} \tag{6.51}$$

with

$$\begin{aligned} S_{31} &= \frac{-2^{2-d}\pi}{\Gamma(d/2)} \sum_{k=0}^{\infty} \frac{(\beta\mu)^k\, \Gamma(d-k-1)\cos\left(\frac{\pi}{2}(k+2)\right)}{\Gamma\left(\frac{k+1}{2}\right)\Gamma\left(\frac{d-k-1}{2}\right)} \\ &\quad \times \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} \frac{e^{\beta\mu(a+b)}}{a^{\frac{d-k}{2}}\, b^{\frac{d-k}{2}-1}}\, {}_2F_1\left(\frac{d-k}{2}, 1+\frac{k}{2}, \frac{3}{2}, -\frac{b}{a}\right) \end{aligned} \tag{6.52}$$

and

$$\begin{aligned} S_{32} &= \frac{2^{1-d}\pi}{\Gamma(d/2)} \sum_{k=0}^{\infty} \frac{(\beta\mu)^k\, \Gamma(d-k-1)\cos\left(\frac{\pi}{2}(k+1)\right)}{\Gamma\left(1+\frac{k}{2}\right)\Gamma\left(\frac{d-k}{2}\right)} \\ &\quad \times \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} \frac{e^{\beta\mu(a+b)}}{(ab)^{\frac{d-k-1}{2}}}\, {}_2F_1\left(\frac{k+1}{2}, \frac{d-k-1}{2}, \frac{1}{2}, -\frac{b}{a}\right). \end{aligned} \tag{6.53}$$

As we will see later on, it is easier to transform the argument of the hypergeometric function in (6.52) from $-b/a$ to $b/(b+a)$:

$$\begin{aligned} S_{31} &= \frac{-2^{2-d}\pi}{\Gamma(d/2)} \sum_{k=0}^{\infty} \frac{(\beta\mu)^k\, \Gamma(d-k-1)\cos\left(\frac{\pi}{2}(k+2)\right)}{\Gamma\left(\frac{k+1}{2}\right)\Gamma\left(\frac{d-k-1}{2}\right)} \\ &\quad \times \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} \frac{e^{\beta\mu(a+b)}}{a^{d/2-k-1}\, b^{\frac{d-k}{2}-1}\,(a+b)^{1+\frac{k}{2}}}\, {}_2F_1\left(1+\frac{k}{2}, \frac{3-d+k}{2}, \frac{3}{2}, \frac{b}{b+a}\right) \end{aligned} \tag{6.54}$$

and

$$\begin{aligned} S_{32} &= \frac{2^{1-d}\pi}{\Gamma(d/2)} \sum_{k=0}^{\infty} \frac{(\beta\mu)^k\, \Gamma(d-k-1)\cos\left(\frac{\pi}{2}(k+1)\right)}{\Gamma\left(1+\frac{k}{2}\right)\Gamma\left(\frac{d-k}{2}\right)} \\ &\quad \times \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} \frac{e^{\beta\mu(a+b)}}{a^{d/2-k-1}\, b^{\frac{d-k-1}{2}}\,(a+b)^{\frac{k+1}{2}}}\, {}_2F_1\left(\frac{k+1}{2}, 1+\frac{k-d}{2}, \frac{1}{2}, \frac{b}{b+a}\right) \end{aligned} \tag{6.55}$$

We use the series representation of hypergeometric functions (5.62) and the Schwinger trick (B.1) to make contact with polylogarithmic functions:

$$
\begin{aligned}
S_{31} &= \frac{-2^{1-d}\pi^{\frac{3}{2}}}{\Gamma(d/2)} \sum_{k=0}^{\infty} \frac{(\beta\mu)^k \Gamma(d-k-1)\cos\left(\frac{\pi}{2}(k+2)\right)}{\Gamma\left(\frac{k+1}{2}\right)\Gamma(\frac{d-k-1}{2})\Gamma(1+\frac{k}{2})\Gamma(\frac{3-d+k}{2})} \\
&\quad \times \sum_{q=0}^{\infty} \frac{\Gamma(\frac{3-d+k}{2}+q)}{q!\Gamma(\frac{3}{2}+q)} \int_0^\infty dx\, x^{\frac{k}{2}+q} \zeta_{d/2-k-1}(ze^{-x})\zeta_{\frac{d-k}{2}-1-q}(ze^{-x}) \qquad (6.56)
\end{aligned}
$$

and

$$
\begin{aligned}
S_{32} &= \frac{2^{1-d}\pi^{\frac{3}{2}}}{\Gamma(d/2)} \sum_{k=0}^{\infty} \frac{(\beta\mu)^k \Gamma(d-k-1)\cos\left(\frac{\pi}{2}(k+1)\right)}{\Gamma\left(1+\frac{k}{2}\right)\Gamma\left(\frac{d-k}{2}\right)\Gamma(\frac{k+1}{2})\Gamma(1+\frac{k-d}{2})} \\
&\quad \times \sum_{q=0}^{\infty} \frac{\Gamma(1+q+\frac{k-d}{2})}{q!\Gamma(\frac{1}{2}+q)} \int_0^\infty dx\, x^{\frac{k-1}{2}+q} \zeta_{d/2-k-1}(ze^{-x})\zeta_{\frac{d-k-1}{2}-q}(ze^{-x}) . \qquad (6.57)
\end{aligned}
$$

Here, z denotes the fugacity $z = e^{\beta\mu}$.

Singular Terms The UV divergencies only arise from the $k = 0$ contribution of S_{31}

$$
S_{31}^{k=0} = \frac{\sqrt{\pi}}{2} \sum_{q=0}^{\infty} \frac{\Gamma(\frac{3-d}{2}+q)}{q!\Gamma(\frac{3}{2}+q)} \int_0^\infty dx\, x^q \zeta_{d/2-1}(ze^{-x})\zeta_{d/2-1-q}(ze^{-x}) . \qquad (6.58)
$$

If we insert only the singular terms of the polylogarithmic functions (A.4), we obtain

$$
S_{31}^{k=0,\text{sing}} = \frac{\sqrt{\pi}}{2}(-\beta\mu)^{d-3} \sum_{q=0}^{\infty} \frac{\Gamma(\frac{3-d}{2}+q)}{q!\Gamma(\frac{3}{2}+q)} \int_0^\infty dx\, x^q (1+x)^{d-q-4} . \qquad (6.59)
$$

The x-integral represents Gamma functions yielding

$$
S_{31}^{k=0,\text{sing}} = \frac{\sqrt{\pi}}{2}(-\beta\mu)^{d-3}\Gamma(d-3)\Gamma(2-d/2) \sum_{q=0}^{\infty} \frac{\Gamma(\frac{3-d}{2}+q)\Gamma(2+q-d/2)}{\Gamma(\frac{3}{2}+q)\Gamma(4+q-d)} . \qquad (6.60)
$$

The remaining sum can be reduced to a geometric one by simplifying the Gamma functions with the identities in [55]

$$
S_{31}^{k=0,\text{sing}} = \frac{\sqrt{\pi}}{2}(-\beta\mu)^{d-3}\Gamma(d-3)\Gamma(2-d/2) \frac{4-2^d}{(d-2)(d-3)} . \qquad (6.61)
$$

This yields in $d = 3 - 2\epsilon$ dimensions

$$
S_{31}^{k=0,\text{sing}} = \pi \left(\frac{1}{2\epsilon} - 3\ln 2 - \gamma - \ln x + 1 \right) . \qquad (6.62)
$$

To calculate terms with $k > 0$ it is more convenient to start at (6.52). As there are no UV divergencies for $k > 0$, we can set $d = 3$ from the beginning. The cosine function in the numerator enables us to transform the index from k to $2k$, because all odd contributions vanish. Furthermore, we use the series representation of the hypergeometric function to obtain

$$\begin{aligned} S_{31}^{k>0} &= \frac{\pi}{2} \sum_{k=1}^{\infty} \frac{(-1)^k (\beta\mu)^{2k} \Gamma(2-2k)}{\Gamma(k+\frac{1}{2})\Gamma(1-k)\Gamma(\frac{3}{2}-k)\Gamma(1+k)} \\ &\times \sum_{q=0}^{\infty} \frac{(-1)^q \Gamma(\frac{3}{2}-k+q)\Gamma(1+k+q)}{q!\Gamma(\frac{3}{2}+q)} \zeta_{\frac{3}{2}-k+q}(z)\zeta_{\frac{1}{2}-k-q}(z) . \end{aligned} \tag{6.63}$$

Considering the singular parts of the polylogarithmic functions and solving the q sum by simplifying the Gamma functions as before, we get gives:

$$S_{31}^{k>0,\text{sing}} = -\frac{\sqrt{\pi}}{4} \sum_{k=1}^{\infty} \left(-\frac{1}{4}\right)^k \frac{\Gamma(2-2k)\Gamma(k-\frac{1}{2})}{\Gamma(1-k)k} , \tag{6.64}$$

which is evaluated to be

$$S_{31}^{k>0,\text{sing}} = \frac{\pi}{2} \sum_{k=1}^{\infty} \left(\frac{1}{16}\right)^k \frac{1}{k} = -\frac{\pi}{2} \ln \frac{15}{16} . \tag{6.65}$$

A similar calculation for S_{32}^{sing}, where all even terms vanish, yields:

$$S_{32}^{\text{sing}} = \frac{\pi}{2} \ln \frac{5}{3} . \tag{6.66}$$

Thus we conclude

$$S_3^{\text{sing}} = \pi \left(\frac{1}{2\epsilon} - 3\ln 2 - \gamma - \ln x + 1 + \ln \frac{4}{3} \right) . \tag{6.67}$$

Regular terms A dimensional analysis shows that all regular terms with $k, q > 0$ in S_{32} are of Order $\mathcal{O}(-\beta\mu)$. So we only need to evaluate:

$$S_{31}^{k=q=0} = \frac{2^{2-d}\sqrt{\pi}\Gamma(d-1)}{\Gamma(d/2)\Gamma(\frac{d-1}{2})} \int_0^{\infty} dx \zeta_{d/2-1}(ze^{-x})^2 = \int_0^{\infty} dx \zeta_{d/2-1}(ze^{-x})^2 \tag{6.68}$$

We already calculated this integral, when we considered the basketball diagram (5.83). The result was:

$$S_{31}^{k=q=0} = S_{31}^{k=q=0,\text{sing}} - 4\sqrt{\pi}\sqrt{-\beta\mu}\zeta(1/2) + 4\pi C_1 + \mathcal{O}(-\beta\mu) , \tag{6.69}$$

where $S_{31}^{k=q=0,\mathrm{sing}}$ comes from the singular Robinson terms, that are included in S_{31}^{sing}. A similar analysis for S_{32} shows, that we only need to consider $k=1$ and $q=0$:

$$S_{32}^{k=1,q=0} = \frac{(-\beta\mu)}{d-2}\int_0^\infty dx\zeta_{d/2-2}(ze^{-x})\zeta_{d/2-1}(ze^{-x})\,. \tag{6.70}$$

The Robinson expansion (A.4) and separating the singular terms yields

$$S_{32}^{k=1,q=0} = S_{32}^{k=1,q=0,\mathrm{sing}} - 2\frac{\zeta(d/2-1)}{(d-2)(d-4)}(-\beta\mu)^{d/2-2} + \mathcal{O}[(-\beta\mu)^{\frac{d-1}{2}}]\,. \tag{6.71}$$

This is evaluated in $d=3$ dimensions

$$S_{32}^{k=1,q=0} = S_{32}^{k=1,q=0,\mathrm{sing}} + 2\sqrt{\pi}\sqrt{-\beta\mu}\zeta(\frac{1}{2}) + \mathcal{O}[(-\beta\mu)]\,. \tag{6.72}$$

Finally, we add all contributions (6.67), (6.69) and (6.72) for S_3 to obtain

$$S_3 = \pi\left(\frac{1}{2\epsilon} - 3\ln 2 - \gamma - \ln x + 1 + \ln\frac{4}{3} - 2\sqrt{\pi}\sqrt{-\beta\mu}\zeta(\frac{1}{2})\right) \tag{6.73}$$

Final result Now we have calculated all pieces S_1, S_2 and S_3 that belong to the sunset diagram:

$$\begin{aligned} S = \frac{4a^2V}{\lambda^2}\Bigg[&\frac{\pi}{\epsilon} + 2\pi - 2\pi\gamma - 2\pi\ln x + 4\pi\ln\lambda - 4\pi\ln 3 \\ &+8\pi C_1 - 6\sqrt{\pi}\sqrt{-\beta\mu}\,\zeta(\frac{1}{2}) + \mathcal{O}(-\beta\mu)\Bigg]\,. \end{aligned} \tag{6.74}$$

For comparison with the high temperature limit we multiply the part of the sunset corresponding to singular Robinson terms

$$S^{\mathrm{sing}} = S_2^{\mathrm{sing}} + S_3^{\mathrm{sing}} = \frac{4a^2V}{\lambda^2}\left(\frac{\pi}{\epsilon} + 2\pi - 2\pi\gamma - 2\pi\ln x + 4\pi\ln\lambda - 4\pi\ln 3\right) \tag{6.75}$$

with the MS scale $\left(\frac{e^\gamma s^2}{4\pi}\right)^{2\epsilon}$ and recall that $\lambda = (2\pi\hbar^2\beta/m)^{1/2}$ is the thermal wavelength to get

$$S_{MS}^{\mathrm{sing}} = 4\frac{a^2V\pi}{\lambda^2}\left[\frac{1}{\epsilon} + 4\ln\left(\frac{s}{2M}\right) + 2 + 4\ln\frac{2}{3}\right]\,, \tag{6.76}$$

where $M=\sqrt{-2m\mu}$. This agrees with the sunset diagram of classical ϕ^4-field theory [92]. Contrary to the calculation of the basketball diagram (5.99), the matching calculation of Arnold et al. [31] allows no comparison with the finite temperature contributions in (6.74)

$$K_{\mathrm{S}} = 8\pi C_1 - 6\sqrt{\pi}\sqrt{-\beta\mu}\,\zeta(\frac{1}{2})\,. \tag{6.77}$$

Chapter 7

Shift of Critical Temperature

As a first application of our results in Chapters 5 and 6 we answer the question how the critical temperature has changed due to weak interactions. In analogy to (1.9) the starting point for calculating the critical temperature is the particle density

$$n = -\frac{1}{V}\frac{\partial \Omega}{\partial \mu} = -\frac{1}{V}\frac{\partial}{\partial \mu}\left(\Omega^{(0)} + \Omega^{(1)} + \Omega^{(2)}\right) , \tag{7.1}$$

which turns out to be with (5.1)-(5.4), (5.12), and (5.99):

$$\begin{aligned} n\lambda^d &= \zeta_{d/2}(z) - \frac{4a_s}{\lambda}\zeta_{d/2}(z)\zeta_{d/2-1}(z) + \frac{16a_s^2}{\lambda^2}\zeta_{d/2}(z)\zeta_{d/2-1}(z)^2 + \frac{8a_s^2}{\lambda^2}\zeta_{d/2}(z)^2\zeta_{d/2-2}(z) \\ &\quad + \frac{8a_s^2}{\lambda^2}\frac{\pi^{3/2}}{\sqrt{x}}\left[\frac{1}{\epsilon} + 2 - 4\ln 2 + 6\ln\left(\frac{s}{2M}\right) + 8C_1\right] \\ &\quad + \frac{8a_s^2}{\lambda^2}\left[8\pi C_1\zeta(1/2) - 8\pi\zeta(1/2) - 4\pi C_2\right] + \mathcal{O}(a_s^3) , \end{aligned} \tag{7.2}$$

where $z = \exp(-x) = \exp(\beta\mu)$ is the fugacity and the second-order contribution has already been evaluated in $d = 3 - 2\epsilon$ dimensions. From (4.38) we know that the phase transition is determined from the vanishing of the renormalized chemical potential, which can be obtained from the self-energy calculated in (6.1)-(6.3), (6.5), and (6.74):

$$\begin{aligned} x_r &= x - \hbar\beta\Sigma(\mathbf{p} = \mathbf{0}, \omega_m = 0) = x + \frac{4a_s}{\lambda}\zeta_{d/2}(z) - \frac{16a_s^2}{\lambda^2}\zeta_{d/2}(z)\zeta_{d/2-1}(z) \\ &\quad - \frac{8a_s^2\pi}{\lambda^2}\left[\frac{1}{\epsilon} + 4\ln\left(\frac{s}{2M}\right) + 2 + 4\ln\frac{2}{3} + 8C_1 - \frac{6\sqrt{x}}{\sqrt{\pi}}\zeta(1/2)\right] + \mathcal{O}(a_s^3) , \end{aligned} \tag{7.3}$$

where $z_r = \exp(-x_r) = \exp(\beta\mu_r)$. Now we replace the bare chemical potential μ in (7.2) in favor of the renormalized chemical potential μ_r. To this end we invert relationship

(7.3) to obtain

$$
\begin{aligned}
x &= x_r - \frac{4a_s}{\lambda}\zeta_{d/2}(z_r) + \frac{8a_s^2\pi}{\lambda^2}\left[\frac{1}{\epsilon} + 4\ln\left(\frac{s}{2M}\right) + 2\right. \\
&\left. +4\ln\frac{2}{3} + 8C_1 - \frac{8\sqrt{x_r}}{\sqrt{\pi}}\zeta(1/2)\right]. \qquad (7.4)
\end{aligned}
$$

Inserting (7.4) into (7.2) yields three different contributions to the renormalized particle density coming from the zeroth, first and second order term.

Contributions from $\mathcal{O}(a_s^0)$: We start with the free energy for the free gas

$$
n\lambda^d \stackrel{(0)}{=} \zeta_{d/2}(z(z_r)) . \qquad (7.5)
$$

Inserting (7.4) and evaluating up to the order $\mathcal{O}(a_s^3)$ yields:

$$
\begin{aligned}
n\lambda^d &\stackrel{(0)}{=} \zeta_{d/2}(z_r) + \frac{4a_s}{\lambda}\zeta_{d/2}(z_r)\zeta_{d/2-1}(z_r) + \frac{8a_s^2}{\lambda^2}\zeta_{d/2}(z_r)^2\zeta_{d/2-2}(z_r) \\
&-\frac{8a_s^2\pi}{\lambda^2}\zeta_{d/2-1}(z_r)\left[\frac{1}{\epsilon} + 4\ln\left(\frac{s}{2M}\right) + 2 + 4\ln\frac{2}{3} + 8C_1 - \frac{8\sqrt{x_r}}{\sqrt{\pi}}\zeta(1/2)\right] . \qquad (7.6)
\end{aligned}
$$

To evaluate this expression to order $\mathcal{O}(\epsilon^0)$ for $d = 3 - 2\epsilon$, we remember that the right-hand side of (7.5) has to be multiplied with the scale $(e^\gamma s^2/4\pi)^\epsilon$ as soon as we work in the MS scheme, see for instance (5.99). With that modification we get

$$
\begin{aligned}
n\lambda^3 &\stackrel{(0)}{=} \zeta_{3/2}(z_r) + \frac{4a_s}{\lambda}\zeta_{3/2}(z_r)\zeta_{1/2}(z_r) + \frac{8a_s^2}{\lambda^2}\zeta_{3/2}(z_r)^2\zeta_{-1/2}(z_r) \\
&-\frac{8a_s^2\pi^{3/2}}{\lambda^2}\frac{1}{\sqrt{x}}\left[\frac{1}{\epsilon} + 6\ln\left(\frac{s}{2M}\right) + 2 + 4\ln\frac{2}{3} + 8C_1 - \frac{8\sqrt{x}}{\sqrt{\pi}}\zeta(1/2)\right] \\
&-\frac{8a_s^2\pi^{3/2}}{\lambda^2}\zeta\left(\frac{1}{2}\right)\left[\frac{1}{\epsilon} + 4\ln\left(\frac{s}{2M}\right) + 2 + 4\ln\frac{2}{3} + 8C_1\right. \\
&\left.+\frac{1}{4}\left(2\gamma - 14\ln 2 - 6\ln\pi - \pi\right) + 2\ln\lambda s\right] . \qquad (7.7)
\end{aligned}
$$

Contributions from $\mathcal{O}(a_s^1)$: The vacuum contribution of order $\mathcal{O}(a_s^1)$ reads:

$$
n\lambda^d \stackrel{(1)}{=} -\frac{4a_s}{\lambda}\zeta_{d/2}(e^{-x(x_r)})\zeta_{d/2-1}(e^{-x(x_r)}) . \qquad (7.8)
$$

The renormalization yields in $d = 3 - 2\epsilon$ dimensions:

$$
\begin{aligned}
n\lambda^3 &= -\frac{4a_s}{\lambda}\zeta_{1/2}(z_r)\zeta_{3/2}(z_r) - \frac{16a_s^2}{\lambda^2}\zeta_{1/2}(z_r)^2\zeta_{3/2}(z_r) \\
&-\frac{16a_s^2}{\lambda^2}\zeta_{-1/2}(z_r)\zeta_{3/2}(z_r)^2 \qquad (7.9)
\end{aligned}
$$

Contributions from $\mathcal{O}(a_s^2)$: In the second order contribution to the particle density (7.2), we only need to replace x by x_r and set $d = 3$:

$$
\begin{aligned}
n\lambda^3 \stackrel{(2)}{=} & \frac{16a_s^2}{\lambda^2}\zeta_{3/2}(z_r)\zeta_{1/2}(z_r)^2 + \frac{8a_s^2}{\lambda^2}\zeta_{3/2}(z_r)^2\zeta_{-1/2}(z_r) \\
& + \frac{8a_s^2}{\lambda^2}\frac{\pi^{3/2}}{\sqrt{x_r}}\left[\frac{1}{\epsilon} + 2 - 4\ln 2 + 6\ln\left(\frac{s}{2M}\right) + 8C_1\right] \\
& + \frac{8a_s^2\pi}{\lambda^2}\left[8C_1\zeta(1/2) - 8\zeta(1/2) - 4C_2\right] . \qquad (7.10)
\end{aligned}
$$

Final result We collect the results (7.7), (7.9), (7.10) and expand for small x_r to obtain

$$
\begin{aligned}
n\lambda^3 = & \zeta(3/2) - 2\sqrt{\pi}\sqrt{x_r} - 32\pi^{3/2}\ln\frac{4}{3}\frac{a_s^2}{\lambda^2}\frac{1}{\sqrt{x_r}} - 8\pi\zeta(1/2)\frac{a_s^2}{\lambda^2}\left[\frac{1}{\epsilon} + 4\ln\left(\frac{s}{2M}\right)\right. \\
& \left. + 2 + 4\ln\frac{2}{3} + \frac{1}{4}(2\gamma - 14\ln 2 - 6\ln\pi - \pi) + 2\ln\lambda s + 4C_2/\zeta(1/2)\right] . \qquad (7.11)
\end{aligned}
$$

On the basis of equation (7.11) we deal now with some questions, which we set up in the introduction of this work.

Classical Field Limit Let us first consider only the terms in (7.11) stemming from the classical limit of field theory, e.g. zeroth- and second-order terms that are proportional to $1/\sqrt{x_r}$. The leading shift of the critical temperature can be obtained from (7.11) as soon as we consider the critical limit $x_r = 0$ and make the ansatz

$$
T_c = T_c^{(0)} + \Delta T_c \, . \qquad (7.12)
$$

Inserting (7.12) into (7.11) yields

$$
\frac{\Delta T_c}{T_c^{(0)}} = a_0\sqrt{x_r^{(0)}} + \frac{a_2}{\sqrt{x_r^{(0)}}}\left(a_s n^{1/3}\right)^2 , \qquad (7.13)
$$

where

$$
x_r^{(0)} = -\frac{\mu_r}{k_{\mathrm{B}}T_c^{(0)}} , \qquad a_0 = \frac{4\sqrt{\pi}}{3\zeta(3/2)} , \qquad a_2 = \frac{64\pi^{3/2}\ln(4/3)}{3\zeta(3/2)^{5/3}} . \qquad (7.14)
$$

Thus perturbation theory shows no first order shift of the critical temperature (7.13) due to weak two-particle delta interactions. Now the question may arise: How does this result fit with the fact that in many publications such a linear contribution

$$
\frac{\Delta T_c}{T_c^{(0)}} = c_1 \, a_s n^{1/3} \qquad (7.15)
$$

was computed? The reason is, that those are non-perturbative results stemming from the term in (7.13) that is proportional to $1/\sqrt{x_r^{(0)}}$. If we compare (7.15) with (7.13) we can read off the coefficient

$$c_1 = \frac{1}{g}\, f_2(g)\,, \tag{7.16}$$

where

$$f_2(g) = a_0 + a_2 g^2\,, \qquad g = \frac{a_s n^{1/3}}{\sqrt{x_r^{(0)}}}\,. \tag{7.17}$$

Inserting (7.17) into (7.16) shows that c_1 is infrared (IF) divergent at the critical point, where $x_r^{(0)} = 0$, e.g. $g = \infty$. But as the particle density and the shift of the critical temperature is a finite quantity even in the thermodynamic limit, their resummation should also be finite. Thus the calculation of (7.16) is a typical strong-coupling problem. We master this problem with the help of variational perturbation theory. To this end we follow the procedure in Chapter 3 and identify (7.17) with (3.1) for $N = 2$ and $a_1 = 0$. As the renormalized chemical potential μ_r defines the natural scale of our theory, it corresponds to the artificial scale κ in (3.3). Thus it follows from dimensional reasons that we have to choose $p = 1/2$ and $q = 1/2$ in (3.3). Next we introduce a variational parameter K according to (3.4) and reexpand $f_2(g,K)$ similar to (3.9):

$$f_2(g,K) = \frac{3}{8}\sqrt{K}a_0 + \frac{1}{\sqrt{K}}a_0 - \frac{3}{8}\frac{1}{K^{7/2}}a_0 + \frac{g^2}{\sqrt{K}}a_2\,. \tag{7.18}$$

Using the principle of minimal sensitivity (3.10), the strong-coupling limit of the variational parameter (3.12) turns out to be

$$K_2(g) = \frac{8a_2}{3a_0}g^2 + \mathcal{O}(g^{-2})\,. \tag{7.19}$$

Inserting (7.19) into (7.18) yields

$$f_2(g) = 2g\sqrt{\frac{3a_0a_2}{8}} + \mathcal{O}(g^{-3})\,. \tag{7.20}$$

Thus the leading coefficient (7.16) becomes

$$c_1 = 2\sqrt{\frac{3a_0a_2}{8}} \approx 3.059\,. \tag{7.21}$$

Of course this has to be understood as a very rough approximation for c_1 as the above resummation was based on only two weak-coupling coefficients a_0 and a_2. However, we have observed that the leading shift of critical temperature is solely determined by the classical field limit. Thus the physics at $T_c^{(0)}$ can be described in terms of an effective three-dimensional field theory for the Matsubara mode $m = 0$. As the high temperature or classical limit of the Green function (2.63) is much simpler than the full temperature dependent one (2.60), one was able to calculate diagrams of higher orders in the coupling constant g [92] which were also connected with IF divergencies at the critical point. Recently, a resummation of these IF divergent terms was accomplished in our group with the help of VPT up to five loops resulting in a linear shift of the critical temperature with the proportionality constant $c_1 = 1.3$ [35]. In the meantime this five loop calculation has been extended to six loops [43] with $c_1 = 1.25$, which is the most accurate analytical calculation so far. This result has to be compared with recent Monte Carlo data which estimate $c_1 \approx 1.30$ [40]. Other analytic estimates are $c_1 \approx 2.90$ [25], 2.33 from a $1/N$-expansion [26], 1.71 from an improved $1/N$-expansion [30], and 3.06 from an inapplicable δ-expansion [32] to three loops, and 1.48 from the same δ-expansion to five loops, with a questionable evaluation at a complex extremum [33]. Note that all these results have in common that the shift in the critical temperature is positive. which can be explained within a reasonable physical argument: In a gas with the expansion parameter $a_s n^{1/3}$ the shift of the critical temperature is determined by two competing effects: For positive s-wave scattering lengths one expects the shift to become negative as the repulsive interaction suppresses condensation. On the other hand, the density of the system and thus the long-range correlations becomes larger, which stimulates condensation. As the second effect dominates for small interactions, the leading shift in the critical temperature is positive.

Quantum Fluctuations We now consider the terms in (7.11) coming from nonzero Matsubara modes. They still contain an ultraviolet (UV) divergency connected with the ϵ pole, which at first forbids the further evaluation of this expression. We assume that this UV divergence is waived by the renormalization of the physical mass m and therefore the computation of the second term in the expansion (4.30) becomes necessary. At the time of the delivery of this diploma thesis the renormalization of the physical mass was not yet final. However dimensional arguments indicate that it has the general form

$$m = m_r \left[1 + 8\pi \frac{a_s^2}{\lambda^2} \left(\frac{1}{\epsilon} + c \right) \right] , \tag{7.22}$$

where c is an unknown second-order coefficient that depends on the mass scale s. With (7.22) a mass renormalization of the second term in (7.11), which is proportional to the square root of the physical mass as $T_c^{(0)} \sim m$ (see (1.11)), cancels the UV divergence. Thus, using (7.12), the shift of the critical temperature turns out to have the general form

$$\frac{\Delta T_c}{T_c^{(0)}} = c_1 a_s n^{1/3} + a_s n^{1/3} (c_2' \ln a_s n^{1/3} + c_2) , \tag{7.23}$$

where c_1 is solely determined by the classical field limit. The result (7.23) has also been found by Arnold et al [31] with the coefficients $c_2' = -64\pi\zeta(1/2)/3\zeta(3/2)^{5/3} \approx 19.75$ and $c_2 \approx 75.7$. If one enters these results into the finite temperature phase diagram of Fig. 10.1, a very unsatisfactory result shows up. Even at infinitely high temperatures the existence of a BEC is forecast. Unfortunately, we cannot indicate own values for the coefficients c_2' and c_2 as we did not calculate the coefficient c in (7.22) up to now. However, in Part 3 of this work a physically meaningful result for the phase diagram has been computed without explicitly calculating the renormalization of the physical mass.

Part III:

Finite-Temperature

Loop Expansion

Chapter 8

Background Method

In many cases a perturbation expansion in terms of free fields, as elaborated in Part 2 of this thesis, cannot produce a useful insight into the physics of a many-body system. In particular, if the average of the field $\psi(\mathbf{x},\tau)$ is not zero, even small fluctuations show huge effects and can drive the system to a nonzero field configuration. If this equilibrium value is not small, perturbation theory is not applicable.
In Section 2.3 we introduced the effective action by a functional Legendre transformation as an ideal tool to describe a many-body system for non-vanishing field configurations. In practice, this procedure is quite cumbersome. Therefore, we present now an alternative way to obtain the effective action by using the so-called background method. This method is based on the idea to decompose the Bose field $\psi(\mathbf{x},\tau)$ in a non-vanishing background field $\Psi(\mathbf{x},\tau)$, which can be identified as the order parameter of our theory, and fluctuations $\delta\psi(\mathbf{x},\tau)$ around it. As we will apply this method to effectively homogeneous systems, the background field can be assumed to be constant: $\Psi(\mathbf{x},\tau) = \Psi$. Thus the effective action reduces to an effective potential $\mathcal{V}(\Psi,\Psi^*)$ whose optimal value with respect to Ψ,Ψ^* is the grand-canonical potential valid for $T < T_c$.
In the following we evaluate this effective potential $\mathcal{V}(\Psi,\Psi^*)$ in the framework of a loop expansion where the fluctuations around the constant background fields Ψ,Ψ^* are treated as small. By doing so, we investigate the global structure of the finite temperature phase diagram for weakly interacting gases as well as strong correlated bosons in optical lattice potentials.

8.1 Effective Potential

Like in perturbation theory the starting point of our considerations is the functional integral for the partition function

$$\mathcal{Z} = \oint \mathcal{D}\psi \oint \mathcal{D}\psi^* e^{-\mathcal{A}[\psi(x,\tau),\psi^*(x,\tau)]/\hbar} . \tag{8.1}$$

The action of a dilute, weakly interacting Bose gas was already mentioned in (1.17). We now expand the Bose fields around the so-called background field Ψ:

$$\psi(\mathbf{x},\tau) := \Psi + \delta\psi(\mathbf{x},\tau)\,, \qquad \psi^*(\mathbf{x},\tau) := \Psi^* + \delta\psi^*(\mathbf{x},\tau)\,. \tag{8.2}$$

Here we identify $|\Psi|^2$ with the order parameter, e.g. the condensate density, which is constant in space as long as we deal with homogeneous systems. With the above expressions the functional measure transforms like

$$\oint \mathcal{D}\psi \oint \mathcal{D}\psi^* \to \oint \mathcal{D}\delta\psi \oint \mathcal{D}\delta\psi^*\,, \tag{8.3}$$

and the action (1.17) decomposes into three parts

$$\mathcal{A} \;=\; \mathcal{A}^{(0)} + \mathcal{A}^{(\mathrm{quad})} + \mathcal{A}^{(\mathrm{int})}\,. \tag{8.4}$$

Here $\mathcal{A}^{(0)}$ denotes the tree-level contribution

$$\mathcal{A}^{(0)} \;=\; \hbar\beta V\left\{-\mu|\Psi|^2 + \frac{g}{2}|\Psi|^4\right\}\,, \tag{8.5}$$

$\mathcal{A}^{(\mathrm{quad})}$ contains all terms, which are quadratic in the fluctuations $\delta\psi, \delta\psi^*$ around the background field Ψ, Ψ^*

$$\mathcal{A}^{(\mathrm{quad})} \;=\; \int_0^{\hbar\beta} d\tau \int d^dx \left\{\delta\psi^*(\mathbf{x},\tau)\left[\hbar\partial_\tau + h(\mathbf{x}) - \mu + 2g|\Psi|^2\right]\delta\psi(\mathbf{x},\tau) + \frac{g}{2}\Psi^2\delta\psi^*(\mathbf{x},\tau)^2 + \frac{g}{2}\Psi^{*2}\delta\psi(\mathbf{x},\tau)^2\right\}, \tag{8.6}$$

and $\mathcal{A}^{(\mathrm{int})}$ is the interaction term

$$\mathcal{A}^{(\mathrm{int})} \;=\; \int_0^{\hbar\beta} d\tau \int d^dx \left\{g\Psi\delta\psi^*(\mathbf{x},\tau)^2\delta\psi(\mathbf{x},\tau) + g\Psi^*\delta\psi(\mathbf{x},\tau)^2\delta\psi^*(\mathbf{x},\tau) + \frac{g}{2}\delta\psi(\mathbf{x},\tau)^2\delta\psi^*(\mathbf{x},\tau)^2\right\}. \tag{8.7}$$

Note that the linear terms of the fluctuations $\delta\psi$ and $\delta\psi^*$ were neglected to guarantee that only the one-particle irreducible diagrams survive in the following diagrammatic analysis. The quadratic part of the action $\mathcal{A}^{(\mathrm{quad})}$ can be written in matrix form:

$$\mathcal{A}^{(\mathrm{quad})} = \frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \int d^dx \int d^dx' (\delta\psi^*, \delta\psi)(\mathbf{x},\tau) G^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') \begin{pmatrix}\delta\psi \\ \delta\psi^*\end{pmatrix}(\mathbf{x}',\tau')\,. \tag{8.8}$$

Here, we call $G^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau')$ the inverse Green function:

$$G^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') \;=\; \frac{1}{\hbar}M(\mathbf{x},\tau)\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau') \tag{8.9}$$

with the 2×2-matrix

$$M(\mathbf{x},\tau) \;=\; \begin{pmatrix} \hbar\partial_\tau + h(\mathbf{x}) - \mu + 2g|\Psi|^2 & g\Psi^2 \\ g\Psi^{*2} & -\hbar\partial_\tau + h(\mathbf{x}) - \mu + 2g|\Psi|^2 \end{pmatrix}. \tag{8.10}$$

The partition function has now become a functional of the background fields Ψ, Ψ^*:

$$\mathcal{Z}[\Psi,\Psi^*] \;=\; e^{-\mathcal{A}^{(0)}/\hbar} \oint \mathcal{D}\delta\psi\mathcal{D}\delta\psi^*\, e^{-\left\{\mathcal{A}^{(\mathrm{quad})}+\mathcal{A}^{(\mathrm{int})}\right\}/\hbar}. \tag{8.11}$$

In the following we will expand the weight factor $e^{-\mathcal{A}^{(\mathrm{int})}/\hbar}$ into a Taylor series. This leads to a series expansion in powers of $\hbar$ for the effective potential, which is defined by

$$e^{\mathcal{V}(\Psi,\Psi^*)} = \mathcal{Z}[\Psi,\Psi^*]\,. \tag{8.12}$$

According to (2.73), extremizing the effective action with respect to the background field leads to the grand-canonical potential.

Zero-loop Effective Potential The leading term in the saddle point approximation of the functional integral (8.11) reads

$$\mathcal{Z}^{(0)}[\Psi,\Psi^*] = \exp\left[-\beta V\left(-\mu|\Psi|^2 + \frac{g}{2}|\Psi|^4\right)\right] \tag{8.13}$$

and corresponds to the $\hbar^0$ contribution to the effective action:

$$\mathcal{V}^{(0)}[\Psi,\Psi^*] = -\beta V\left(-\mu|\Psi|^2 + \frac{g}{2}|\Psi|^4\right). \tag{8.14}$$

One-loop Effective Potential The leading order is obtained by only taking into account the zeroth term in the Taylor expansion $e^{-\mathcal{A}^{(\mathrm{int})}/\hbar} \approx 1$ and performing the functional integral over the quadratic part of the action:

$$\begin{aligned}\mathcal{Z}^{(1)}[\Psi,\Psi^*] \;=\; & \oint \mathcal{D}\delta\psi\mathcal{D}\delta\psi^* \exp\Bigg\{-\frac{1}{2\hbar}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \int d^dx \int d^dx' \\ & \times(\delta\psi^*,\delta\psi)(\mathbf{x},\tau)G^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau')\begin{pmatrix}\delta\psi\\ \delta\psi^*\end{pmatrix}(\mathbf{x}',\tau')\Bigg\}.\end{aligned} \tag{8.15}$$

This functional integral can be treated analogous to the simple integral

$$\int_{-\infty}^{\infty}\frac{d\delta\psi}{\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{d\delta\psi^*}{\sqrt{\pi}}\exp\left\{-(\delta\psi^*,\delta\psi)\,M\begin{pmatrix}\delta\psi\\ \delta\psi^*\end{pmatrix}\right\} = \frac{1}{\sqrt{\det M}} = e^{-\frac{1}{2}\mathrm{Tr}\log\mathrm{M}}. \tag{8.16}$$

Hence, the one-loop effective potential can be written as

$$\mathcal{V}^{(1)}[\psi,\psi^*] = -\frac{1}{2}\mathrm{Tr}\log G^{-1}\,. \tag{8.17}$$

Of course, the derivation presented here is a rather symbolic one. Instead the functional integral must be calculated using a Matsubara decomposition of the fluctuations $\delta\psi$ and $\delta\psi^*$. How to do this calculation will be shown in Section 8.3.

Two-loop Effective Potential One gets the two-loop contribution by taking into account the linear and quadratic terms of the Taylor expansion of the exponential function $e^{-\mathcal{A}^{(int)}/\hbar}$

$$\begin{aligned}\mathcal{Z}^{(2)}[\Psi,\Psi^*] &= \oint\mathcal{D}\psi\oint\mathcal{D}\psi^* e^{-\mathcal{A}^{(\mathrm{quad})}[\psi,\psi^*]/\hbar}\left\{\frac{g}{2\hbar}\int_1\psi_1^2\psi_1^{*2}+\frac{g^2\Psi^2}{2\hbar^2}\int_1\int_2\psi_1^{*2}\psi_1\psi_2^{*2}\psi_2\right.\\ &+\left.\frac{g^2\Psi^{*2}}{2\hbar^2}\int_1\int_2\psi_1^*\psi_1^2\psi_2^*\psi_2^2+\frac{g^2|\Psi|^2}{\hbar^2}\int_1\int_2\psi_1^{*2}\psi_1\psi_2^*\psi_2^2\right\}\,,\end{aligned} \tag{8.18}$$

where we used the short hand notation:

$$\int_0^{\hbar\beta} d\tau_1\int d^dx_1 = \int_1\,,\qquad \delta\psi(\mathbf{x_1},\tau_1)=\psi_1\,,\ \delta\psi^*(\mathbf{x_1},\tau_1)=\psi_1^*. \tag{8.19}$$

Here, we neglected odd terms in $\delta\psi$ and evaluated up to the sixth order in powers of the deviations $\delta\psi,\delta\psi^*$. Defining the ensemble average

$$\begin{aligned}\langle f(\psi^*,\psi)\rangle &:= \frac{\oint\mathcal{D}\psi\oint\mathcal{D}\psi^* f(\psi^*,\psi)e^{-\mathcal{A}^{(\mathrm{quad})}[\psi,\psi^*]/\hbar}}{\oint\mathcal{D}\psi\oint\mathcal{D}\psi^* e^{-\mathcal{A}^{(\mathrm{quad})}[\psi,\psi^*]/\hbar}}\\ &= e^{\frac{1}{2}\mathrm{Tr}\log G^{-1}}\oint\mathcal{D}\psi\oint\mathcal{D}\psi^* f(\psi^*,\psi)e^{-\mathcal{A}^{(\mathrm{quad})}[\psi,\psi^*]/\hbar}\,,\end{aligned} \tag{8.20}$$

we can write:

$$\begin{aligned}\mathcal{Z}^{(2)}[\Psi,\Psi^*] &= e^{\frac{1}{2}\mathrm{Tr}\log G^{-1}}\left(-\frac{g}{2\hbar}\int_1\langle\psi_1^2\psi_1^{*2}\rangle+\frac{g^2\Psi^2}{2\hbar^2}\int_1\int_2\langle\psi_1^{*2}\psi_1\psi_2^{*2}\psi_2\rangle\right.\\ &\left.+\frac{g^2\Psi^{*2}}{2\hbar^2}\int_1\int_2\langle\psi_1^*\psi_1^2\psi_2^*\psi_2^2\rangle+\frac{g^2|\Psi|^2}{\hbar^2}\int_1\int_2\langle\psi_1^{*2}\psi_1\psi_2^*\psi_2^2\rangle\right)\,.\end{aligned} \tag{8.21}$$

In order to obtain a cumulant expansion, we rewrite the terms in the brackets into the exponent:

$$1+\langle x\rangle = e^{\ln(1+\langle x\rangle)}\approx e^{\langle x\rangle}+\mathcal{O}(\langle x\rangle^2)\,. \tag{8.22}$$

Thus the two-loop effective potential reads:

$$\begin{aligned} \mathcal{V}^{(2)}[\Psi,\Psi^*] &= -\frac{g}{2\hbar}\int_1 \langle \psi_1^2 \psi_1^{*2}\rangle_c + \frac{g^2\Psi^2}{2\hbar^2}\int_1\int_2 \langle \psi_1^{*2}\psi_1\psi_2^{*2}\psi_2\rangle_c \\ &+ \frac{g^2\Psi^{*2}}{2\hbar^2}\int_1\int_2 \langle \psi_1^*\psi_1^2\psi_2^*\psi_2^2\rangle_c + \frac{g^2|\Psi|^2}{\hbar^2}\int_1\int_2 \langle \psi_1^{*2}\psi_1\psi_2^*\psi_2^2\rangle_c \,. \end{aligned} \tag{8.23}$$

Here the subscript c denotes the fact that in the cumulant expansion (8.22) only the connected diagrams survive. At the moment, we only want to consider two-loop diagrams up to first order in the coupling constant:

$$\mathcal{V}^{(2)}[\Psi,\Psi^*] = -\frac{g}{2\hbar}\int_1 \langle \psi_1^2\psi_1^{*2}\rangle_c + \mathcal{O}(g^2)\,. \tag{8.24}$$

The ensemble average in (8.24) is reduced to products of two-point correlation functions via Wick's rule (4.9):

$$\langle \psi_1\psi_1\psi_1^*\psi_1^*\rangle = \langle \psi_1\psi_1\rangle\langle \psi_1^*\psi_1^*\rangle + 2\langle \psi_1\psi_1^*\rangle\langle \psi_1\psi_1^*\rangle\,. \tag{8.25}$$

Here, both contributions represent connected diagrams and thus survive in (8.24). In the next section we will show that the matrix elements of the Green function itself

$$G(\mathbf{x},\mathbf{x}';\tau) = \begin{pmatrix} G_{\psi\psi^*}(\mathbf{x},\mathbf{x}';\tau) & G_{\psi\psi}(\mathbf{x},\mathbf{x}';\tau) \\ G_{\psi^*\psi^*}(\mathbf{x},\mathbf{x}';\tau) & G_{\psi^*\psi}(\mathbf{x},\mathbf{x}';\tau) \end{pmatrix} \tag{8.26}$$

consists of the connected two-point correlation functions via

$$\begin{aligned} \langle \psi_1\psi_2^*\rangle &= G_{\psi\psi^*}(\mathbf{x}_1,\mathbf{x}_2,\tau_1-\tau_2)\,, \\ \langle \psi_1^*\psi_2\rangle &= G_{\psi^*\psi}(\mathbf{x}_1,\mathbf{x}_2,\tau_1-\tau_2)\,, \\ \langle \psi_1\psi_2\rangle &= G_{\psi\psi}(\mathbf{x}_1,\mathbf{x}_2,\tau_1-\tau_2)\,, \\ \langle \psi_1^*\psi_2^*\rangle &= G_{\psi^*\psi^*}(\mathbf{x}_1,\mathbf{x}_2,\tau_1-\tau_2)\,. \end{aligned} \tag{8.27}$$

Thus we write the final result for the two-loop effective action up to $\mathcal{O}(g)$ with the help of relationship (8.27) as:

$$\mathcal{V}^{(2)}[\Psi,\Psi^*] = -\frac{g\beta V}{2}\left[G_{\psi\psi}(\mathbf{0},0)G_{\psi^*\psi^*}(\mathbf{0},0) + 2G_{\psi\psi^*}(\mathbf{0},0)^2\right] + \mathcal{O}(g^2)\,, \tag{8.28}$$

where we used the fact that the propagators (8.26) are translationally invariant in space for homogeneous systems $G(\mathbf{x}_1,\mathbf{x}_2;\tau) = G(\mathbf{x}_1-\mathbf{x}_2;\tau)$ (see next section).

8.2 Green Functions

In the last section we have shown that the inverse Green functions are given by (8.9). The Green functions themselves follow from the relationship

$$\int_0^{\hbar\beta} d\tau'' \int d^d x'' G^{-1}(\mathbf{x},\tau;\mathbf{x}'',\tau'')G(\mathbf{x}'',\tau'';\mathbf{x}',\tau') = \delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{8.29}$$

Inserting (8.9) into (8.29) yields

$$M(\mathbf{x},\tau)G(\mathbf{x},\tau,\mathbf{x}',\tau') = \hbar\delta(\tau-\tau')\delta(\mathbf{x}-\mathbf{x}')\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{8.30}$$

Using the translational invariance of the Green functions with respect to the imaginary times

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = G(\mathbf{x},\mathbf{x}';\tau-\tau') \tag{8.31}$$

and performing a Matsubara decomposition, we obtain

$$G(\mathbf{x},\mathbf{x}';\tau) = \sum_{\mathbf{k}'} \sum_{m'=-\infty}^{\infty} G_{m'\mathbf{k}'}(\mathbf{x}')\psi_{\mathbf{k}'}(\mathbf{x})e^{-i\omega_{m'}\tau} . \tag{8.32}$$

Inserting (8.32) into (8.30), we get

$$\sum_{\mathbf{k}'} \sum_{m'=-\infty}^{\infty} G_{m'\mathbf{k}'}(\mathbf{x}')\psi_{\mathbf{k}'}(\mathbf{x})e^{-i\omega_{m'}\tau}M(\mathbf{k}',m') = \hbar\delta(\tau)\delta(\mathbf{x}-\mathbf{x}')\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{8.33}$$

with

$$M(\mathbf{k},m) = \begin{pmatrix} -i\hbar\omega_m + \tilde{\epsilon}(\mathbf{k}) & g\Psi^2 \\ g\Psi^{*2} & i\hbar\omega_m + \tilde{\epsilon}(\mathbf{k}) \end{pmatrix} \tag{8.34}$$

and

$$\tilde{\epsilon}(\mathbf{k}) = \epsilon(\mathbf{k}) - \mu + 2g|\Psi|^2 . \tag{8.35}$$

Multiply Eq.(8.33) with

$$\int d^d x\, \psi^*_{\mathbf{k}}(\mathbf{x}) \int_0^{\hbar\beta} d\tau e^{i\omega_m\tau} \tag{8.36}$$

and using the orthogonality relations (2.8) yields

$$\hbar\beta \sum_{\mathbf{k}'} \sum_{m'=-\infty}^{\infty} G_{m'\mathbf{k}'}(\mathbf{x}')\delta_{\mathbf{k},\mathbf{k}'}\delta_{m,m'}M(\mathbf{k}',\omega_{m'}) = \hbar\psi^*_{\mathbf{k}}(\mathbf{x}')\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{8.37}$$

Therefore, the Matsubara coefficients in (8.32) are determined by

$$G_{m\mathbf{k}}(\mathbf{x}') = \frac{1}{\beta} \frac{\psi_{\mathbf{k}}^*(\mathbf{x}')}{\hbar^2\omega_m^2 + \tilde{\epsilon}(\mathbf{k})^2 - g^2|\Psi|^4} \bar{M}(\mathbf{k}, \omega_m) \tag{8.38}$$

with

$$\bar{M}(\mathbf{k}, m) := \begin{pmatrix} i\hbar\omega_m + \tilde{\epsilon}(\mathbf{k}) & -g\Psi^2 \\ -g\Psi^{*2} & -i\hbar\omega_m + \tilde{\epsilon}(\mathbf{k}) \end{pmatrix} . \tag{8.39}$$

Thus, the Green functions read

$$G(\mathbf{x}, \mathbf{x}'; \tau) = \frac{1}{\beta} \sum_{\mathbf{k}} \sum_{m=-\infty}^{\infty} \frac{\psi_{\mathbf{k}}^*(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x})e^{-i\omega_m\tau}}{\hbar^2\omega_m^2 + \tilde{\epsilon}(\mathbf{k})^2 - g^2|\Psi|^4} \bar{M}(\mathbf{k}, \omega_m) . \tag{8.40}$$

From Eq.(8.40) we define the Green functions $G_{\psi\psi^*}, G_{\psi\psi}, G_{\psi^*\psi^*}, G_{\psi^*\psi}$ via (8.26). In the next section we show explicitly that these four functions represent the fundamental two-point correlation functions, respectively. With help of the short-hand notation

$$E(\mathbf{k})^2 := \tilde{\epsilon}(\mathbf{k})^2 - g^2|\Psi|^4 \tag{8.41}$$

we calculate at first the off-diagonal propagator

$$\begin{aligned} G_{\psi\psi}(\mathbf{x}, \mathbf{x}'; \tau) &= -g\psi^2 \frac{1}{\beta} \sum_{\mathbf{k}} \psi_{\mathbf{k}}^*(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x}) \sum_{m=-\infty}^{\infty} \frac{e^{-i\omega_m\tau}}{\hbar^2\omega_m^2 + E(\mathbf{k})^2} \\ &= -g\psi^2 \frac{1}{\beta} \sum_{\mathbf{k}} \frac{\psi_{\mathbf{k}}^*(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})} \sum_{m=-\infty}^{\infty} \left[\frac{e^{-i\omega_m\tau}}{-i\hbar\omega_m + E(\mathbf{k})} + \frac{e^{-i\omega_m\tau}}{i\hbar\omega_m + E(\mathbf{k})} \right] \\ &= -g\psi^2 \sum_{\mathbf{k}} \frac{\psi_{\mathbf{k}}^*(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})} \left[S_{\mathbf{k}}(\tau) + S_{\mathbf{k}}(-\tau) \right] , \end{aligned} \tag{8.42}$$

$$G_{\psi^*\psi^*}(\mathbf{x}, \mathbf{x}'; \tau) = -g\psi^{*2} \sum_{\mathbf{k}} \frac{\psi_{\mathbf{k}}^*(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})} \left[S_{\mathbf{k}}(\tau) + S_{\mathbf{k}}(-\tau) \right] . \tag{8.43}$$

Here $S_{\mathbf{k}}(\tau)$ denotes the Matsubara sum

$$S_{\mathbf{k}}(\tau) = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} \frac{e^{-i\omega_m\tau}}{-i\hbar\omega_m + E(\mathbf{k})} . \tag{8.44}$$

It is the same function (2.57) as in Section 2.1 except the different dispersion relation (8.41). Therefore, we only restate the result:

$$S_{\mathbf{k}}(\tau) = \frac{\Theta(\tau)e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau-\hbar\beta/2)} + \Theta(-\tau)e^{-\frac{1}{\hbar}E(\mathbf{k})(\tau+\hbar\beta/2)}}{2\sinh\beta E(\mathbf{k})/2} . \tag{8.45}$$

The calculation of the remaining diagonal Green functions can be obtained from the above formula by differentiating with respect to the imaginary time τ:

$$
\begin{aligned}
G_{\psi\psi^*}(\mathbf{x},\mathbf{x}';\tau) &= \frac{1}{\beta}\sum_{\mathbf{k}} \psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x}) \sum_{m=-\infty}^{\infty} \frac{e^{-i\omega_m\tau}}{\hbar^2\omega_m^2 + E(\mathbf{k})^2}\left[i\hbar\omega + \tilde{\epsilon}(\mathbf{k})\right] \\
&= \frac{1}{g\psi^2}\left[\hbar\frac{\partial}{\partial\tau} - \tilde{\epsilon}(\mathbf{k})\right] G_{\psi\psi}(\mathbf{x},\mathbf{x}';\tau) \\
&= \sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})}\left\{\left[\tilde{\epsilon}(\mathbf{k}) - \hbar\frac{\partial}{\partial\tau}\right]\left[S_{\mathbf{k}}(\tau) + S_{\mathbf{k}}(-\tau)\right]\right\}, \qquad (8.46) \\
G_{\psi^*\psi}(\mathbf{x},\mathbf{x}';\tau) &= \frac{1}{\beta}\sum_{\mathbf{k}} \psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x}) \sum_{m=-\infty}^{\infty} \frac{e^{-i\omega_m\tau}}{\hbar^2\omega_m^2 + E(\mathbf{k})^2}\left[-i\hbar\omega + \tilde{\epsilon}(\mathbf{k})\right] \\
&= \sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})}\left\{\left[\tilde{\epsilon}(\mathbf{k}) + \hbar\frac{\partial}{\partial\tau}\right]\left[S_{\mathbf{k}}(\tau) + S_{\mathbf{k}}(-\tau)\right]\right\}. \qquad (8.47)
\end{aligned}
$$

With the property

$$
\frac{\partial}{\partial\tau}\left[S_{\mathbf{k}}(\tau) + S_{\mathbf{k}}(-\tau)\right] = -\frac{E(\mathbf{k})}{\hbar}\left[S_{\mathbf{k}}(\tau) - S_{\mathbf{k}}(-\tau)\right] \qquad (8.48)
$$

we write our final results for the propagators as follows

$$
\begin{aligned}
G_{\psi\psi^*}(\mathbf{x},\mathbf{x}';\tau) &= \sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})}\left\{S_{\mathbf{k}}(\tau)\left[\tilde{\epsilon}(\mathbf{k}) + E(\mathbf{k})\right] + S_{\mathbf{k}}(-\tau)\left[\tilde{\epsilon}(\mathbf{k}) - E(\mathbf{k})\right]\right\}, \\
G_{\psi\psi}(\mathbf{x},\mathbf{x}';\tau) &= -g\psi^2\sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})}\left[S_{\mathbf{k}}(\tau) + S_{\mathbf{k}}(-\tau)\right], \\
G_{\psi^*\psi}(\mathbf{x},\mathbf{x}';\tau) &= \sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})}\left\{S_{\mathbf{k}}(-\tau)\left[\tilde{\epsilon}(\mathbf{k}) + E(\mathbf{k})\right] + S_{\mathbf{k}}(\tau)\left[\tilde{\epsilon}(\mathbf{k}) - E(\mathbf{k})\right]\right\}, \\
G_{\psi^*\psi^*}(\mathbf{x},\mathbf{x}';\tau) &= -g\psi^{*2}\sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})}\left[S_{\mathbf{k}}(\tau) + S_{\mathbf{k}}(-\tau)\right]. \qquad (8.49)
\end{aligned}
$$

As expected, one obtains the correct Green function (2.58) above T_c , if one sets the background field Ψ, Ψ^* to zero

$$
G(\mathbf{x},\mathbf{x}';\tau)^{T>T_c} = \sum_{\mathbf{k}} \psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x}) \begin{pmatrix} S_{\mathbf{k}}(\tau) & 0 \\ 0 & S_{\mathbf{k}}(-\tau) \end{pmatrix}. \qquad (8.50)
$$

This also justifies to identify the background field Ψ, Ψ^* with the order parameter, which is the condensate density. We end this section by specializing (8.49) to three important cases.

Special case 1: Equal arguments In case of a homogeneous Bose gas the functions $\psi^*_{\mathbf{k}}(\mathbf{x})\,,\psi_{\mathbf{k}}(\mathbf{x})$ represent plane waves. From this follows that the Green functions possess a translation invariance in space and time:

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = G(\mathbf{x}-\mathbf{x}',\tau-\tau')\,. \tag{8.51}$$

Therefore, the diagonal Green functions reduce for equal time and space arguments to

$$G_{\psi\psi^*}(\mathbf{0},0) \;=\; G_{\psi^*\psi}(\mathbf{0},0) = \sum_{\mathbf{k}} S_{\mathbf{k}}(0)^+ = \sum_{\mathbf{k}} \frac{e^{\beta E(\mathbf{k})/2}}{2\sinh \beta E(\mathbf{k})/2} = \sum_{\mathbf{k}} \frac{1}{e^{\beta E(\mathbf{k})}-1} \tag{8.52}$$

Special case 2: Low temperature limit In the low temperature limit $T \to 0$ or $\beta \to \infty$ neighboured Matsubara frequencies stick together and the frequency spectrum becomes very dense:

$$\Delta\omega_m = \omega_{m+1} - \omega_m = \frac{2\pi}{\hbar\beta} \overset{T\to 0}{=} 0\,. \tag{8.53}$$

This means that the Matsubara sum in (8.44) can be replaced by an integral

$$S_{\mathbf{k}}(\tau) = \frac{1}{\beta}\sum_{m=-\infty}^{\infty} \frac{e^{-i\omega_m\tau}}{-i\hbar\omega_m + E(\mathbf{k})} \overset{T\to 0}{=} \frac{\hbar}{2\pi}\int_{-\infty}^{\infty} d\omega_m\, \frac{e^{-i\omega_m\tau}}{-i\hbar\omega_m + E(\mathbf{k})} = \theta(\tau)e^{-E(\mathbf{k})\tau/\hbar}\,. \tag{8.54}$$

In this low temperature limit we get for the propagators (8.49)

$$\begin{aligned}
G_{\psi\psi^*}(\mathbf{x},\mathbf{x}';\tau) &= \sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})} \left\{\theta(\tau)e^{-E(\mathbf{k})\tau/\hbar}[\tilde\epsilon(\mathbf{k})+E(\mathbf{k})] + \theta(-\tau)e^{E(\mathbf{k})\tau/\hbar}[\tilde\epsilon(\mathbf{k})-E(\mathbf{k})]\right\}\,,\\
G_{\psi\psi}(\mathbf{x},\mathbf{x}';\tau) &= -g\psi^2\frac{1}{\beta}\sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})} \left[\theta(\tau)e^{-E(\mathbf{k})\tau/\hbar} + \theta(-\tau)e^{E(\mathbf{k})\tau/\hbar}\right]\,,\\
G_{\psi^*\psi}(\mathbf{x},\mathbf{x}';\tau) &= \sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})} \left\{\theta(-\tau)e^{E(\mathbf{k})\tau/\hbar}[\tilde\epsilon(\mathbf{k})+E(\mathbf{k})] + \theta(\tau)e^{-E(\mathbf{k})\tau/\hbar}[\tilde\epsilon(\mathbf{k})-E(\mathbf{k})]\right\}\,,\\
G_{\psi^*\psi^*}(\mathbf{x},\mathbf{x}';\tau) &= -g\psi^{*2}\frac{1}{\beta}\sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x})}{2E(\mathbf{k})} \left[\theta(\tau)e^{-E(\mathbf{k})\tau/\hbar} + \theta(-\tau)e^{E(\mathbf{k})\tau/\hbar}\right]\,.
\end{aligned} \tag{8.55}$$

Special case 3: High temperature limit Consider the Matsubara sum (8.44). For high temperatures $T \to \infty$ or $\beta \to 0$ all Matsubara frequencies, except the zero mode, become infinite and thus give no contribution. As only the zero mode survives, we get:

$$S_{\mathbf{k}}(\tau) \overset{T\to\infty}{=} \frac{1}{\beta E(\mathbf{k})}\,. \tag{8.56}$$

Thus the propagator (8.49) read in this high temperature limit:

$$\begin{aligned} G_{\psi\psi^*}(\mathbf{x},\mathbf{x}';\tau) = G_{\psi^*\psi}(\mathbf{x},\mathbf{x}';\tau) &= \frac{1}{\beta}\sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{E(\mathbf{k})^2}\,\tilde{\epsilon}(\mathbf{k})\,, \\ G_{\psi\psi}(\mathbf{x},\mathbf{x}';\tau) &= -g\psi^2\frac{1}{\beta}\sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{E(\mathbf{k})^2}\,, \\ G_{\psi^*\psi^*}(\mathbf{x},\mathbf{x}';\tau) &= -g\psi^{*2}\frac{1}{\beta}\sum_{\mathbf{k}} \frac{\psi^*_{\mathbf{k}}(\mathbf{x}\,')\psi_{\mathbf{k}}(\mathbf{x})}{E(\mathbf{k})^2}\,. \end{aligned} \tag{8.57}$$

The above limit process is also referred to as the classical limit, because $\beta \to 0$ is equivalent to $\hbar \to 0$ as follows from equation (8.53).

8.3 Generating Functional

We consider now the quadratic action

$$\begin{aligned} \mathcal{A}^{(\mathrm{quad})}[\psi,\psi^*;j,j^*] &= \frac{1}{2}\int_\tau\int_{\tau'}\int_{\mathbf{x}}\int_{\mathbf{x}'}(\psi^*,\psi)(\mathbf{x},\tau)G^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau')\begin{pmatrix}\psi\\ \psi^*\end{pmatrix}(\mathbf{x}',\tau') \\ &\quad -(j^*,j)(\mathbf{x},\tau)\begin{pmatrix}\psi\\ \psi^*\end{pmatrix}(\mathbf{x},\tau) - (\psi^*,\psi)(\mathbf{x},\tau)\begin{pmatrix}j\\ j^*\end{pmatrix}(\mathbf{x},\tau)\,, \end{aligned} \tag{8.58}$$

where $G^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau')$ is the inverse Greens function given by (8.9) and $j(\mathbf{x},\tau), j(\mathbf{x},\tau)^*$ is a current which couples linearly to the Bose fields $\delta\psi(\mathbf{x},\tau), \delta\psi(\mathbf{x},\tau)$ and shall also be periodic in imaginary time. This action defines the generating functional

$$\mathcal{Z}[j,j^*] = \oint \mathcal{D}\psi\mathcal{D}\psi^* e^{-\mathcal{A}^{(\mathrm{quad})}[\psi,\psi^*;j,j^*]/\hbar}\,. \tag{8.59}$$

from which all n-point correlation functions are obtained by successive differentiations with respect to the currents. For example, the two-point correlation function $\langle\psi(\mathbf{x}_1,\tau_1)\psi^*(\mathbf{x}_2,\tau_2)\rangle$ is given by a functional derivation with respect to $j^*(\mathbf{x}_1,\tau_1)$ and $j(\mathbf{x}_2,\tau_2)$:

$$\langle\delta\psi(\mathbf{x}_1,\tau_1)\delta\psi^*(\mathbf{x}_2,\tau_2)\rangle = \left.\frac{\hbar^2\,\delta^2\mathcal{Z}[j,j^*]}{\delta j(\mathbf{x}_2,\tau_2)\delta j^*(\mathbf{x}_1,\tau_1)}\right|_{j,j^*=0}. \tag{8.60}$$

We calculate the generating functional (8.59) via a Matsubara decomposition of the Bose fields

$$\psi(\mathbf{x},\tau) = \sum_{\mathbf{k}}\sum_{m=-\infty}^{\infty} c_{\mathbf{k}m}\psi_{\mathbf{k}}(\mathbf{x})e^{-i\omega_m\tau}\,, \qquad \psi^*(\mathbf{x},\tau) = \sum_{\mathbf{k}}\sum_{m=-\infty}^{\infty} c^*_{\mathbf{k}m}\psi^*_{\mathbf{k}}(\mathbf{x})e^{i\omega_m\tau} \tag{8.61}$$

and the currents

$$j(\mathbf{x},\tau)=\sum_{\mathbf{k}}\sum_{m=-\infty}^{\infty}j_{\mathbf{k}m}\psi_{\mathbf{k}}(\mathbf{x})e^{-i\omega_m\tau}\,,\qquad j^*(\mathbf{x},\tau)=\sum_{\mathbf{k}}\sum_{m=-\infty}^{\infty}j^*_{\mathbf{k}m}\psi^*_{\mathbf{k}}(\mathbf{x})e^{i\omega_m\tau}\,. \tag{8.62}$$

We have already performed such a transformation in the previous section and thus only state the results for the functional measure

$$\oint\mathcal{D}\psi(\mathbf{x},\tau)\mathcal{D}\psi^*(\mathbf{x},\tau)\to\prod_{\mathbf{k}}\prod_{m=-\infty}^{\infty}\int dc_{\mathbf{k}m}\int dc^*_{\mathbf{k}m}\frac{\beta}{2\pi} \tag{8.63}$$

and the action

$$\begin{aligned}\mathcal{A}^{(\mathrm{quad})}[c_{\mathbf{k}m},c^*_{\mathbf{k}m};j_{\mathbf{k}m},j^*_{\mathbf{k}m}] &= \sum_{\mathbf{k}}\sum_{m=-\infty}^{\infty}\{\hbar\beta\left[-i\hbar\omega_m+\tilde{\epsilon}(\mathbf{k})\right]c^*_{\mathbf{k}m}c_{\mathbf{k}m}+\frac{1}{2}g\hbar\beta\Psi^2c^*_{\mathbf{k}-m}c^*_{\mathbf{k}m}\\ &+\frac{1}{2}g\hbar\beta\Psi^{*2}c_{\mathbf{k}-m}c_{\mathbf{k}m}-c^*_{\mathbf{k}m}j_{\mathbf{k}m}-c_{\mathbf{k}m}j^*_{\mathbf{k}m}\}\,. \end{aligned}\tag{8.64}$$

This can be written in the more compact way

$$\mathcal{A}^{(\mathrm{quad})}[\mathbf{c}_{\mathbf{k}m},\mathbf{j}_{\mathbf{k}m}] = \hbar\sum_{\mathbf{k}}\sum_{m}\left[\mathbf{c}^\dagger_{\mathbf{k}m}M(\mathbf{k},m)\mathbf{c}_{\mathbf{k}m}-\mathbf{c}^\dagger_{\mathbf{k}m}\mathbf{j}_{\mathbf{k}m}-\mathbf{j}^\dagger_{\mathbf{k}m}\mathbf{c}_{\mathbf{k}m}\right] \tag{8.65}$$

with the four component vector

$$\mathbf{c}^\dagger_{\mathbf{k}m} = \left(c^*_{\mathbf{k}m},c_{\mathbf{k}m},c^*_{\mathbf{k}-m},c_{\mathbf{k}-m}\right)\,,\qquad \mathbf{j}^\dagger_{\mathbf{k}m}=\left(j^*_{\mathbf{k}m},j_{\mathbf{k}m},j^*_{\mathbf{k}-m},j_{\mathbf{k}-m}\right) \tag{8.66}$$

and the matrix

$$M(\mathbf{k},m)=\frac{1}{4}\begin{pmatrix}\beta\left[-i\hbar\omega_m+\tilde{\epsilon}(\mathbf{k})\right] & 0 & 0 & g\beta\Psi^2\\ 0 & \beta\left[-i\hbar\omega_m+\tilde{\epsilon}(\mathbf{k})\right] & g\beta\Psi^{*2} & 0\\ 0 & g\beta\Psi^{*2} & \beta\left[-i\hbar\omega_m+\tilde{\epsilon}(\mathbf{k})\right] & 0\\ g\beta\Psi^2 & 0 & 0 & \beta\left[-i\hbar\omega_m+\tilde{\epsilon}(\mathbf{k})\right]\end{pmatrix} \tag{8.67}$$

Thus the generating functional becomes:

$$\mathcal{Z}[j,j^*] = \prod_{\mathbf{k}}\prod_{m}\int dc_{\mathbf{k}m}\int dc^*_{\mathbf{k}m}\frac{\beta}{2\pi}\exp\left\{-\sum_{\mathbf{k}}\sum_{m}\left[\mathbf{c}^\dagger_{\mathbf{k}m}M(\mathbf{k},m)\mathbf{c}_{\mathbf{k}m}-\mathbf{c}^\dagger_{\mathbf{k}m}\mathbf{j}_{\mathbf{k}m}-\mathbf{j}^\dagger_{\mathbf{k}m}\mathbf{c}_{\mathbf{k}m}\right]\right\}\,. \tag{8.68}$$

To calculate this generating functional, we perform the following transformation:

$$\mathbf{c}_{\mathbf{k}m}\to T\mathbf{c}_{\mathbf{k}m}+\mathbf{a}\,,\qquad \mathbf{c}^\dagger_{\mathbf{k}m}\to\mathbf{c}^\dagger_{\mathbf{k}m}T^\dagger+\mathbf{a}^\dagger\,, \tag{8.69}$$

where the translation vectors $\mathbf{a}\,,\mathbf{a}^\dagger$ and the matrices $T,T^\dagger$ are still not known. The corresponding transformation of the functional measure

$$\oint\mathcal{D}\psi\oint\mathcal{D}\psi^*\to\oint\mathcal{D}\psi\oint\mathcal{D}\psi^*\det TT^\dagger \tag{8.70}$$

implies the following result for the generating functional

$$\begin{aligned}\mathcal{Z}[j,j^*] &= \prod_{\mathbf{k}}\prod_{m=-\infty}^{\infty}\int dc_{\mathbf{k}m}\int dc^*_{\mathbf{k}m}\frac{\beta}{2\pi}\det TT^\dagger \exp\Big\{-\sum_{\mathbf{k}}\sum_m\Big\{\mathbf{c}^\dagger_{\mathbf{k}m}T^\dagger M(\mathbf{k},m)^{-1}T\mathbf{c}_{\mathbf{k}m}\\ &\quad+\mathbf{c}^\dagger_{\mathbf{k}m}T^\dagger\left[M(\mathbf{k},m)^{-1}\mathbf{a}+\mathbf{j}_{\mathbf{k}m}\right]+\left[M(\mathbf{k},m)^{-1}\mathbf{a}+\mathbf{j}_{\mathbf{k}m}\right]^\dagger T\mathbf{c}_{\mathbf{k}m}\\ &\quad+\mathbf{a}^\dagger M(\mathbf{k},m)^{-1}\mathbf{a}+\mathbf{j}^\dagger_{\mathbf{k}m}\mathbf{a}+\mathbf{a}^\dagger\mathbf{j}_{\mathbf{k}m}\Big\}\,.\end{aligned} \tag{8.71}$$

Now we will choose our transformation parameter such that the following equations are fulfilled:

$$M(\mathbf{k},m)^{-1}\mathbf{a}+\mathbf{j}_{\mathbf{k}m}=0\,, \tag{8.72}$$

and

$$T^\dagger M(\mathbf{k},m)^{-1}T=M(\mathbf{k},m)^{-1}_{\text{diag}}\,. \tag{8.73}$$

The latter means that the matrix T is unitary and thus the generating functional simplifies to

$$\mathcal{Z}[j,j^*] \;=\; \mathcal{Z}[0,0]\,\mathcal{Z}^{(\text{corr})}[j,j^*] \tag{8.74}$$

where

$$\mathcal{Z}[0,0]=\prod_{\mathbf{k}}\prod_m\int dc_{\mathbf{k}m}\int dc^*_{\mathbf{k}m}\,\frac{\beta}{2\pi}\exp\left\{-\sum_{\mathbf{k}}\sum_m\mathbf{c}^\dagger_{\mathbf{k}m}M^{-1}(\mathbf{k},m)_{\text{diag}}\mathbf{c}_{\mathbf{k}m}\right\} \tag{8.75}$$

and

$$\mathcal{Z}^{\text{corr}}[j,j^*]=\exp\left\{\sum_{\mathbf{k}}\sum_m\mathbf{j}^\dagger_{\mathbf{k}m}M^{-1}(\mathbf{k},m)\mathbf{j}_{\mathbf{k}m}\right\}\,. \tag{8.76}$$

8.3.1 Correlation Functions

For $\mathcal{Z}^{\text{corr}}[j,j^*]$ we can state the result of the Matsubara back transformation

$$\begin{aligned}\mathbf{j}_{\mathbf{k},m} &= \frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\int d^dx\,\mathbf{j}(\mathbf{x},\tau)\psi^*_{\mathbf{k}}(\mathbf{x})e^{i\omega_m\tau}\\ \mathbf{j}^*_{\mathbf{k},m} &= \frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\int d^dx\,\mathbf{j}^*(\mathbf{x},\tau)\psi_{\mathbf{k}}(\mathbf{x})e^{-i\omega_m\tau}\,.\end{aligned} \tag{8.77}$$

Correspondingly, we get

$$\mathcal{Z}^{\text{corr}}[j,j^*] \;=\; \exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\int d^dx\int d^dx'\,\mathbf{j}^*(\mathbf{x},\tau)G(\mathbf{x},\mathbf{x}',\tau)\mathbf{j}(\mathbf{x}',\tau')\right\}\,, \tag{8.78}$$

where $G(\mathbf{x}, \mathbf{x}', \tau)$ is the Green function (8.39), (8.40). From (8.58) we read off that the two-point correlation functions are given by differentiations of the generating functional with respect to the currents. In Eq. (8.74) we see that the currents occur only in $\mathcal{Z}^{\rm corr}[j, j^*]$. Thus the correlation functions are connected with the fundamental propagators

$$\begin{aligned}
\langle \psi(\mathbf{x}_1, \tau_1)\psi^*(\mathbf{x}_2, \tau_2)\rangle &= \hbar^2 \left.\frac{\delta^2 \mathcal{Z}^{\rm corr}[j, j^*]}{\delta j(\mathbf{x}_2, \tau_2)\delta j^*(\mathbf{x}_1, \tau_1)}\right|_{j,j^*=0} = G_{\psi\psi^*}(\mathbf{x}_1, \tau_1; \mathbf{x}_2\tau_2)\,, \\
\langle \psi^*(\mathbf{x}_1, \tau_1)\psi(\mathbf{x}_2, \tau_2)\rangle &= \hbar^2 \left.\frac{\delta^2 \mathcal{Z}^{\rm corr}[j, j^*]}{\delta j^*(\mathbf{x}_2, \tau_2)\delta j(\mathbf{x}_1, \tau_1)}\right|_{j,j^*=0} = G_{\psi^*\psi}(\mathbf{x}_1, \tau_1; \mathbf{x}_2\tau_2)\,, \\
\langle \psi(\mathbf{x}_1, \tau_1)\psi(\mathbf{x}_2, \tau_2)\rangle &= \hbar^2 \left.\frac{\delta^2 \mathcal{Z}^{\rm corr}[j, j^*]}{\delta j^*(\mathbf{x}_2, \tau_2)\delta j^*(\mathbf{x}_1, \tau_1)}\right|_{j,j^*=0} = G_{\psi\psi}(\mathbf{x}_1, \tau_1; \mathbf{x}_2\tau_2)\,, \\
\langle \psi^*(\mathbf{x}_1, \tau_1)\psi^*(\mathbf{x}_2, \tau_2)\rangle &= \hbar^2 \left.\frac{\partial^2 \mathcal{Z}^{\rm corr}[j, j^*]}{\partial j(\mathbf{x}_2, \tau_2)\partial j(\mathbf{x}_1, \tau_1)}\right|_{j,j^*=0} = G_{\psi^*\psi^*}(\mathbf{x}_1, \tau_1; \mathbf{x}_2\tau_2)\,. \qquad (8.79)
\end{aligned}$$

8.3.2 TraceLog

By setting $\mathbf{j}_{\mathbf{k}m} = \mathbf{j}^\dagger_{\mathbf{k}m} = 0$ in (8.74) the generating functional reduces to the one-loop contribution (8.15). Because of the terms containing $c_{\mathbf{k}-m}$ and $c^*_{\mathbf{k}-m}$ in the action, we split the Matsubara sum in the $m = 0$ term and the remaining $m \neq 0$ terms. In the sum running over negative Matsubara frequencies we perform a global transformation $-m \to m$ yielding

$$\begin{aligned}
\mathcal{Z}[0,0] &= \prod_{\mathbf{k}} \prod_{m=1}^{\infty} \int_{-\infty}^{\infty} dc_{\mathbf{k}m} \int_{-\infty}^{\infty} dc^*_{\mathbf{k}m} \int_{-\infty}^{\infty} dc_{\mathbf{k}-m} \int_{-\infty}^{\infty} dc^*_{\mathbf{k}-m} \frac{\beta}{2\pi} \exp\left[-\mathbf{c}^\dagger_{\mathbf{k}m} M(\mathbf{k}, m)\mathbf{c}_{\mathbf{k}m}\right] \\
&\times \int_{-\infty}^{\infty} dc_{\mathbf{k}0} \int_{-\infty}^{\infty} dc^*_{\mathbf{k}0} \exp\left[-\mathbf{c}^\dagger_{\mathbf{k}0} M(\mathbf{k}, 0)\mathbf{c}_{\mathbf{k}0}\right]. \qquad (8.80)
\end{aligned}$$

Using the standard integral

$$\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_1^* \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_2^* \exp\left\{-\mathbf{x}^\dagger M \mathbf{x}\right\} = \frac{\pi^2}{\sqrt{\det M}} \qquad (8.81)$$

for the four-component vector $\mathbf{x}^\dagger = (x_1, x_1^*, x_2, x_2^*)$, we obtain

$$\mathcal{Z}[0,0] = \prod_{\mathbf{k}} \frac{\beta}{2\sqrt{\det M(\mathbf{k}, 0)}} \prod_{m=1}^{\infty} \frac{\beta^2}{4\sqrt{\det M(\mathbf{k}, m)}}\,, \qquad (8.82)$$

where the respective determinants follow from (8.67)

$$\det M(\mathbf{k}, m) = \left(\frac{\beta}{2}\right)^4 \left[\hbar^2\omega_m^2 + E(\mathbf{k})^2\right]^2, \qquad (8.83)$$

$$\det M(\mathbf{k}, 0) = \left(\frac{\beta}{2}\right)^2 E(\mathbf{k})^2\,, \qquad (8.84)$$

where $E(\mathbf{k})$ is defined by (8.41). Because they do not longer depend on the sign of m, we rewrite the one-loop contribution as:

$$\mathcal{Z}[0,0] = \prod_{\mathbf{k}} \prod_{m=-\infty}^{\infty} \frac{1}{\sqrt{\hbar^2\omega_m^2 + E(\mathbf{k})^2}} = \exp\left\{-\frac{1}{2}\sum_{\mathbf{k}}\sum_{m=-\infty}^{\infty} \ln[\hbar^2\omega_m^2 + E(\mathbf{k})^2]\right\} . \quad (8.85)$$

The calculation of the above Matsubara sum has already been done in Section 2.1 of this thesis. There we got the final result (2.33), so we have here

$$\mathcal{Z}[0,0] = \exp\left\{-\frac{\beta}{2}\sum_{\mathbf{k}} E(\mathbf{k}) - \sum_{\mathbf{k}} \ln\left[1 - e^{-\beta E(\mathbf{k})}\right]\right\} . \quad (8.86)$$

Chapter 9

Density of Non-Condensed Atoms

With the results of the previous chapter, we are now able to calculate the effective potential. From (8.12), (8.28), (8.17), and (8.86) we get

$$\begin{aligned}\mathcal{V}[\Psi, \Psi^*] &= V(-\mu|\Psi|^2 + \frac{g}{2}|\Psi|^4) + \frac{\eta}{2}\sum_{\mathbf{k}} E(\mathbf{k}) + \frac{\eta}{\beta}\sum_{\mathbf{k}} \ln\left[1 - e^{-\beta E(\mathbf{k})}\right] \\ &\quad -\eta^2 \frac{g}{V}\left[\sum_{\mathbf{k}} \frac{1}{e^{\beta E(\mathbf{k})} - 1}\right]^2 + \mathcal{O}(g^2, \eta^2)\,. \end{aligned} \tag{9.1}$$

Here we introduced the parameter $\eta = 1$, which counts the loop order. Note that the last term of (9.1) is the first-order g-contribution of the two-loop approximation. We will need this term only in Section 10.3, where a perturbation expansion in the coupling constant is carried out to calculate the leading shift in the critical temperature of BEC due to weak interactions.

9.1 Bogoliubov Approximation

In the Bogoliubov approximation the starting point of a thermodynamic discussion of the condensate is the effective potential up to one loop:

$$\frac{\mathcal{V}[\Psi, \Psi^*]}{V} = -\mu|\Psi|^2 + \frac{g}{2}|\Psi|^4 + \frac{\eta}{2V}\sum_{\mathbf{k}} E(\mathbf{k}) + \frac{\eta}{\beta V}\sum_{\mathbf{k}} \ln\left[1 - e^{-\beta E(\mathbf{k})}\right]\,, \tag{9.2}$$

where the dispersion relation $E(\mathbf{k})$ follows from (8.35) and (8.41)

$$E(\mathbf{k}) = \sqrt{[\epsilon(\mathbf{k}) - \mu + 2g|\Psi|^2]^2 - g^2|\Psi|^4}\,. \tag{9.3}$$

Here, the effective potential is still a function of the absolute value of the background field $|\Psi|$. In fact, this function is not a thermodynamic potential for all background fields, but only at its extremum. The extremalization of (9.2)

$$\frac{\partial \mathcal{V}[\Psi,\Psi^*]}{\partial|\Psi|^2} = 0 \tag{9.4}$$

leads to

$$\begin{aligned} 0 &= -\mu + g|\Psi|^2 + \frac{\eta}{2V}\sum_{\mathbf{k}} \frac{2g[\epsilon(\mathbf{k}) - \mu + 2g|\Psi|^2] - g^2|\Psi|^2}{E(\mathbf{k})} \\ &+ \frac{\eta}{V}\sum_{\mathbf{k}} \frac{2g[\epsilon(\mathbf{k}) - \mu + 2g|\Psi|^2] - g^2|\Psi|^2}{E(\mathbf{k})} \frac{1}{e^{\beta E(\mathbf{k})} - 1} \,. \end{aligned} \tag{9.5}$$

The resulting extremal value for the background field is our order parameter, the condensate density n_0:

$$n_0 = |\Psi|^2 = \frac{\mu}{g} - \frac{\eta}{V}\sum_{\mathbf{k}} \frac{2\epsilon(\mathbf{k}) + \mu}{\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}} - 1}\right) + \mathcal{O}(\eta^2)\,. \tag{9.6}$$

This result is obtained from (9.4) by performing a systematic expansion in the loop order parameter η, where the zero-loop approximation for the condensate density $n_0 = \mu/g + \mathcal{O}(\eta)$ is called the tree-level. With this tree-level the dispersion relation (9.3) reduces to

$$E(\mathbf{k}) = \sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}\,, \tag{9.7}$$

which was first derived by Bogoliubov [93]. Inserting (9.6) and (9.7) into (9.2) yields the extremal value of the effective potential, which coincides with the grand-canonical potential Ω according to (2.73):

$$\frac{\Omega(\mu,T)}{V} = -\frac{\mu^2}{2g} + \frac{\eta}{2V}\sum_{\mathbf{k}} \sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})} + \frac{\eta}{\beta V}\sum_{\mathbf{k}} \ln\left(1 - e^{-\beta\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}}\right) + \mathcal{O}(\eta^2) \tag{9.8}$$

From that, we obtain the particle density by differentiating with respect to the chemical potential μ:

$$n = -\frac{1}{V}\frac{\partial \mathcal{V}(\mu,T)}{\partial\mu} = \frac{\mu}{g} - \frac{\eta}{V}\sum_{\mathbf{k}} \frac{\epsilon(\mathbf{k})}{\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}} - 1}\right) + \mathcal{O}(\eta^2) \tag{9.9}$$

This dependency on the chemical potential μ is not helpful, as it is rather the condensate density, which is observed in the experiment. Therefore we eliminate μ in favor of n_0 via relationship (9.6):

$$n - n_0 = \frac{\eta}{V}\sum_{\mathbf{k}} \frac{\epsilon(\mathbf{k}) + gn_0}{\sqrt{\epsilon(\mathbf{k})^2 + 2gn_0\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2 + 2gn_0\epsilon(\mathbf{k})}} - 1}\right) + \mathcal{O}(\eta^2)\,. \tag{9.10}$$

The right hand-side of Eq.(9.10) denotes the number of non-condensed particles in the Bogoliubov approximation.

9.2 Popov Approximation via VPT

The result (9.10) is valid only for $n \approx n_0$, i.e. for small η. However, the quantum phase transition takes place for $n \gg n_0$, i.e. at strong η, which can be reached by applying variational perturbation theory according to the rules developed in Chapter 3 of this thesis. Here we introduce a dummy variational parameter M by replacing

$$\mu \to M + \eta\Delta \tag{9.11}$$

with the abbreviation

$$\Delta = \frac{\mu - M}{\eta} \, . \tag{9.12}$$

By inserting (9.11) into the grand-canonical potential (9.8), we have to consider Δ as being independent of the expansion parameter η. By doing so we re-expand (9.8) consistently up to the first power in η:

$$\begin{aligned}\frac{\Omega^{\rm trial}(M,\mu,T)}{V} &= -\frac{M^2}{2g} - \eta\frac{M}{g}\Delta + \frac{\eta}{2V}\sum_{\mathbf{k}}\sqrt{\epsilon(\mathbf{k})^2 + 2M\epsilon(\mathbf{k})} \\ &\quad + \frac{\eta}{\beta V}\sum_{\mathbf{k}}\ln\left(1 - e^{-\beta\sqrt{\epsilon(\mathbf{k})^2+2M\epsilon(\mathbf{k})}}\right)\end{aligned} \tag{9.13}$$

and replace Δ afterwards by its definition (9.12)

$$\begin{aligned}\frac{\Omega^{\rm trial}(M,\mu,T)}{V} &= \frac{M^2}{2g} - \frac{M\mu}{g} + \frac{\eta}{2V}\sum_{\mathbf{k}}\sqrt{\epsilon(\mathbf{k})^2 + 2M\epsilon(\mathbf{k})} \\ &\quad + \frac{\eta}{\beta V}\sum_{\mathbf{k}}\ln\left(1 - e^{-\beta\sqrt{\epsilon(\mathbf{k})^2+2M\epsilon(\mathbf{k})}}\right) \, .\end{aligned} \tag{9.14}$$

Subsequently, we extremize this trial expression for the grand-canonical potential with respect to the variational parameter M

$$\frac{1}{V}\frac{\partial\Omega^{\rm trial}(M,\mu,T)}{\partial M} = 0 \, , \tag{9.15}$$

which leads to

$$\begin{aligned}0 &= \frac{M^{\rm opt} - \mu}{g} + \frac{\eta}{V}\sum_{\mathbf{k}}\frac{\epsilon(\mathbf{k})}{\sqrt{\epsilon(\mathbf{k})^2 + 2M^{\rm opt}\epsilon(\mathbf{k})}} \\ &\quad \times\left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2+2M^{\rm opt}\epsilon(\mathbf{k})}} - 1}\right) \, .\end{aligned} \tag{9.16}$$

Thus we obtain the optimal variational parameter as a solution of the equation

$$M^{\rm opt} = \mu - \frac{\eta g}{V} \sum_{\mathbf{k}} \frac{\epsilon(\mathbf{k})}{\sqrt{\epsilon(\mathbf{k})^2 + 2M^{\rm opt}\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2+2M^{\rm opt}\epsilon(\mathbf{k})}} - 1} \right) . \tag{9.17}$$

Inserting (9.17) into (9.14) yields the optimized grand-canonical potential

$$\Omega(\mu, T) = \Omega^{\rm trial}(M^{\rm opt}, \mu, T) . \tag{9.18}$$

However, we are more interested in a resummation of equation (9.10). At first we compute the particle density

$$\begin{aligned} n &= -\frac{1}{V}\frac{\partial\Omega(\mu,T)}{\partial\mu}\bigg|_T = -\frac{1}{V}\frac{\partial\Omega^{\rm trial}(M^{\rm opt},\mu,T)}{\partial\mu}\bigg|_{M^{\rm opt},T} \\ &= -\frac{1}{V}\frac{\partial\Omega^{\rm trial}}{\partial\mu}\bigg|_{M^{\rm opt},T} - \frac{1}{V}\frac{\partial\Omega^{\rm trial}}{\partial M^{\rm opt}}\bigg|_{\mu,T}\frac{\partial M^{\rm opt}}{\partial\mu} . \end{aligned} \tag{9.19}$$

Because of equation (9.15) this reduces to

$$n = -\frac{1}{V}\frac{\partial\Omega^{\rm trial}}{\partial\mu} = \frac{M^{\rm opt}}{g} . \tag{9.20}$$

Second, we insert the substitution (9.11) in the condensate density (9.6) and perform a similar variational resummation for the condensate density

$$n_0 = \frac{M}{g} + \eta\frac{\Delta}{g} - \frac{\eta}{V}\sum_{\mathbf{k}} \frac{2\epsilon(\mathbf{k}) + M}{\sqrt{\epsilon(\mathbf{k})^2 + 2M\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2+2M\epsilon(\mathbf{k})}} - 1} \right) . \tag{9.21}$$

Taking into account the abbreviation (9.12), we obtain

$$n_0 = \frac{\mu(M)}{g} - \frac{\eta}{V}\sum_{\mathbf{k}} \frac{2\epsilon(\mathbf{k}) + M}{\sqrt{\epsilon(\mathbf{k})^2 + 2M\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2+2M\epsilon(\mathbf{k})}} - 1} \right) . \tag{9.22}$$

Evaluating this expression for the optimal value of the variational parameter

$$n_0 = \frac{\mu(M^{\rm opt})}{g} - \frac{\eta}{V}\sum_{\mathbf{k}} \frac{2\epsilon(\mathbf{k}) + M^{\rm opt}}{\sqrt{\epsilon(\mathbf{k})^2 + 2M^{\rm opt}\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2+2M^{\rm opt}\epsilon(\mathbf{k})}} - 1} \right) \tag{9.23}$$

and inserting the relationship (9.17) yields:

$$n_0 = \frac{M^{\rm opt}}{g} - \frac{\eta}{V}\sum_{\mathbf{k}} \frac{\epsilon(\mathbf{k}) + M^{\rm opt}}{\sqrt{\epsilon(\mathbf{k})^2 + 2M^{\rm opt}\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2+2M^{\rm opt}\epsilon(\mathbf{k})}} - 1} \right) . \tag{9.24}$$

Finally we replace M^{opt} by gn according to (9.20) and get the final result

$$\boxed{n - n_0 = \frac{\eta}{V} \sum_{\mathbf{k}} \frac{\epsilon(\mathbf{k}) + gn}{\sqrt{\epsilon(\mathbf{k})^2 + 2gn\epsilon(\mathbf{k})}} \left(\frac{1}{2} + \frac{1}{e^{\beta \sqrt{\epsilon(\mathbf{k})^2 + 2gn\epsilon(\mathbf{k})}} - 1} \right)} \, . \tag{9.25}$$

This result is known as the Popov approximation [18] and turns out to have the same form as in (9.10), except that the condensate density n_0 on the right-hand side is replaced by the total particle density n.

Chapter 10

Application to Weakly Interacting Gases

We first discuss the formation of a condensate for the free-particle spectrum

$$\epsilon(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m} \,. \tag{10.1}$$

Here, the quantum numbers $\mathbf{k}$ denote the eigenvalues of the non-interacting gas, which represent continuous wave vectors in d dimensions. Therefore the sum in (9.25) can be converted for big volumes V into an integral over all wave vectors $\mathbf{k}$:

$$\sum_{\mathbf{k}} = V \int_{\mathcal{R}} \frac{d^d k}{(2\pi)^d} \,. \tag{10.2}$$

At first, we want to show in Section 10.1 how the early results of Lee and Yang [94] for the special case of zero temperature can be obtained within our formalism. Second, we extend these calculations in Section 10.2 for finite temperatures and show how to calculate the whole phase diagram with the help of VPT, thereby predicting a surprising reentrant phenomenon. Furthermore, we perform in Section 10.3 a high temperature expansion of the effective potential (9.1) and show that the leading shift of the critical temperature vanishes.

10.1 Zero Temperature Limit

With the above specialization the temperature independent part of the grand-canonical potential (9.2) and the particle density (9.25) become

$$\frac{\mathcal{V}(\mu,T)}{V} = -\frac{\mu^2}{2g} + \frac{\eta}{2} \int_{\mathcal{R}} \frac{d^d k}{(2\pi)^d} \sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})} \,, \tag{10.3}$$

$$n = n_0 + \frac{\eta}{2} \int_{\mathcal{R}} \frac{d^d k}{(2\pi)^d} \frac{\epsilon(\mathbf{k}) + gn}{\sqrt{\epsilon(\mathbf{k})^2 + 2gn\epsilon(\mathbf{k})}} . \tag{10.4}$$

The free particle spectrum (10.1) depends only on the absolute value of the wave vector $\mathbf{k}$, so that we can transform both zero-temperature integrals (10.3) and (10.4) into one-dimensional ones

$$\begin{aligned} \frac{\mathcal{V}(\mu,T)}{V} &= -\frac{\mu^2}{2g} + \frac{\eta}{2\Gamma(d/2)} \left(\frac{m}{2\pi\hbar^2}\right)^{d/2} \int_0^\infty dx x^{d/2-1} \sqrt{x^2 + 2\mu x} \\ &= -\frac{\mu^2}{2g} + \frac{\eta}{2} I_d(0, -1/2, 2\mu) , \end{aligned} \tag{10.5}$$

$$\begin{aligned} n &= n_0 + \frac{\eta}{2\Gamma(d/2)} \left(\frac{m}{2\pi\hbar^2}\right)^{d/2} \int_0^\infty dx x^{d/2-1} \frac{x + gn}{\sqrt{x^2 + 2gnx}} \\ &= n_0 + \frac{\eta}{2} \left[I_d(1, 1/2, 2gn) + gn I_d(0, 1/2, 2gn)\right] . \end{aligned} \tag{10.6}$$

All of these integrals are of the general form:

$$I_d(\alpha, \beta, a) = \frac{1}{\Gamma(d/2)} \left(\frac{m}{2\pi\hbar^2}\right)^{d/2} \int_0^\infty dx x^{d/2-1} \frac{x^\alpha}{(x^2 + ax)^\beta} . \tag{10.7}$$

Therefore, we first calculate this integral and apply the result afterwards to physics. By using the Schwinger trick (B.1), we obtain

$$I_d(\alpha, \beta, a) = \frac{1}{\Gamma(d/2)} \left(\frac{m}{2\pi\hbar^2}\right)^{d/2} \int_0^\infty dx \, \frac{x^{d/2+\alpha-\beta-1}}{(x + a)^\beta} . \tag{10.8}$$

Interchanging both integrals and taking into account again (B.1) yields

$$I_d(\alpha, \beta, a) = \frac{\Gamma(d/2 + \alpha - \beta)\Gamma(-d/2 - \alpha + 2\beta)}{\Gamma(d/2)\Gamma(\beta)} \left(\frac{m}{2\pi\hbar^2}\right)^{d/2} a^{d/2+\alpha-2\beta} . \tag{10.9}$$

In the following we make use of some special cases of this master integral:

$$I_3(1, 1/2, 2gn) = \frac{8}{3\pi^2} \frac{m^{3/2}(gn)^{3/2}}{\hbar^3} , \tag{10.10}$$

$$I_3(0, 1/2, 2gn) = -\frac{2}{\pi^2} \frac{m^{3/2}(gn)^{1/2}}{\hbar^3} , \tag{10.11}$$

$$I_3(0, -1/2, 2\mu) = \frac{16}{15\pi^2} \frac{m^{3/2}\mu^{5/2}}{\hbar^3} . \tag{10.12}$$

Thus we get for the grand-canonical potential (10.5) and the particle density (10.6) in $d = 3$ dimensions

$$\frac{\mathcal{V}(\mu,T)}{V} = -\frac{\mu^2}{2g} + \eta \frac{8}{15\pi^2} \frac{m^{3/2}\mu^{5/2}}{\hbar^3} , \tag{10.13}$$

$$n = n_0 + \eta \frac{1}{3\pi^2} \frac{m^{3/2}(gn)^{3/2}}{\hbar^3} . \tag{10.14}$$

Depletion The depletion is defined by the ratio of the number of excited particles to the number of particles. From (10.14) we read off the depletion

$$\frac{n-n_0}{n} = \frac{\eta}{3\pi^2}\frac{m^{3/2}g^{3/2}n^{1/2}}{\hbar^3}\,. \tag{10.15}$$

Inserting the relationship between the coupling constant and the s-wave scattering length (1.14) leads to the well-known result for the depletion [93]:

$$\boxed{\frac{n-n_0}{n} = \frac{8}{3}\sqrt{\frac{a_s^3 n}{\pi}}}\,. \tag{10.16}$$

Ground-state energy The relationship between the internal energy

$$dU = TdS - pdV + \mu dN\,, \tag{10.17}$$

and the grand-canonical potential

$$d\Omega = -SdT - pdV - Nd\mu \tag{10.18}$$

is given by the Legendre transformation

$$U = \Omega + TS + \mu N\,. \tag{10.19}$$

The ground-state energy is the internal energy per volume in the zero temperature limit. Using (10.13) we get

$$E_0 = \left.\frac{U}{V}\right|_{T=0} = \frac{\mathcal{V}}{V} + \mu\frac{N}{V} = -\frac{\mu^2}{2g} + \eta\frac{8}{15\pi^2}\frac{m^{3/2}\mu^{5/2}}{\hbar^3} + \mu n\,. \tag{10.20}$$

The chemical potential in zero-loop order is given by (9.9): $\mu = gn + \mathcal{O}(\eta)$. With a consistent expansion of (10.20) up to $\mathcal{O}(\eta^2)$ we obtain

$$E_0 = \frac{1}{2}gn^2\left(1 + \eta\frac{16}{15\pi^2}\frac{m^{3/2}g^{3/2}n^{1/2}}{\hbar^3}\right)\,. \tag{10.21}$$

Inserting (1.14) we get

$$\boxed{E_0 = \frac{2\pi\hbar^2}{m}a_s n^2\left(1 + \frac{128}{15}\sqrt{\frac{a_s^3 n}{\pi}}\right)}\,, \tag{10.22}$$

which is related to the depletion (10.16) according to:

$$E_0 = \frac{2\pi\hbar^2}{m}a_s n^2\left(1 + \frac{16}{5}\frac{n-n_0}{n}\right)\,. \tag{10.23}$$

Sound velocity The expression for the sound velocity can be obtained from the $\mathbf{p} \to 0$ behavior of the Bogoliubov spectrum (9.7) with $\mathbf{k} = \mathbf{p}/\hbar$. For the free one-particle spectrum (10.1) the dispersion relation (9.7) has the important property to be linear for small momenta $\mathbf{p}$:

$$E(\mathbf{p}) = \sqrt{\left(\frac{\mathbf{p}^2}{2m}\right)^2 + 2\mu\frac{\mathbf{p}^2}{2m}} \overset{\mathbf{p}\to 0}{=} \sqrt{\frac{\mu}{m}}|\mathbf{p}| = \sqrt{\frac{gn}{m}}|\mathbf{p}| = c|\mathbf{p}| \,. \tag{10.24}$$

Equation (10.24) shows a typical quasi-particle behavior indicating the condensed state, where all particles are energetically in the same state. With (1.14), the result for the sound velocity reads

$$\boxed{c = \sqrt{\frac{4\pi\hbar^2 n a_s}{m^2}}}\,. \tag{10.25}$$

Thus the sound velocity depends only on the density n. Recently, this Bogoliubov sound velocity could be measured [95] in the research group of Ketterle at MIT . Their measurements coincided very well with the theoretical prediction (10.25). Note that for large values of $\mathbf{k}$ the Bogoliubov spectrum (9.7) becomes classical $E(\mathbf{k}) \approx \epsilon(\mathbf{k})$.

10.2 Nonzero Temperatures

We will now take into consideration the full temperature dependent one-loop result for the particle density (9.25), where $\epsilon(\mathbf{k})$ is the free one-particle energy spectrum (10.1) and the zero temperature integral has already been calculated in (10.15). After substituting the integration variable in $d = 3$ dimensions this leads to:

$$a_s\, n^{1/3} = \left(\frac{n - n_0}{n}\right)^{2/3} \left(\frac{9\pi}{64}\right)^{1/3} \left[1 + \frac{3\alpha}{16} I(\alpha)\right]^{-2/3} \,, \tag{10.26}$$

where $I(\alpha)$ abbreviates the integral

$$I(\alpha) = \int_0^\infty dx \, \frac{x\alpha + 8}{2\sqrt{x\alpha + 16}\,\left(e^{\sqrt{x^2\alpha/16 + x}} - 1\right)} \,. \tag{10.27}$$

Taking into account (1.14) the dimensionless parameter α is given by

$$\alpha = \left(\frac{t}{a_s n^{1/3} \zeta(3/2)^{2/3}}\right)^2 \,, \tag{10.28}$$

where $t = T/T_c^{(0)}$ denotes the reduced temperature.

10.2.1 Phase Diagram

The phase transition is defined by the vanishing of the order parameter, i.e. $n_0 = 0$. Thus the transition line in our phase diagram follows from (10.26) to be:

$$\boxed{a_{sc}\, n^{1/3} = \left(\frac{9\pi}{64}\right)^{1/3} \left[1 + \frac{3\alpha_c}{16} I(\alpha_c)\right]^{-2/3}}\,. \tag{10.29}$$

Near $T = 0$ we perform a Taylor expansion in the parameter α_c and obtain for the first four coefficients of this expansion:

$$a_{sc} n^{\frac{1}{3}} = a_0 + a_1\alpha_c + a_2\alpha_c^2 + a_3\alpha_c^3 + \mathcal{O}(\alpha_c^4)\,. \tag{10.30}$$

with

$$a_0 = \left(\frac{9\pi}{64}\right)^{1/3} \approx 0.762\,,\;\; a_1 \approx -0.313\,,\;\; a_2 \approx 0.200\,,\;\; a_3 \approx -0.207\,. \tag{10.31}$$

We observe that this Taylor expansion is not valid for small coupling constants as the expansion parameter α_c diverges in the weak-coupling limit $a_{sc} \to 0$. However, the whole expression in (10.29) has a well defined weak-coupling limit. Evaluating the integral (10.27) numerically leads to the dotted curve in Fig. 10.1. There we plotted the whole phase diagram parametrically, which means that we computed $a_{sc}n^{1/3}(\alpha_c)$ and $t(\alpha_c)$ as functions of the parameter α_c separately.

10.2.2 Critical Temperature Shift

The behavior near $T_c^{(0)}$ can even be calculated analytically. Therefore we rescale and expand the integrand in (10.27) in the limit $\alpha \to \infty$, yielding:

$$I(\alpha) \;=\; \frac{\sqrt{\alpha}}{2}\int_0^\infty dz\sqrt{z}\frac{1}{\exp\left(\sqrt{\alpha}z/4 + 2/\sqrt{\alpha}\right) - 1} + \mathcal{O}\left(\frac{1}{\alpha}\right)\,. \tag{10.32}$$

Using the series representation of the Bose distribution function, we obtain

$$I(\alpha) \;=\; \frac{\sqrt{\alpha}}{2}\sum_{m=1}^{\infty} e^{-2m/\sqrt{\alpha}}\int_0^\infty dz z^{1/2} e^{-m\sqrt{\alpha}z/4} + \mathcal{O}\left(\frac{1}{\alpha}\right)\,, \tag{10.33}$$

where the integral gives a Gamma function:

$$I(\alpha) \;=\; \frac{4\Gamma(3/2)}{\alpha^{1/4}}\sum_{m=1}^{\infty}\frac{e^{-2m/\sqrt{\alpha}}}{m^{3/2}} + \mathcal{O}\left(\frac{1}{\alpha}\right)\,. \tag{10.34}$$

The remaining sum is a polylogarithmic function (A.1):

$$I(\alpha) \;=\; \frac{4\Gamma(3/2)}{\alpha^{1/4}}\,\zeta_{3/2}(e^{-2/\sqrt{\alpha}}) + \mathcal{O}(\frac{1}{\alpha}). \tag{10.35}$$

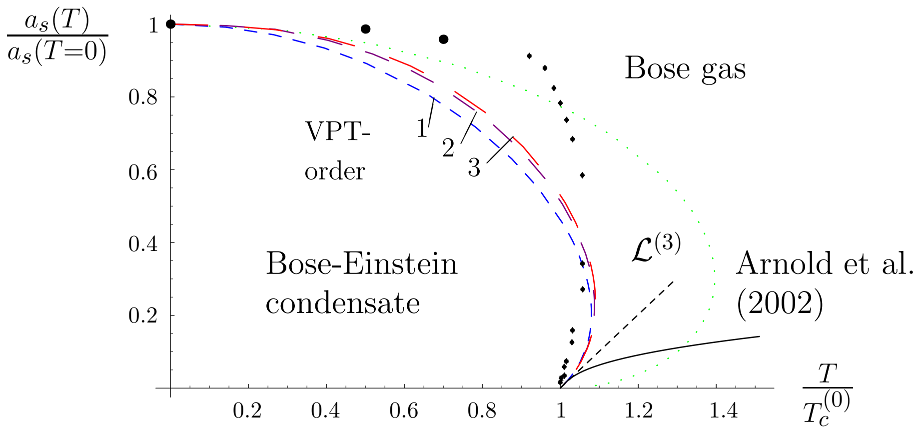


Figure 10.1: Phase diagram of Bose-Einstein condensation in variationally improved one-loop approximation without (dashed) and with properly imposed higher-loop slope properties at $T_c^{(0)}$. The short curves starting at $T = T_c^{(0)}$ is due to Arnold et al.[31]. The dashed straight line indicates the slope of our curve. The diamonds correspond to the Monte-Carlo data of Ref. [28] which are scaled to their value $a_{\rm eff}(T=0) \approx 0.63$, whereas the dots show simulation results obtained for helium [96].

With the help of the Robinson expansion (A.4) we now expand this result for large α and obtain

$$I(\alpha) \;=\; \frac{2\sqrt{\pi}\zeta(3/2)}{\alpha^{1/4}} - \frac{4\sqrt{2}\pi}{\sqrt{\alpha}} + \mathcal{O}\left(\frac{1}{\alpha^{3/4}}\right) . \tag{10.36}$$

Inserting (10.36) into (10.29) yields:

$$\boxed{1 = t_c^{3/2} - \frac{2\sqrt{2\pi a_s n^{1/3}} t_c}{\zeta(3/2)^{2/3}}} . \tag{10.37}$$

To get the leading shift in the critical temperature, we expand

$$t_c = 1 + \frac{\Delta T_c}{T_c^0} , \tag{10.38}$$

and thus obtain from (10.37)

$$t_c = 1 + \frac{4\sqrt{2\pi}}{3\zeta(3/2)^{2/3}} \sqrt{a_{sc} n^{1/3}} + \mathcal{O}(a_{sc} n^{1/3}) . \tag{10.39}$$

Although a similar square-root contribution was also found in the Refs [21, 22], recent Monte-Carlo simulations [39, 40, 42] and precise high-temperature calculations [35, 43] indicate that the leading critical temperature shift is linear in the s-wave scattering length

$$t_c = 1 + c_1 a_{sc} n^{1/3} + \mathcal{O}(a_{sc}^2 n^{2/3}) \tag{10.40}$$

with the numerical value $c_1 \approx 1.3$. Thus it becomes necessary to improve our resummed one-loop approximation (10.29) for the transition line via variational perturbation theory (see Chapter 3) in such a way that the $\alpha_c \to \infty$ behavior of the expansion (10.30) is given by (10.40) and not by (10.39).

10.2.3 Resummation Improved Results

A more reliable curve is obtained by extrapolating the weak-coupling expansions (10.30)

$$a_{sc}n^{1/3} = \sum_{k=0}^{N} a_k \alpha_c^k \tag{10.41}$$

to a strong-coupling one

$$a_{sc}n^{1/3} = \alpha_c^{p/q} \sum_{k=0}^{N} b_k \alpha_c^{-2k/q} \tag{10.42}$$

with the help of variational perturbation theory. Note that the series (10.30) has Borel character, which means that the sign of the coefficients (10.31) changes from term to term. At last this circumstance enables us to do a resummation via VPT.

Determination of p and q For the resummation we have first to determine the exponents p and q, which characterize the strong-coupling behavior. Our starting point is the strong-coupling expansion (10.42) for $N = 1$:

$$a_{sc}n^{1/3} = \alpha_c^{p/q}\left(b_0 + b_1 \alpha_c^{-2/q}\right) . \tag{10.43}$$

Imposing the definition of the parameter α in (10.28) and the critical temperature (10.38), we obtain

$$b_0 - \left(a_{sc}n^{1/3}\right)^{1+2p/q} \zeta(3/2)^{4p/3q} + b_0\,\frac{2p}{q}\,\frac{\Delta T_c}{T_c^{(0)}} + b_1 \zeta(3/2)^{8/3q}\left(a_{sc}n^{1/3}\right)^{4/q} = 0 \,. \tag{10.44}$$

Thus we get from (10.44) the correct asymptotic behavior (10.40) when p and q are fixed according to

$$1 + \frac{2p}{q} = 0\,, \qquad \frac{4}{q} = 1\,. \tag{10.45}$$

Therefore we have to choose our strong-coupling exponents p and q to be

$$p = -2\,, \qquad q = 4\,. \tag{10.46}$$

With that choice a comparison between (10.40) and (10.44) leads to

$$b_0 = \frac{1}{\zeta(3/2)^{2/3}}\,, \qquad b_1 = \frac{c_1 b_0}{\zeta(3/2)^{2/3}} = \frac{c_1}{\zeta(3/2)^{4/3}}\,. \tag{10.47}$$

VPT Resummation We now want to improve our resummed one-loop approximation (10.29) for the transition line. The philosophy will be to trust only the first $W+1$ weak-coupling coefficients $a_0, \ldots, a_W$ in (10.41) and impose the first two strong-coupling coefficients b_0 and b_1 in (10.42) near $T_c^{(0)}$. Using VPT we calculate with this information two successive weak-coupling coefficients $\tilde{a}_{W+1}$ and $\tilde{a}_{W+2}$:

$$a_{sc} n^{1/3} = \sum_{k=0}^{W} a_k \alpha_c^k + \tilde{a}_{W+1} \alpha_c^{W+1} + \tilde{a}_{W+2} \alpha_c^{W+2} . \tag{10.48}$$

Afterwards we determine the whole phase diagram by resumming the new weak-coupling series (10.48) to be valid for all values of α_c.

Leading VPT Order Let us illustrate this procedure for $W = 0$ and determine the subsequent weak-coupling coefficients $\tilde{a}_1, \tilde{a}_2$ from the strong-coupling coefficients b_0, b_1. To this end we identify $\alpha_c \equiv g$ and follow the VPT procedure of Chapter 3 by specifying (3.9) for $N = 2, p = -2$ and $q = 4$:

$$f_2(g, K) = \frac{3a_0}{K^2} - \frac{3a_0}{K^4} + \frac{a_0 + 4g\tilde{a}_1}{K^6} - \frac{3g\tilde{a}_1}{K^8} + \frac{\tilde{a}_2 g^2}{K^{10}} , \tag{10.49}$$

where the last two coefficients in (3.9) were replaced by $\tilde{a}_1, \tilde{a}_2$. According to the principle of minimal sensitivity we have to optimize this equation with respect to K and solve (3.10) with the ansatz (3.12) containing the two leading coefficients $K_2^{(0)}$ and $K_2^{(1)}$:

$$K_2(g) = K_2^{(0)} g^{1/4} + K_2^{(1)} g^{-1/4} + \mathcal{O}(g^{-3/4}) . \tag{10.50}$$

Inserting this ansatz for $K_2(g)$ into (3.10)

$$0 = -\frac{6a_0}{K^3} + \frac{12a_0}{K^5} - 6\frac{a_0 + 4g\tilde{a}_1}{K^7} + \frac{24g\tilde{a}_1}{K^9} - \frac{10\tilde{a}_2 g^2}{K^{11}} \tag{10.51}$$

and comparing the coefficients of the two leading powers $g^{-1/2}$, $g^{-1/4}$ in the coupling constant g, yields the following two equations:

$$0 = 3{K_2^{(0)}}^8 a_0 + 12{K_2^{(1)}}^4 \tilde{a}_1 + 5\tilde{a}_2 , \tag{10.52}$$
$$0 = 6{K_2^{(0)}}^7 a_0 + 9{K_2^{(0)}}^8 K_2^{(1)} a_0 + 12{K_2^{(0)}}^3 \tilde{a}_1 + 84{K_2^{(0)}}^4 K_2^{(1)} \tilde{a}_1 + 55 K_2^{(1)} \tilde{a}_2 . \tag{10.53}$$

As we have four unknown variables $\tilde{a}_1, \tilde{a}_2, K_2^{(0)}$, and $K_2^{(1)}$, we need two more equations for their unique determination. They can be obtained from the known strong-coupling coefficients b_0 and b_1 in (10.49). Inserting (10.50) into (10.49) and comparing with (3.13) yields:

$$b_0 = \frac{1}{K_2^{(0)^{10}}}\left(3K_2^{(0)^8}a_0 + 4K_2^{(0)^4}\tilde{a}_1 + \tilde{a}_2\right), \tag{10.54}$$

$$b_1 = \frac{1}{K_2^{(0)^{11}}}\Big(-3K_2^{(0)^7}a_0 + 6K_2^{(0)^8}K_2^{(1)}a_0 + 3K_2^{(0)^3}\tilde{a}_1 + 24K_2^{(0)^4}K_2^{(1)}\tilde{a}_1 + 10K_2^{(1)}\tilde{a}_2\Big). \tag{10.55}$$

From (10.52) and (10.54), we get $\tilde{a}_1$ and $\tilde{a}_2$ as functions of $K_2^{(0)}$:

$$\tilde{a}_1 = -\frac{3}{2}K_2^{(0)^4}\left(a_0 - \frac{5}{12}b_0K_2^{(0)^2}\right), \tag{10.56}$$

$$\tilde{a}_2 = 3K_2^{(0)^8}\left(a_0 - \frac{1}{2}b_0K_2^{(0)^2}\right). \tag{10.57}$$

Furthermore, Eq.(10.53) can be solved for $K_2^{(1)}$:

$$K_2^{(1)} = -K_2^{(0)^3}\frac{b_1K_2^{(0)^8} + 3a_0K_2^{(0)^4} + 3\tilde{a}_1}{6K_2^{(0)^8}a_0 + 24K_2^{(0)^4}\tilde{a}_1 + 10\tilde{a}_2}. \tag{10.58}$$

This expression has the interesting property, that the denominator is zero, if we insert (10.56) and (10.57). As $K_2^{(1)}$ should be a finite quantity, we have to demand that the numerator also vanishes. This leads to an explicit algebraic expression for $K_2^{(0)}$, which is solved by

$$K_2^{(0)} = \pm\left(-\frac{3a_0}{2b_1} + \sqrt{\frac{9a_0^2}{4b_1^2} - \frac{3a_1}{b_1}}\right)^{1/4}. \tag{10.59}$$

Note that with that choice (10.55) is satisfied although (10.55) was not needed for deriving (10.59). We now insert the weak-coupling coefficient $a_0 \approx 0.76$ from (10.31) and the correct strong-coupling coefficients (10.47) with $c_1 \approx 1.3$ to yield $K_2^{(0)} \approx \pm 0.93461$. This result leads via (10.56) and (10.57) to the new coefficients:

$$\tilde{a}_1 \approx -0.654\,, \qquad \tilde{a}_2 \approx 0.935\,. \tag{10.60}$$

Finally, the trial function (10.49) follows to be

$$f_2(g,K) \approx 2.284\frac{1}{K^2} - 2.284\frac{1}{K^4} + (0.761 - 2.616g)\frac{1}{K^6} + 1.962g\frac{1}{K^8} + 0.935g^2\frac{1}{K^{10}} \tag{10.61}$$

and leads together with (3.10) to our first resummation improved transition line that is valid for arbitrary values of the coupling constant. The result, shown in Fig. 10.1 as the first VPT order, has now the correct asymptotic behavior near $T_c^{(0)}$ as well as near $T = 0$.

Higher VPT Orders Finally, we state the new computed weak-coupling coefficients of the improved resummed one-loop approximation for the orders $W = 0, 1, 2$:

$$W = 0: \qquad \tilde{a}_1 = -0.654 \qquad \tilde{a}_2 = 0.935 \tag{10.62}$$
$$W = 1: \qquad \tilde{a}_2 = -1.864 \qquad \tilde{a}_3 = 16.66 \tag{10.63}$$
$$W = 2: \qquad \tilde{a}_3 = -29.53 \qquad \tilde{a}_3 = 622.0 \tag{10.64}$$

A resummation of the corresponding weak-coupling series (10.48) shows the fast converging phase curves with the second and third VPT order in Fig. 10.1. It is interesting that the new computed coefficients in (10.63) and (10.64) deviate significantly from the original ones in (10.31). The reason is that the influence of higher orders becomes smaller in a weak-coupling expansion and it needs higher deviations to obtain the correct strong-coupling behavior.

The phase diagram in Fig. 10.1 has the interesting property that there exists a characteristic reentrant transition [47, 48] above $T_c^{(0)}$, a nose in the transition curve, where a condensate can be produced by increasing a_s, which disappears upon a further increase of a_s. Such a reentrant behavior was also found in a previous Monte-Carlo simulation [28] as shown in Fig. 10.1. However the validity of their calculations can be doubted as their value of the constant $c_1 \approx 0.3$ in (10.40) deviates significantly from recent Monte-Carlo [39, 40, 42] and analytic calculations [35, 43] with $c_1 \approx 1.3$. Experimentally, one could probe this behavior in two different ways, i.e. by thermal and by quantum heating. Quantum heating means that one works at a certain temperature, which is slightly higher than $T_c^{(0)}$ and then, coming from higher a_s, one decreases the s-wave scattering length by Feshbach resonances [51]. Contrary to that, thermal heating means to decrease the temperature for a given scattering length a_s. This procedure has to be done at least for three different gases with different scattering length a_s to be able to observe the phase diagram in Fig. 10.1. Independent from the heating process the phases can be observed by probing the coherence properties with time-flight measurements [97].

10.3 High-Temperature Expansion

In this section we will show that a high temperature expansion of the effective potential (9.1) is consistent with perturbation theory at weak couplings above T_c. At a first glance, this is astonishing as BEC takes place at very low temperature near $T \approx 0$ compared to room temperatures at $T \approx 300K$. But this is not really a contradiction, as in this context "high" means that $T_c^{(0)}$ is much larger than the characteristic temperature where the Bogoliubov spectrum becomes classical (10.24). With the result in (10.25) this takes place at the momentum $|\tilde{\mathbf{p}}| = 2mc = 2\sqrt{\mu m}$ and at the energy $\tilde{E} = 2\mu$ corresponding to the temperature $\tilde{T} = 2\mu/k_B$. Thus, we effectively perform a perturbation expansion in the dimensionless parameter $\tilde{T}/T$, which is indeed a small parameter at temperatures $T \approx T_c^{(0)}$. To do so, we consider the effective potential (9.1) with the free spectrum (10.1) and replace the sum by an integral (10.2), yielding

$$\frac{\mathcal{V}[\Psi,\Psi^*]}{V} = -\mu|\Psi|^2 + \frac{g}{2}|\Psi|^4 + \frac{1}{\beta\Gamma(D/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\int_0^\infty dx x^{D/2-1}\ln(1-e^{-\beta E(x)})$$
$$-\frac{gV}{\Gamma(D/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\left(\int_0^\infty dx\,\frac{x^{D/2-1}}{e^{\beta E(x)}-1}\right)^2 . \tag{10.65}$$

Here the $\mathcal{O}(g)$-contribution of the two-loop effective potential (8.28) is included, as we carry out a consistent calculation in the coupling constant g, and $E(x)$ is the dispersion relation

$$E(x) = \sqrt{(x-\mu+2g|\Psi|^2)^2 - g^2|\Psi|^4} \tag{10.66}$$

stemming from (9.3). At first we substitute βx by x and expand the argument of the exponential function in (10.65) in powers of β:

$$\beta E(x) \rightarrow \sqrt{[x-\beta\mu+2\beta g|\Psi|^2]^2 - \beta^2 g^2|\Psi|^4}$$
$$= x - \beta\left(\mu - 2g\beta|\Psi|^2\right) + \mathcal{O}(\beta^2) . \tag{10.67}$$

One-Loop contribution In this approximation the one-loop contribution to the effective potential becomes

$$\mathcal{V}^{(1)}[\Psi,\Psi^*] = V\frac{T^{D/2+1}}{\Gamma(D/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\int_0^\infty dx x^{D/2-1}\ln\left[1-\exp\left(-x+\beta\mu-2g\beta|\Psi|^2\right)\right] . \tag{10.68}$$

Thus the series representation of the logarithm

$$\ln(1-e^{-y}) = \sum_{n=1}^{\infty}\frac{e^{-yn}}{n} \tag{10.69}$$

yields:

$$\mathcal{V}^{(1)}[\Psi,\Psi^*] = V\frac{T^{D/2+1}}{\Gamma(D/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\sum_{n=1}^{\infty}\frac{1}{n}\exp\left\{(\beta\mu-2\beta g|\Psi|^2)n\right\}\int_0^\infty dx x^{D/2-1}e^{-xn} \tag{10.70}$$

Evaluating the integral gives $n^{-d/2}\Gamma(d/2)$ and the remaining sum represents a polylogarithmic function:

$$\mathcal{V}^{(1)}[\Psi,\Psi^*] = -V\frac{T^{D/2+1}}{\Gamma(D/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\Gamma(D/2)\zeta_{D/2+1}\left[\exp\left(\beta\mu-2\beta g|\Psi|^2\right)\right] \tag{10.71}$$

A perturbative evaluation of the zeta function up to first order in the coupling constant, i.e.

$$\zeta_\nu(e^{\beta\mu-2\beta g|\Psi|^2}) = \zeta_\nu(e^{\beta\mu}) - 2\beta g|\Psi|^2\zeta_{\nu-1}(e^{\beta\mu})\,, \tag{10.72}$$

setting $d=3$ and using the thermal wavelength $\lambda = \sqrt{2\pi\hbar^2\beta/m}$ results in

$$\mathcal{V}^{(1)}[\Psi,\Psi^*] \;=\; -\frac{T}{\lambda^3}\zeta_{5/2}(e^{\beta\mu}) + \frac{2g}{\lambda^3}\zeta_{3/2}(e^{\beta\mu})|\Psi|^2 + \mathcal{O}(g^2,\sqrt{T})\,. \tag{10.73}$$

Two-Loop contribution The two-loop contribution reads

$$\mathcal{V}^{(2)}[\Psi,\Psi^*] = V^2\frac{g}{\Gamma(D/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\left[\int_0^\infty dx\,\frac{x^{D/2-1}}{e^{x-\beta\mu}-1}\right]^2. \tag{10.74}$$

This time we use the series representation of the Bose distribution function

$$\frac{1}{e^y-1} = \sum_{n=1}^\infty e^{-yn} \tag{10.75}$$

to obtain

$$\mathcal{V}^{(2)}[\Psi,\Psi^*] \;=\; V^2\frac{g}{\Gamma(D/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\left[\sum_{n=1}^\infty e^{\beta\mu n}\int_0^\infty dx\,x^{D/2-1}\,e^{-xn}\right]^2. \tag{10.76}$$

As before the integral is proportional to a Gamma function and the remaining sum gives a polylogarithmic function

$$\mathcal{V}^{(2)}[\Psi,\Psi^*] \;=\; gV\Gamma(D/2)\left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\zeta_{D/2}(e^{\beta\mu})^2 + O(g^2)\,. \tag{10.77}$$

Finally we set $d=3$ and use again the thermal wavelength $\lambda = \sqrt{2\pi\hbar^2\beta/m}$:

$$\mathcal{V}^{(2)}[\Psi,\Psi^*] \;=\; \frac{g}{\lambda^6}\zeta_{3/2}(e^{\beta\mu})^2 + O(g^2)\,. \tag{10.78}$$

Landau expansion Collecting the results above and reordering the effective potential in powers of the order parameter yields:

$$\frac{\mathcal{V}[\Psi,\Psi^*]}{V} \;=\; -\frac{T}{\lambda^3}\zeta_{5/2}(e^{\beta\mu}) + \frac{g}{\lambda^6}\zeta_{3/2}(e^{\beta\mu})^2 - \mu_r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + \mathcal{O}(g^2) \tag{10.79}$$

By doing so, we identify the coefficient of the $|\Psi|^2$-contribution to the effective potential with the renormalized chemical potential

$$\mu_r = \mu - \frac{2g}{\lambda^3}\,\zeta_{3/2}(e^{\beta\mu}) + \mathcal{O}(g^2) \tag{10.80}$$

which shows how the bare chemical potential $-\mu$ changes due to weak interactions. It is important to note that this renormalized chemical potential is positive so that the coefficient of the quadratic term in (10.79) is negative, leading to a potential of a form resembling a mexican hat. The typical mexican hat shape shows two possible equilibrium values at nonzero order parameters, where the effective potential reduces to the grand-canonical potential. In reality, the system is of course disturbed by different environmental influences so that the system will prefer only one equilibrium value. With this choice the symmetry of the system is broken and that is why this phenomena is called spontaneous symmetry breaking.
One may ask: How can one see that μ_r is really positive? The answer can be obtained by optimizing the effective potential leading to the determination of the condensate density $|\Psi|^2$ which turns out to be $\mu_r = g|\Psi|^2$ in lowest order.

Critical temperature An interesting application for the above Landau form of the grand-canonical potential deals with the question, whether the critical temperature has changed due to weak interactions. From the above discussion of the Landau form, we know that the critical point is determined by the vanishing of the renormalized chemical potential (10.80). Indeed, this condition coincides with determining the critical point within the framework of finite temperature perturbation theory (4.38). From Eq. (10.80) we would get T_c as a function of the bare chemical potential μ

$$k_B T_c = \frac{2\pi\hbar^2}{m}\left(\frac{\mu}{2g\zeta(3/2)}\right)^{2/3} . \tag{10.81}$$

Since this temperature is large for small g compared with $\tilde{T}$, the high-temperature expansion is consistent with the weak-coupling assumption of perturbation theory. This proves that classical thermal fluctuations dominate at $T_c^{(0)}$ over quantum fluctuations. This also justifies the zero Matsubara approximation for the leading shift in the critical temperature in (7.13).

An experimentally more accessible quantity is the particle density n, which is obtained by differentiating the grand-canonical potential (10.79) with respect to μ:

$$n(T,\mu) = -\frac{1}{V}\frac{\partial\mathcal{V}(T_c,\mu,V)}{\partial\mu} = \frac{1}{\lambda_c^3}\zeta_{3/2}(e^{\beta_c\mu}) - \frac{2g\beta_c}{\lambda_c^6}\zeta_{3/2}(e^{\beta_c\mu})\zeta_{1/2}(e^{\beta_c\mu}) \tag{10.82}$$

Here, we have already set $|\Psi|^2 = 0$ which is true at the critical point. If one now insert the critical condition $\mu_r = 0$ for the chemical potential (10.81) and expand up to $O(g)$, this reduces to the free Bose gas expression:

$$n(T_c,\mu) = \frac{1}{\lambda^3}\zeta_{3/2}(e^{\beta\mu_r}) + \mathcal{O}(g^2) \overset{\mu_r=0}{=} \frac{1}{\lambda_c^3}\zeta(3/2) + \mathcal{O}(g^2) . \tag{10.83}$$

Thus the effective potential evaluated up to the first perturbative order does not lead to a shift in the condensation temperature which agrees with the result of Ref. [98].

Chapter 11

Application to Optical Boson Lattices

In this chapter we return to the problem of an effectively homogeneous Bose gas confined in an optical lattice. For the lowest band the one-particle dispersion relation is given by (1.25):

$$\epsilon(\mathbf{k}) = 2J \sum_{i=1}^{d} (1 - \cos k_i \delta) \,. \tag{11.1}$$

Here the wave vectors $\mathbf{k}$ are also continous but they are restricted to the first Brillouin zone $k_i \in (-\pi/\delta, \pi/\delta)$. Thus the sum in (9.25) reduces to the integral

$$\sum_{\mathbf{k}} = V \int_{\mathcal{BZ}} \frac{d^d k}{(2\pi)^d} = V \prod_{i=1}^{d} \int_{-\pi/\delta}^{\pi/\delta} \frac{dk_i}{2\pi} \,. \tag{11.2}$$

These integrals are evaluated using the hopping expansion [99], in which one expands the integrand in powers of the cosines of (9.25). This is formally implemented by inserting in (11.1) an artificial parameter κ according to

$$\epsilon(\mathbf{k}) = 2J \sum_{i=1}^{d} (1 - \kappa \cos k_i \delta) \tag{11.3}$$

and by expanding the resulting expressions in powers of κ, where we set $\kappa = 1$ at the end. By doing so, we introduce the on-site interaction $U = gn$ and the particle density by $n = \delta^{-d}$ for an integer filling factor in the periodic potential. So the resulting transition line ($n_0 = 0$) turns out to be defined by the implicit equation

$$F_d\left(\frac{k_B T_c}{J}, \frac{U}{J}\right) = 0 \,. \tag{11.4}$$

11.1 Zeroth Hopping Order

In zeroth hopping order, where $\kappa = 0$, the function F_d is given by:

$$F_d^{(0)}(x,y) = x - \frac{2\sqrt{d^2+dy}}{\ln \dfrac{4\sqrt{d^2+dy}+y+2d}{4\sqrt{d^2+dy}-y-2d}}\,. \tag{11.5}$$

In this lowest approximation one obtains analytic expressions for the value of the interaction parameter U/J at $T = 0$

$$\left.\frac{U}{J}\right|_{T=0} = 2(3+2\sqrt{3})d \approx 12.93d\,, \tag{11.6}$$

the critical temperature of the interaction free model ($U = 0$)

$$T_c^{(0)} = \frac{2dJ}{k_b \ln 3}\,, \tag{11.7}$$

and the shift in the critical temperature $\Delta T_c = T_c - T_c^0$ due to small interactions, which turns out to be linear

$$\frac{\Delta T_c}{T_c^{(0)}} = \frac{1}{2d}\frac{U}{J}\,. \tag{11.8}$$

The resulting transition curve for $d = 3$ and the next three approximations coming from successive hopping orders (see next section) are shown in Fig. 11.1. Qualitatively we observe a similar reentrant behavior [47] like in the homogeneous case of BEC, which is not really surprising as we deal with an effectively homogenous system in the lowest band. However, the nose is more pronounced than in the case of the free one-particle dispersion (10.1) and therefore it may be easier to experimentally observe this reentrant transition in the experiment of optical Boson lattices. Furthermore, the measurement process is much easier here, because quantum heating can be carried out by just varying the intensity of the laser beam at a certain temperature.

11.2 Higher Hopping Orders

The convergence of the transition line in Fig. 11.1 can be observed with the approximation sequence of transition points U/J at $T = 0$ shown in Fig. 11.2, converging towards the value 30.8. From that one can compute the corrections due to higher hopping orders:

$$\left.\frac{U}{J}\right|_{T=0} = 38.8 - 4.7\kappa^2 - 1.3\kappa^4 - 0.6\kappa^6 - 0.4\kappa^8 - 0.3\kappa^{10} - 0.2\kappa^{12} + \mathcal{O}(\kappa^{14})\,, \tag{11.9}$$

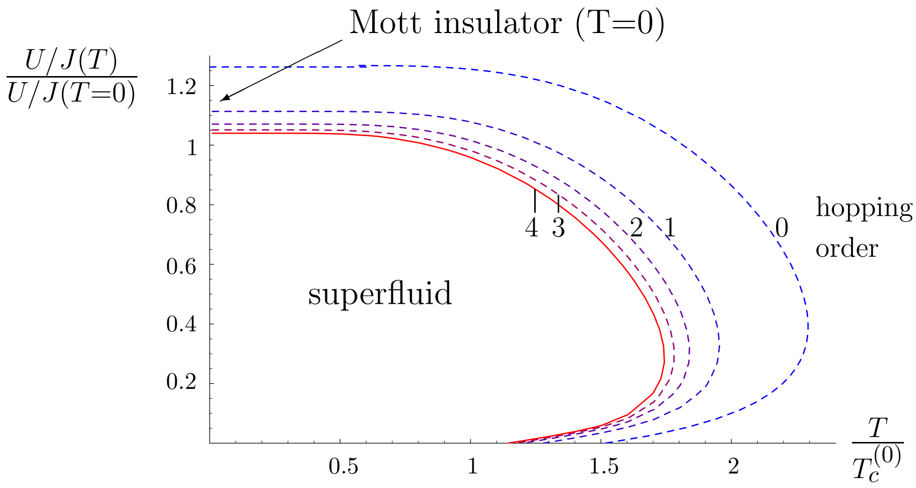


Figure 11.1: Phase diagram of superfluid-Mott insulator transition in optical lattices for increasing hopping order.

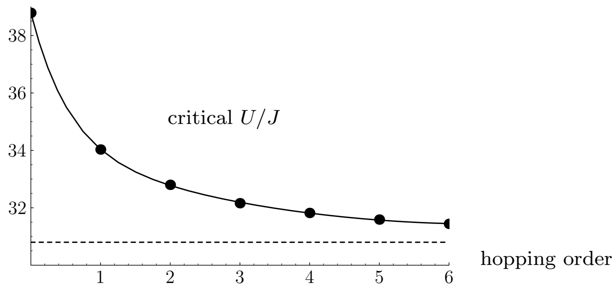


Figure 11.2: Convergence of hopping expansion for the critical value of U/J at the zero-temperature quantum phase transition.

where the expansion parameter $\kappa = 1$ has been introduced whose power serves to count the hopping order. Thus our value is smaller than the mean-field result $U/J|_{T=0} \approx 34.8$ [16, 100–102] derived from the Bose-Hubbard model (1.22) and the experimental number $U/J|_{T=0} \approx 36$ [15].
In the same way the sequence of transition temperatures at $U = 0$ converges to $T_c \approx 3.6\, J/k_B$ with the corresponding expansion:

$$\frac{k_B T_c}{J} = 5.46 - 0.85\kappa^2 - 0.29\kappa^4 - 0.16\kappa^6 - 0.09\kappa^8 - 0.07\kappa^{10} + \mathcal{O}(\kappa^{12})\,. \qquad (11.10)$$

The higher-loop slope for the lattice spectrum (11.1) is unknown, so that we cannot improve the result near T_c in the same way as for the free-particle spectrum. By analogy, we may, however, assume that the characteristic reentrant transition will also here survive higher-loop corrections.

For the experimentalist it is important to know whether this phenomenon persists if the optical lattice is stabilized by an overall weak magnetic trap of a typical frequency $\omega_{\rm trap} \approx 2\pi \times 24$ Hz which is necessary to prevent the particles from escaping the optical lattice. According to the result of Ref. [41], the nose in the transition curve could disappear since for the free-particle spectrum an external trap causes a reversal of the slope of the transition curve at $T_c^{(0)}$ [49, 103, 104], the shift becoming

$$t_c \approx 1 - 3.427\sqrt{r_1} \times r_2 \times a_{sc} n^{1/3} = 1 - 0.136\sqrt{r_1} \times r_2 \times U/J, \tag{11.11}$$

where $r_1 \equiv k_B T_c^{(0)}/2\pi\hbar\omega_{\rm trap}$ and $r_2 \equiv 1/\lambda_{\omega_{\rm trap}} n^{1/3}$ is the ratio between the length scale $\delta/f^{1/3}$ and the width of the trap $\lambda_{\omega_{\rm trap}} \equiv \sqrt{\hbar/M\omega_{\rm trap}}$. These numbers have the ranges $r_1 \in (0.27, 2.0)$ and $r_2 \in (0.52, 1.4)$ so that $0.136 \times \sqrt{r_1} \times r_2$ lies between 0.037 and 0.27, experimentally.

We end by mentioning that after our paper [47] appeared on the Los Alamos server, P.J.H. Denteneer drew our attention to a preprint of his written with D.B.M. Dickerscheid, D. van Oosten, and H.T.C. Stoof (eprint: `cond-mat/0306573`) in which they also found a nose in the phase diagram (see their Figure 6). According to his private communication they did not, however, interpret their nose as a signal for a reentrant transition but considered it as an artefact of their slave boson approach.

Appendix A

Robinson Formula

Here we derive a series representation of the polylogarithmic function

$$\zeta_\nu(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\nu}, \tag{A.1}$$

where $z = e^{\beta\mu}$ is the fugacity, which is valid for small negative chemical potential μ. Naively, one would expect that this is carried out by a simple Taylor expansion of the exponential function:

$$\zeta_\nu(e^{\beta\mu}) = \sum_{n=1}^{\infty} \frac{1}{n^\nu} \sum_{k=0}^{\infty} \frac{(\beta\mu n)^k}{k!} = \sum_{k=0}^{\infty} \frac{(\beta\mu)^k}{k!} \sum_{n=1}^{\infty} \frac{1}{n^{\nu-k}}. \tag{A.2}$$

Applying the sum representation of the zeta function $\zeta(\nu) = \zeta_\nu(1)$ this yields:

$$\zeta_\nu(e^{\beta\mu}) = \sum_{k=0}^{\infty} \frac{(\beta\mu)^k}{k!} \zeta(\nu - k). \tag{A.3}$$

However, this result is wrong for negative chemical potential μ, as the sums cannot be interchanged. Instead, the correct series representation turns out to be:

$$\boxed{\zeta_\nu(e^{\beta\mu}) = \Gamma(1-\nu)(-\beta\mu)^{\nu-1} + \sum_{k=0}^{\infty} \frac{(\beta\mu)^k}{k!}\zeta(\nu - k), \;\; \mu < 0.} \tag{A.4}$$

This was first proven by Robinson [105] using the Mellin transformation as elaborated in Section A.1. In Section A.2 we show that it can also be shown by invoking the Poisson formula [49, Chap. 2].

A.1 Proof via Mellin Transformation

The Mellin transformation of a function $f(x)$ is defined by

$$F(s) = \int_0^\infty f(x)\, x^{s-1}\, dx. \tag{A.5}$$

The inverse Mellin transformation is then given by

$$f(x) \;=\; \frac{1}{2\pi i}\oint_{c-i\infty}^{c+i\infty} F(s)\, x^{-s}\, ds\,, \tag{A.6}$$

where the integral has to be performed over the so-called Bromwich path [106]. Now, we apply these formulas to the polylogarithmic function (A.1). Its Mellin transformed follows from (A.5) to be

$$F(s) = \int_0^\infty \sum_{n=1}^\infty \frac{e^{-xn}}{n^\nu} x^{s-1}\, dx = \sum_{n=1}^\infty \frac{1}{n^\nu}\int_0^\infty e^{-xn} x^{s-1}\, dx = \Gamma(s)\zeta(\nu+s)\,. \tag{A.7}$$

Of course, the inverse Mellin transformation (A.6) should give back the polylogarithmic function itself

$$f(x) = \zeta_\nu(e^{-x}) = \frac{1}{2\pi i}\oint_{c-i\infty}^{c+i\infty} x^{-s}\Gamma(s)\zeta(\nu+s)\, ds\,. \tag{A.8}$$

From that we derive a series representation of the polylogarithmic function by calculating the complex integral with the help of the residue theorem, which states that a complex integral is given by a sum over all residues of the integrand $f(x)$ at its singularities a_k:

$$\oint_C f(z)dz = 2\pi i \sum_{k=1}^n \mathrm{Res}(f, a_k)\,. \tag{A.9}$$

The function $\zeta(s+\nu)$ has a simple pole at $s = 1-\nu$ with the residue 1, which will give the first part of the Robinson formula (A.4). The second part comes from the simple poles of the gamma function $\Gamma(s)$ at $s = -n$ with residues $(-1)^n/n!$.

A.2 Proof via Poisson Formula

A.2.1 Derivation of Poisson Formula

We consider a periodic delta function

$$\delta^{(p)}(x) := \sum_{m=-\infty}^{\infty} \delta(x-m) \tag{A.10}$$

and its Fourier representation

$$\delta^{(p)}(x) = \sum_{n=-\infty}^{\infty} \delta_n^{(p)}\, e^{-2\pi i n x}\,, \tag{A.11}$$

where the coefficients $\delta_n^{(p)}$ are given by

$$\delta_n^{(p)} = \int_0^1 \delta^{(p)}(x) e^{-2\pi i n x}\, dx\,. \tag{A.12}$$

The last integral can be done, by inserting the definition (A.10):

$$\delta_n^{(p)} = \sum_{m=-\infty}^{\infty} \int_0^1 \delta(x-m) e^{-2\pi i n x}\, dx = \int_0^1 \left[\delta(x-1) + \delta(x)\right] e^{-2\pi i n x}\, dx = 1\,. \tag{A.13}$$

Inserting (A.13) in (A.11) yields together with (A.10) the fundamental identity

$$\sum_{m=-\infty}^{\infty} \delta(x-m) = \sum_{n=-\infty}^{\infty} e^{-2\pi i n x}\,. \tag{A.14}$$

We apply this distribution identity to a test function $f(x)$ and multiply the resulting equation with an integral over the whole real axis to obtain the bosonic Poisson formula:

$$\boxed{\sum_{m=-\infty}^{\infty} f(m) = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) e^{-2\pi i n x}\, dx}\,. \tag{A.15}$$

Applying the Poisson formula in many-body theory has the effect of converting a high-temperature in a low-temperature expansion, as can be seen in Section 2.1 . Integrating over only one half of the real axis, we get

$$\lim_{\epsilon \downarrow 0} \sum_{m=-\infty}^{\infty} \int_{\epsilon}^{\infty} f(x) \delta(x-m)\, dx = \lim_{\epsilon \downarrow 0} \sum_{n=-\infty}^{\infty} \int_{\epsilon}^{\infty} f(x) e^{-2\pi i n x}\, dx\,, \tag{A.16}$$

so that extracting the $n = 0$ contribution yields the modified bosonic Poisson formula:

$$\boxed{\sum_{m=1}^{\infty} f(m) = \int_0^{\infty} f(x)\, dx + 2 \sum_{n=1}^{\infty} \int_0^{\infty} f(x) \cos(2\pi n x)\, dx}\,. \tag{A.17}$$

A.2.2 Derivation of Robinson's Formula

Now we apply the modified bosonic Poisson formula (A.17) to the function $f(x) = x^{-\nu} e^{\beta\mu x}$:

$$\zeta_\nu(e^{\beta\mu}) = \sum_{n=1}^{\infty} \frac{e^{\beta\mu n}}{n^\nu} = \int_0^{\infty} x^{-\nu} e^{\beta\mu x}\, dx + 2 \sum_{n=1}^{\infty} \int_0^{\infty} x^{-\nu} e^{\beta\mu x} \cos(2\pi n x)\, dx\,. \tag{A.18}$$

The first part of the above equation can be calculated immediately. It gives the additional contribution to the Taylor expansion in (A.4):

$$\int_0^{\infty} x^{-\nu} e^{\beta\mu x}\, dx = (-\beta\mu)^{\nu-1} \int_0^{\infty} x^{-\nu} e^{-x}\, dx = \Gamma(1-\nu)(-\beta\mu)^{\nu-1}\,. \tag{A.19}$$

The calculation of the second part

$$I_2 := 2\sum_{n=1}^{\infty}\int_0^{\infty} x^{-\nu} e^{\beta\mu x}\cos(2\pi n x)\,dx = 2\mathrm{Re}\sum_{n=1}^{\infty}\int_0^{\infty} x^{-\nu} e^{-(-\beta\mu-2\pi i n)x}\,dx \tag{A.20}$$

is a little bit more involved. There, it is allowed to expand the exponential function into a Taylor series

$$I_2 = 2\Gamma(1-\nu)\mathrm{Re}\sum_{n=1}^{\infty}(-2\pi i n)^{\nu-1}\left(1+\frac{\beta\mu}{2\pi i n}\right)^{\nu-1} . \tag{A.21}$$

As $\beta\mu/(2\pi i n)^{\nu-1}$ is a small parameter, we evaluate the last bracket in a power series

$$I_2 = 2\Gamma(1-\nu)\mathrm{Re}\sum_{n=1}^{\infty}(-2\pi i n)^{\nu-1}\sum_{k=0}^{\infty}\binom{\nu-1}{k}\left(\frac{\beta\mu}{2\pi i n}\right)^{k} , \tag{A.22}$$

so that the sum over index n becomes a zeta function:

$$I_2 = 2\Gamma(1-\nu)\sum_{k=0}^{\infty}\binom{\nu-1}{k}\frac{(\beta\mu)^k\cos(\pi/2(\nu-1+k))}{(2\pi)^{1+k-\nu}}\zeta(1-\nu+k) . \tag{A.23}$$

With the analytic continuation of the zeta function [55]

$$\zeta(1-z) = \frac{2^{1-z}\,\Gamma(z)\cos(\pi z/2)}{\pi^z}\zeta(z) \tag{A.24}$$

we obtain, after some trivial simplifications, the desired result:

$$I_2 = \sum_{k=0}^{\infty}\frac{(\beta\mu)^k}{k!}\zeta(\nu-k) . \tag{A.25}$$

Appendix B

Dimensional Regularization

B.1 Motivation

In perturbation theory the integrals of the second-order Feynman diagrams diverge in $d = 3$ dimensions. With the help of so-called regularization procedures they can be made finite. One of the most popular procedures is dimensional regularization, which was invented by 't Hooft and Veltman [107]. There, the measure of integration is changed by allowing the dimension d in the integrals to be an arbitrary complex number for which convergence is assured. The d-dimensional results can be expanded in powers of the deviation ϵ from three dimensions by setting $d = 3 - 2\epsilon$. The divergencies in the physical quantities then arise as ϵ poles, which vanish in most physical theories by renormalization. Those theories are called renormalizable. Here, we will derive some important formulas which are needed for calculating Feynman diagrams with dimensional regularization in Part 2 and 3 of this work.

B.2 Schwinger Trick

Schwinger observed that a fraction of the form $1/\alpha^x$ with an arbitrary expression α and power x can be rewritten as an integral:

$$\boxed{\frac{1}{\alpha^x} = \frac{1}{\Gamma(x)} \int_0^\infty d\tau \tau^{x-1} e^{-\alpha\tau}}. \tag{B.1}$$

This can be proven with the integral representation of the Gamma function

$$\Gamma(x) = \int_0^\infty dt\, t^{x-1} e^{-t}\,. \tag{B.2}$$

If we substitute t by αt, we get immediately the relationship (B.1). If α is an expression, which can become zero, one has to use the modified Schwinger trick:

$$\boxed{\frac{1}{\alpha} = \text{Re} \lim_{\epsilon \downarrow 0} \int_0^{i\infty} d\tau e^{-(\alpha - i\epsilon)\tau}}\,. \tag{B.3}$$

We proof Eq. (B.3) as follows:

$$\lim_{\epsilon \downarrow 0} \int_0^{i\infty} d\tau e^{-(\alpha - i\epsilon)\tau} = \lim_{\epsilon \downarrow 0} i \frac{1}{\epsilon + i\alpha} = i \lim_{\epsilon \downarrow 0} \frac{\epsilon}{\epsilon^2 + \alpha^2} + \lim_{\epsilon \downarrow 0} \frac{\alpha}{\epsilon^2 + \alpha^2} = i\pi\delta(x) + \frac{1}{\alpha} \tag{B.4}$$

Thus taking the real part of the right-hand side of (B.4) yields the desired result (B.3). A useful application of the Schwinger trick is the following representation of a logarithm:

$$\boxed{\ln \alpha = -\frac{\partial}{\partial x}\, \alpha^{-x}\Big|_{x=0} = -\frac{\partial}{\partial x} \left\{ \frac{1}{\Gamma(x)} \int_0^{\infty} d\tau \tau^{x-1} e^{-\alpha\tau} \right\}\Big|_{x=0}}\,. \tag{B.5}$$

We proof this relationship by considering the function

$$f(x) = \alpha^{-x} = e^{-x \ln \alpha}\,. \tag{B.6}$$

Because of it's derivative $f'(x) = -\ln \alpha f(x)$ and $f(0) = 1$, we write

$$\ln \alpha = -f'(0) = -\frac{\partial}{\partial x}\, \alpha^{-x}\Big|_{x=0}\,. \tag{B.7}$$

Finally we apply (B.1) to (B.7) from which one obtains (B.5).

B.3 Feynman Parameter

For products of different denominators we use Feynman's parametric integral formula

$$\boxed{\frac{1}{A^a B^b} = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \int_0^1 d\tau \frac{\tau^{a-1}(1-\tau)^{b-1}}{[A\tau + B(1-\tau)]^{a+b}}}\,, \tag{B.8}$$

which is a straight-forward generalization of the obvious identity

$$\frac{1}{AB} = \frac{1}{B-A}\left(\frac{1}{A} - \frac{1}{B}\right) = \frac{1}{B-A} \int_A^B dx \frac{1}{\tau^2} = \int_0^1 d\tau \frac{1}{[A\tau + B(1-\tau)]^2}\,. \tag{B.9}$$

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