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Phases and phase transitions in an interacting Bose gas

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Christopher Moseley

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Erstgutachter:	Prof. Dr. Klaus Ziegler
Zweitgutachter:	Priv. Doz. Dr. Sigmund Kohler
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1 Introduction

The quantum statistics of non-interacting particles was established by S. N. Bose in 1924 [1]. Bose was able to deduce Planck's radiation law on the assumption that each quantum state can be occupied by an arbitrary number of indistinguishable photons. By applying this idea to the quantum statistics of an ideal gas of N atoms enclosed in a volume V, A. Einstein predicted the occurrence of a phase transition [2]: Below a critical temperature T_c, a certain fraction of atoms would "condense" in the ground state of the system. This phenomenon is called Bose-Einstein condensation (BEC).

The possibility to study quantum phase transitions in interacting Bose gases experimentally with high accuracy motivates the development of a statistical theory, which is not only valid in weakly interacting but also in strongly interacting systems. The strongly interacting regime has been realised by the application of Feshbach resonances [3]. In this thesis, special attention will be drawn to Bose systems in optical lattices, where a quantum phase transition of a BEC to a Mott-insulator (MI) has been described theoretically [4, 5, 6] by means of the so-called Bose-Hubbard model, as well as observed experimentally [7].

In this thesis, a system of hard-core bosons will be used as a foundation for the theoretical analysis of these phase transitions. This system is characterised by the restriction that each lattice site is either empty, or occupied by one single boson. It differs from the Bose-Hubbard model in the way that the latter allows multiple occupation of lattice sites by the cost of a repulsive interaction energy U. Thus the model of hard-core bosons requires one parameter less than the Bose-Hubbard model. Different approaches shall be presented to make predictions to experimentally relevant physical quantities and the qualitative behaviour of the system at zero temperature as well as non-zero temperatures. The objects of interest are the phase diagram, the particle density and condensate density, the spectrum of quasiparticle excitations, and the static structure factor which can be measured by means of light scattering experiments.

The functional integral formalism provides an adequate approach to this problem of many particle physics [8, 9]. Within this formalism the determination of the quantities mentioned above reduces to the calculation of correlation functions, which can be evaluated by means of appropriate approximations. Four different models to describe a gas of hard-core bosons in an optical lattice will be discussed: A one-dimensional model, a hard-core Bose model constructed by nilpotent field variables, a model describing paired fermions, and a model which is based on the slave-boson approach.

The thesis is organised as follows: In chapter 2 an outline of the theoretical and

experimental developments in the field of Bose-Einstein condensation, which are relevant for the topic, is given. In chapter 3 the functional integral representation is introduced in the form as it is applied to the models. It is shown that all physical quantities can be drawn out of the functional integral representation of the grand canonical partition function. In chapter 4 it is applied to an ideal Bose gas in an optical lattice. The procedure of calculating physical quantities from correlation functions is demonstrated. In the last section a random-walk expansion is performed in order to show that bosons can be illustrated by world-lines along the imaginary time coordinate. This world-line picture will also be applied to motivate the one-dimensional model, the hard-core Bose model and the paired-fermion model.

The aim of chapter 5 is to demonstrate the principle of the saddle-point approximation, which will be applied to all models that will be discussed later, except the one-dimensional model. The first four sections of the chapter give an introduction to Bogoliubov theory. Then it is shown, that the same results are found by applying a saddle point approximation to the action of an interacting Bose gas with weak two-particle interaction: On the mean-field level, which is derived by minimising the action due to the variational principle, the Gross-Pitaevskii equation [10] is found. On the level of Gaussian fluctuations around the mean-field result, all results of Bogoliubov theory are found.

In chapter 6 the one-dimensional system is discussed. Based on the well-known fact that a system of one-dimensional impenetrable bosons can be mapped to ideal fermions, we define the model by a special construction of a bipartite lattice where it is assured that two particles cannot interchange their position. This allows to calculate some physical quantities exactly.

Chapter 7 is devoted to the model which will be referred to as hard-core Bose model. The functional integral representation of its grand canonical partition function is constructed by an algebra of nilpotent commutating field variables. A Hubbard-Stratonovich transformation allows a mapping to a representation with two complex fields, which can be treated by means of a saddle point approximation. Calculations are made on the mean-field level and on the level of Gaussian fluctuations. An extension of this model to a model of N-component bosons is presented, where the limit $N \to \infty$ can be solved exactly and is identical to the mean-field result.

In chapter 8 a fermionic model is discussed, which is constructed such that pairs of fermions always stick together while tunneling through the optical lattice. The Pauli principle forbids multiple occupation on lattice sites. Thus these pairs of fermions are expected to behave physically like hard-core bosons. This system will be referred to as paired-fermion model. Similar to the hard-core Bose model, a Hubbard-Stratonovich transformation leads to a representation of two complex fields. The calculations of the mean-field approximation are presented.

In chapter 9 the slave-boson approach is applied to hard-core bosons. The model is treated in classical approximation, and again a Hubbard-Stratonovich approximation

is applied. The mean-field theory is discussed and used to derive an equation similar to the Gross-Pitaevskii equation, which is applied to a condensate in a harmonic trap potential with and without a vortex through the trap center. The excitation spectrum is calculated from Gaussian fluctuations.

In chapter 10 we summarise the results for the different models, and discuss their common features and differences. The quasiparticle spectra which were calculated, will be compared to results for the Bose-Hubbard model form the literature.

2 Overview of Bose-Einstein condensation

2.1 Definition of the condensate density

In this chapter we shall outline the theoretical and experimental developments in the field of Bose-Einstein condensation as far as they are relevant for this thesis.

In a homogeneous ideal Bose-gas in the absence of an external potential, the condensation temperature of the ideal Bose gas is given as [10, 11, 12, 13, 14]

$$k_{\mathrm{B}} T_c = \frac{2\pi\hbar^2}{m} \left(\frac{n_{\mathrm{tot}}}{\zeta\left(\frac{3}{2}\right)} \right)^{\frac{2}{3}} , \tag{2.1}$$

where k_{B} is Boltzmann's constant, $n_{\mathrm{tot}} = N/V$ is the particle density, m is the mass of the particles and $\zeta(x)$ is Riemann's Zeta-Function. The condensate fraction is given as

$$\frac{n_0}{n_{\mathrm{tot}}} = \begin{cases} 0 & \text{if } T > T_c \\ 1 - \left(\frac{T}{T_c}\right)^{\frac{3}{2}} & \text{if } T < T_c \end{cases} , \tag{2.2}$$

where n_0 is the condensate density.

The first candidate for a possible realisation of Bose-Einstein condensation was the discovery of superfluidity in ^{4}He atoms below $T_c = 2.2$K by P. L. Kapitza in 1934. Although superfluid Helium is far away from the ideal Bose-gas considered by Einstein because of strong interactions between the Helium atoms, the phenomena of superfluidity and BEC are related. Superfluidity was first explained by L. D. Landau in 1941 by an argument which is based on the idea that the viscosity of a fluid depends on the existence of elementary excitations. If the excitation spectrum is linear for small momenta, elementary excitations would not occur below a critical flow velocity v_c [10]. However, it is important to mention that superfluidity and BEC are not identical. For instance, an ideal Bose gas can condense, but it is not superfluid due to Landau's principle.

In an interacting Bose gas of uncharged atoms, the main contribution to the interparticle interaction comes from s-wave scattering between two particles. The characteristic length scale here is the scattering length a_s. We assume a_s to be positive, although it should be mentioned, that it can also be negative in trapped Bose gases (without trapping potential a Bose gas with negative a_s is instable [10]). For theoretical description, the two-body interaction is usually assumed to be hard-core, which means that an

interaction process between two atoms is regarded as a collision of hard spheres with a diameter a_s. In other words, this means that the probability density of two bosons being at the same point in space vanishes. Approximately, the two-body interaction potential can be written in form of a δ-potential:

$$V_{\text{int}}(\mathbf{r}-\mathbf{r}') \approx g\,\delta(\mathbf{r}-\mathbf{r}')\ . \tag{2.3}$$

Here, g is the strength of the repulsive interaction between two bosons. It is connected to the s-wave scattering length by the relation

$$g = \frac{4\pi a_s \hbar^2}{m}\ . \tag{2.4}$$

This approximation is possible, if the a_s is small compared to the thermal de Broglie wavelength, the interparticle spacing, and the characteristic lenght scale of the trapping potential [12]. After the introduction of an external potential V_{ext}, the full Hamiltonian of the Bose system in terms of bosonic field operators is

$$\hat{H} = \int \mathrm{d}^3 r \left[\hat{\psi}^+(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r})\right)\hat{\psi}(\mathbf{r}) + \frac{g}{2}\,\hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\right]\ . \tag{2.5}$$

The ground state of this interacting many-body system is not known, therefore the condensate density cannot be defined by the population density of the ground state like in the ideal Bose gas. An appropriate definition for a homogeneous system is the concept of "off-diagonal long-range order" which was developed in the 1950's [10, 12, 15]. The condensate density is given by the long-range behaviour of the one-particle correlation function

$$n_0 := \lim_{\mathbf{r}-\mathbf{r}'\to\infty} \langle \hat{\psi}^+(\mathbf{r})\hat{\psi}(\mathbf{r}')\rangle\ . \tag{2.6}$$

If the one-particle correlation function decays exponentially or algebraically, the condensate density is zero. An algebraic decay is found in a two-dimensional Bose gas at low temperature and in a one-dimensional Bose gas at zero temperature [8].

2.2 Dilute Bose gas

When the mean distance between atoms is large compared to their spacial extension, which is the case when $n_{\text{tot}} a_s^3 \ll 1$, the system is said to be in the dilute regime. In this case, the effect of interaction is small. A consistent mean-field theory of a dilute Bose gas which is valid for low temperatures $T \ll T_c$ was given by N. N. Bogoliubov in 1947 [10, 11]. The condensed phase is described by replacing the bosonic field-operators by the sum of a complex condensate order parameter Φ_0 and fluctuations out of the condensate as

$$\hat{\psi}(\mathbf{r},t) = \Phi_0(\mathbf{r},t) + \tilde{\psi}(\mathbf{r},t)\ , \tag{2.7}$$

where the field operators $\tilde{\psi}$ of the fluctuations fulfill bosonic commutation relations. This theory finds elementary excitations out of the condensate which have the energy spectrum

$$E_{\mathbf{k}} = \sqrt{\frac{(\hbar\mathbf{k})^2}{2m}\left(2gn_0 + \frac{(\hbar\mathbf{k})^2}{2m}\right)} \tag{2.8}$$

where $\mathbf{k}$ is the wave number vector. It is linear for small momenta ("phonon spectrum") and therefore satisfies Landau's criterion for superfluidity, in contrary to Einstein's non-interacting Bose-gas with a quadratic energy spectrum. In the Bogoliubov approximation, the elementary excitations are regarded as non-interacting. An important feature of an interacting Bose gases is the ground state depletion, which means that even at $T = 0$, the condensate fraction is smaller than 1. This is also found in Bogoliubov theory. In a dilute Bose gas, the condensate depletion is small.

The condensate order parameter Φ_0 is connected to the breaking of the global $U(1)$ symmetry, which reflects the fact that the replacement

$$\Phi_0(\mathbf{r}, t) \to e^{i\alpha}\Phi_0(\mathbf{r}, t) \ , \tag{2.9}$$

where α is a global phase, does not change the physics of the system. The phase α can be chosen arbitrarily, but once it has been chosen, the symmetry is broken. This is the case in the BEC phase. This phase α is responsible for the fact that the quasiparticle spectrum in eq. (2.8) vanishes for $\mathbf{k} = 0$: The Goldstone-theorem states that the existence of a broken $U(1)$ phase symmetry leads to a gapless excitation spectrum [16].

The order parameter in interpreted as a macroscopic wave function and can be split into its modulus and phase:

$$\Phi_0(\mathbf{r}, t) = \rho(\mathbf{r}, t)\, e^{\mathrm{i}\theta(\mathbf{r},t)} \ . \tag{2.10}$$

The local condensate density is related to the modulus squared of the order parameter

$$n_0(\mathbf{r}, t) = |\Phi_0(\mathbf{r}, t)|^2 \ , \tag{2.11}$$

and the gradient of its phase, $\nabla\theta(\mathbf{r}, t)$, is associated with the velocity field of the condensed atoms. Gross and Pitaevskii have independently derived an equation to describe the dynamics of the order parameter, which is known as the Gross-Pitaevskii (GP) equation [10, 12, 13]:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) + g|\Phi_0(\mathbf{r}, t)|^2\right)\Phi_0(\mathbf{r}, t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\Phi_0(\mathbf{r}, t) \ . \tag{2.12}$$

The third order term, which is proportional to the interaction constant g, can be interpreted as the coupling of the order parameter to the local particle density as given in eq. (2.11). If $g = 0$, the GP equation reduces to the Schrödinger equation of a single

particle moving in an external potential $V_{\text{ext}}(\mathbf{r},t)$, therefore it is also called nonlinear Schrödinger equation. The GP energy functional is given as

$$\mathcal{E} = \int \mathrm{d}^3 r\, \Phi_0^*(\mathbf{r},t) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + \frac{g}{2}\left|\Phi_0(\mathbf{r})\right|^2 \right) \Phi_0(\mathbf{r},t)\ . \tag{2.13}$$

For stationary solutions of the GP equation we use the separation ansatz $\Phi_0(\mathbf{r},t) = \Phi_0(\mathbf{r})\exp(-i\mu t/\hbar)$, using the chemical potential

$$\mu = \frac{\partial \mathcal{E}}{\partial N_{\text{tot}}}\ , \tag{2.14}$$

where

$$N_{\text{tot}} \approx N_0 = \int |\Phi_0(\mathbf{r})|^2 \mathrm{d}^3 r \tag{2.15}$$

is the total particle number and N_0 the number of condensed particles. The GP equation then reduces to the stationary form

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) - \mu + g|\Phi_0(\mathbf{r})|^2 \right) \Phi_0(\mathbf{r}) = 0\ . \tag{2.16}$$

2.3 Trapped Bose gas

The experimental realisation of a weakly interacting BEC in a magnetic trap succeeded in 1995 by E. Cornell and C. Wiemann at Boulder and W. Ketterle at MIT in vapors of ^{87}Rb ($a_s = 5.77$nm) and ^{23}Na ($a_s = 2.75$nm). This became possible by a combination of evaporative cooling and laser cooling. This cooling techniques are so effective, that the Bose gas can be brought in the vicinity of the absolute ground state. Experimentally, the condensate is identified from time-of-flight measurements that can image the momentum distribution of the atoms. While the momentum distribution of the non-condensed part of the Bose gas is spherical, the distribution of the condensed part adjusts to the shape of the trap potential. These systems are well described by Bogoliubov theory and the GPE. Since the discovery of magnetic Feshbach resonances it is possible to tune the scattering length over a large range of values (positive as well as negative) to reach the strongly interacting regime, where Bogoliubov theory is not applicable anymore [3, 10, 17]. These magnetic Feshbach resonances became possible after the development of optical trapping as an alternative to magnetic trapping.

For models of the trapped condensates as those realised in experiments, usually a harmonic trap potential of the general form

$$V_{\text{ext}}(\mathbf{r}) = V_{\text{tr}}(\mathbf{r}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \tag{2.17}$$

is assumed. If $\omega_x = \omega_y = \omega_z$, the trap is spherical, in the case $\omega_x = \omega_y < \omega_z$ we speak of a "disk-shaped", and in the case $\omega_x = \omega_y > \omega_z$ of a "cigar-shaped" condensate. For an ideal Bose gas, the condensation temperature is given as [10]

$$k_{\mathrm{B}}T = \hbar\omega_{\mathrm{ho}} \left(\frac{N_{\mathrm{tot}}}{\zeta(3)} \right)^{\frac{1}{3}} \tag{2.18}$$

with the geometrical average of the trap frequencies

$$\omega_{\mathrm{ho}} = (\omega_x \omega_y \omega_z)^{\frac{1}{3}} \ , \tag{2.19}$$

in contrast to the condensation temperature of a homogeneous BEC in eq. (2.1). Instead of eq. (2.2), the condensate fraction in a trapped condensate is

$$\frac{n_0}{n_{\mathrm{tot}}} = \begin{cases} 0 & \text{if } T > T_c \\ 1 - \left(\frac{T}{T_c}\right)^3 & \text{if } T < T_c \end{cases} \ . \tag{2.20}$$

In rotating BECs, quantised vortices and vortex lattices have been observed, a phenomenon which is also known in type-II superconductors and superfluid ^{4}He [18, 19]. The are two ways to achieve the rotation of the condensate. One way is to use a stirring laser beam which has the same effect like a spoon in a cup of coffee. The second way is to use an elongated condensate in a cigar-shaped trap with a weak non-axialsymmetric deformation that rotates about its axis. Vortices are observed by absorption imaging [20].

The GP equation can well describe the vortex formation observed in weakly interacting trapped BECs. If the condensate is in rotational equilibrium at angular velocity Ω around the z-axis, we can transform the order parameter into a rotating frame. This can be done by using the z-component of the angular momentum operator given by

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -\mathrm{i}\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right) \ , \tag{2.21}$$

as the generator of a rotation around the z-axis [21], and substituting

$$\Phi_0 \to e^{-\frac{\mathrm{i}}{\hbar}\Omega\hat{L}_z t}\Phi_0$$

into the time-dependent GP eq. (2.12). Because of the commutation relation $[\nabla^2, \hat{L}_z] = 0$, we get for the rotating frame [18] the equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \Omega\hat{L}_z + V_{\mathrm{ext}}(\mathbf{r}) + g|\Phi_0(\mathbf{r},t)|^2 \right) \Phi_0(\mathbf{r},t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\Phi_0(\mathbf{r},t) \ , \tag{2.22}$$

where the additional term $-\Omega\hat{L}_z\Phi_0$ arises from the time derivative on the right hand side. Correspondingly, the energy functional becomes

$$\mathcal{E}_{\mathrm{rot}}(\Omega) = \int \mathrm{d}^3 r\, \Phi_0^*(\mathbf{r},t)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) - \Omega\hat{L}_z + \frac{g}{2}\left|\Phi_0(\mathbf{r})\right|^2\right)\Phi_0(\mathbf{r},t)\ . \tag{2.23}$$

The critical angular velocity Ω_c, at which the creation of a vortex occurs, as well as the stability and dynamics of vortex cores and vortex lattices have, can be calculated by minimizing the free energy in the GP approach [22, 23, 24, 25, 26].

2.4 Light scattering and structure factor

Light scattering experiments on BECs allow the study of density fluctuations. In so-called Bragg scattering experiments, light scattering is studied as a stimulated process, induced by two laser beams which illuminate the atomic sample [27]. In scattering events elementary excitations are created, and the momentum and energy transfer is pre-determined by the angle and frequency difference between the incident beams.

The most important quantity here is the dynamic structure factor $S(\mathbf{q},\omega)$, which is proportional to the excitation rate per particle, where $\mathbf{q} = \mathbf{q}_{\mathrm{f}} - \mathbf{q}_{\mathrm{i}}$, and $\mathbf{q}_{\mathrm{i}}$ is the wave vector of the incoming, $\mathbf{q}_{\mathrm{f}}$ the wave vector of the reflected light beam, and ω is the frequency difference between the two laser beams. Integrating over all frequencies ω one obtains the static structure factor

$$S(\mathbf{q}) = \int S(\mathbf{q},\omega)\,\mathrm{d}\omega\ , \tag{2.24}$$

which is equivalent to the line strength of the Bragg resonance.

The dynamic structure factor describes a correlation between a density fluctuation at time $t_0 = 0$ and at time $t_1 = t$ and is defined as the expectation value [28]

$$S(\mathbf{q},t) = \frac{1}{N}\left\langle \hat{\rho}_{\mathbf{q}}(t)\hat{\rho}_{\mathbf{q}}^{+}(0)\right\rangle\ , \tag{2.25}$$

with the density operator in momentum space, which is given as

$$\hat{\rho}_{\mathbf{q}}^{+} = \int \hat{n}_{\mathbf{r}}\, e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}\,\mathrm{d}^d r = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}+\mathbf{q}}^{+}\hat{a}_{\mathbf{k}}\ , \tag{2.26}$$

and $\hat{a}_{\mathbf{k}}$, $\hat{a}_{\mathbf{k}}^{+}$ fulfil bosonic commutation relations. The time dependence is due to the Heisenberg picture in real time:

$$\hat{\rho}_{\mathbf{q}}(t) = e^{-\mathrm{i}(\hat{H}-\mu\hat{N})t/\hbar}\hat{\rho}_{\mathbf{q}}\, e^{\mathrm{i}(\hat{H}-\mu\hat{N})t/\hbar}\ . \tag{2.27}$$

If the states $|n\rangle$ are the eigenstates of the extended Hamiltonian $\hat{H}-\mu\hat{N}$ with eigenenergy E_n, we can write, after inserting the unity operator $\sum_n |n\rangle\langle n|$:

$$S(\mathbf{q},t) = \frac{1}{ZN}\sum_{n,m} e^{-\beta E_m/\hbar}\langle m|e^{-\mathrm{i}(\hat{H}-\mu\hat{N})t/\hbar}\hat{\rho}_{\mathbf{q}}\, e^{\mathrm{i}(\hat{H}-\mu\hat{N})t/\hbar}|n\rangle\langle n|\hat{\rho}^{+}_{\mathbf{q}}|m\rangle =$$

$$\frac{1}{ZN}\sum_{n,m} e^{-\beta E_m} e^{\mathrm{i}(E_n-E_m)t/\hbar}\left|\langle n|\hat{\rho}^{+}_{\mathbf{q}}|m\rangle\right|^2 \tag{2.28}$$

with the grand canonical partition function

$$Z = \sum_m e^{-\beta E_m}\ . \tag{2.29}$$

The Fourier transformation of S with respect to time is

$$S(\mathbf{q},\omega) = \int S(\mathbf{q},t)\, e^{-\mathrm{i}\omega t}\,\frac{\mathrm{d}t}{2\pi} = \frac{1}{ZN}\sum_{n,m} e^{-\beta E_m}\left|\langle n|\hat{\rho}^{+}_{\mathbf{q}}|m\rangle\right|^2 \delta(\omega-\omega_{nm})\ , \tag{2.30}$$

where $\hbar\omega_{nm} = E_n - E_m$. This is the quantity which is accessible by Bragg scattering experiments as explained above. The static structure factor is then given by eq. (2.24) as

$$S(\mathbf{q}) = \int S(\mathbf{q},t)\,\frac{\mathrm{d}t}{2\pi}\underbrace{\int e^{-\mathrm{i}\omega t}\,\mathrm{d}\omega}_{=2\pi\delta(t)} = S(\mathbf{q},0) = \frac{1}{N}\,\left\langle\hat{\rho}_{\mathbf{q}}(0)\hat{\rho}^{+}_{\mathbf{q}}(0)\right\rangle\ . \tag{2.31}$$

From eq. (2.30) we then get

$$S(\mathbf{q}) = \frac{1}{ZN}\sum_{n,m} e^{-\beta E_m}\left|\langle n|\hat{\rho}^{+}_{\mathbf{q}}|m\rangle\right|^2\ . \tag{2.32}$$

A very useful property of the dynamic structure factor is the f-sum rule, which is model independent [10, 28, 29]:

$$\int_{-\infty}^{\infty} S(\mathbf{q},\omega)\omega\,\mathrm{d}\omega = N_{\mathrm{tot}}\frac{\hbar^2\mathbf{q}^2}{2m}\ . \tag{2.33}$$

The static response function is given by the dynamic structure factor through the relation [10]

$$N_{\mathrm{tot}}\chi(\mathbf{q}) = 2\int_{-\infty}^{\infty}\frac{1}{\omega}S(\mathbf{q},\omega)\,\mathrm{d}\omega\ . \tag{2.34}$$

The low $\mathbf{q}$ limit of the static response is related to the thermodynamic compressibility via

$$\lim_{\mathbf{q}\to 0}\chi(\mathbf{q}) = \frac{1}{mc_{\mathrm{T}}^2}\ , \tag{2.35}$$

where $1/mc_{\mathrm{T}}^2$ is the isothermal compressibility of the medium. In this regime of long wave lengths there is also a general relation between the static structure factor and the sound velocity c [30, 31]:

$$S(\mathbf{q}) = \frac{\hbar|\mathbf{q}|}{2mc} + \mathcal{O}(q^2) \; . \tag{2.36}$$

In the ground state of a non-interacting condensate, the static structure factor is unity, and in the Bogoliubov ground state, it is given as

$$S(\mathbf{q}) = \frac{\hbar^2\mathbf{q}^2}{2m\,E_{\mathbf{q}}} \; , \tag{2.37}$$

where $E_{\mathbf{q}}$ is the quasiparticle spectrum given in (2.8). This result has originally been derived by R. Feynman for the static structure factor of superfluid ^{4}He [32], and will be reproduced in chapter 5.

2.5 Multi-component and fermionic condensates

The field of ultracold trapped atoms is not restricted to bosonic atoms of one single species. Systems which consist of two or more species of bosonic atoms have been studied as well. Gases of fermionic atoms are a field of interest today, too.

Multi-component BECs have been reached with atoms which occupy nearly degenerate hyperfine states [10, 12, 27]. Although many of these mixtures are unstable against exothermic hyperfine state changing collisions, some of them are relatively long-living because of a suppressed spin exchange collision rate. In the case of magnetic trapping it is required that the hyperfine states are weak-field seeking. This means that they are attracted to regions where the magnetic field is weak due to the Zeeman effect. In optically trapped condensates, a magnetic field can be switched off, such that the atoms are confined regardless of their hyperfine state. This opens the possibility of spinor condensates. The Hamiltonian of an N-component Bose gas is of the general form

$$\hat{H} = \int \mathrm{d}^3r \Bigg[\sum_{i,j=1}^{N} \hat{\psi}_i^+(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\delta_{ij}\nabla^2 + (V_{\mathrm{ext}})_{ij}(\mathbf{r}) \right) \hat{\psi}_j(\mathbf{r}) \\ + \sum_{i,j,k,l=1}^{N} \frac{g_{ij,kl}}{2}\, \hat{\psi}_i^+(\mathbf{r})\hat{\psi}_j^+(\mathbf{r})\hat{\psi}_k(\mathbf{r})\hat{\psi}_l(\mathbf{r}) \Bigg] \; . \tag{2.38}$$

In the case $N = 1$ it reduces to the single-component Hamiltonian (2.5).

A very interesting feature of ultracold fermionic gases with two spin states $\uparrow, \downarrow$ is the so-called BEC-BCS crossover. This appears in the case of attractive interaction ($g < 0$),

which can be reached by means of Feshbach resonances. If the attractive interaction is weak, the system can approximately be described by the BCS-Hamiltonian [10]

$$\hat{H} = \sum_{\sigma=\uparrow,\downarrow} \int \mathrm{d}^3k \left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \mu \right) \hat{c}^+_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \frac{g}{V} \int \mathrm{d}^3k \int \mathrm{d}^3q \, \hat{c}^+_{\mathbf{k},\uparrow} \hat{c}^+_{-\mathbf{k},\uparrow} \hat{c}_{\mathbf{q},\uparrow} \hat{c}_{-\mathbf{q},\uparrow} \, , \tag{2.39}$$

where the operators fulfill fermionic commutation relations. In this case the system forms a condensate of Cooper pairs like in superconductivity and superfluid ^{3}He.

In the regime of strong attractive interaction, the atoms form strongly bound molecules in contrary to the weakly bound Cooper pairs. Those molecules consist of fermionic atoms with opposite spin and thus can be treated like bosonic particles that form an interacting Bose-Einstein condensate. The crossover between the weakly interacting BCS and the strongly interacting BEC regime is of much interest today. The superfluid property of the BEC-BCS crossover regime has been shown in experiments by the observation of quantised vortices, which provides conclusive evidence for superfluid flow [33].

2.6 Optical lattices

A last aspect which is important to mention here, is the field of atoms in optical lattices. There are one-, two- and three-dimensional optical lattices. To create a one-dimensional optical lattice, a laser beam (wave vector $\mathbf{q}$) is reflected into itself such that a standing wave is created. For electrically polarisable atoms this gives rise to a periodic potential $V_{\mathrm{latt}}(\mathbf{r}) = V_0 \sin^2(\mathbf{q} \cdot \mathbf{r})$, where the amplitude V_0 is proportional to the intensity of the laser light. In the case of two or three laser beams, a two- or three-dimensional lattice is formed. The lattice potential of a three-dimensional optical lattice created of three perpendicular laser beams parallel to the coordinate axes, is of the general form

$$V_{\mathrm{latt}}(\mathbf{r}) = V_x \sin^2(q_x x) + V_y \sin^2(q_y y) + V_z \sin^2(q_z z) \, . \tag{2.40}$$

Together with the harmonic trap potential given in eq. (2.17) the external potential of the atoms is $V_{\mathrm{ext}}(\mathbf{r}) = V_{\mathrm{tr}}(\mathbf{r}) + V_{\mathrm{latt}}(\mathbf{r})$. It should be mentioned that the denotation "one- and two-dimensional lattice" does not mean, that the movement of atoms is restricted to one or two dimensions, but is only referred to the dimension of the lattice potential. A two-dimensional lattice (e.g. for $V_x = 0$, $V_y, V_z \neq 0$) has the form of parallel running tubes and a one-dimensional lattice (e.g. for $V_x = V_y = 0$, $V_z \neq 0$) has the form of parallel planes (see fig. 2.1).

A *real* one-dimensional Bose gas, where the movement of atoms is only possible in one direction (e.g. the z-direction), can be created by tightly confining the particle motion in two directions (the x- and y-direction) to zero point oscillations. This can be done by increasing the amplitude V_x and V_y until tunneling of atoms through the lattice wells is prohibited. If $V_z = 0$, the Bose gas is trapped in one-dimensional tubes, and if $V_z \neq 0$

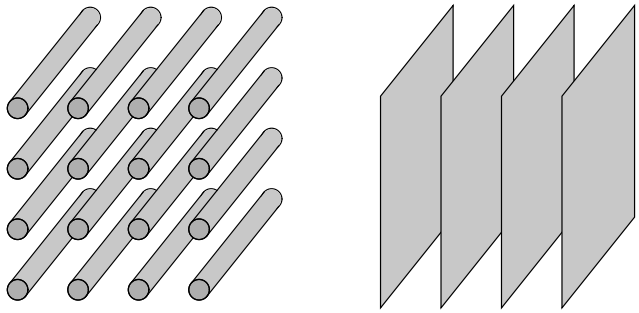

Figure 2.1: Illustration of a two-dimensional (left) and a one-dimensional (right) optical lattice

but small compared to V_x and V_y, a one-dimensional lattice is created where atoms can only tunnel between neighbouring lattice-sites in the z-direction [34].

The conventional model for a single-component system of bosons in an optical lattice is the Bose-Hubbard model. Assuming a d-dimensional simple-cubic lattice potential with $q_x = q_y = q_z \equiv q$ and $V_x = V_y = V_z \equiv V_0/3$, it has the form [4, 5, 6]

$$\hat{H}_{\mathrm{BH}} = -\frac{J}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \hat{a}^+_{\mathbf{r}} \hat{a}_{\mathbf{r}'} + \sum_{\mathbf{r}} V_{\mathbf{r}}\, \hat{a}^+_{\mathbf{r}} \hat{a}_{\mathbf{r}} + \frac{U}{2} \sum_{\mathbf{r}} \hat{a}^+_{\mathbf{r}} \hat{a}^+_{\mathbf{r}} \hat{a}_{\mathbf{r}} \hat{a}_{\mathbf{r}} \,, \tag{2.41}$$

where $\mathbf{r}, \mathbf{r}'$ denote the discrete positions of the lattice sites, $\hat{a}$ and $\hat{a}^+$ are bosonic annihilation and creation operators and the sum of the kinetic term runs over nearest neighbour sites only. The position $\mathbf{r}_i$ of site i is at a minimum of the lattice potential, i.e. $V_{\mathrm{latt}}(\mathbf{r}_i) = 0$. The Bose-Hubbard Hamiltonian is derived from the Hamiltonian (2.5) by means of the tight-binding approximation. Using the Wannier functions $w(\mathbf{r} - \mathbf{r}_i)$ which are located at site i, the parameters of the tunneling rate J, the on-site interaction strength U and the external (trap) potential $V_{\mathbf{r}_i}$ are given by

$$\frac{J}{2d} = \int w^*(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\mathrm{latt}}(\mathbf{r}) \right) w(\mathbf{r})\, \mathrm{d}^d r \tag{2.42}$$

$$U = g \int |w(\mathbf{r})|^4\, \mathrm{d}^d r \tag{2.43}$$

$$V_{\mathbf{r}_i} = \int V_{\mathrm{tr}}(\mathrm{r})\, |w(\mathbf{r} - \mathbf{r}_i)|^2\, \mathrm{d}^d r \approx V_{\mathrm{tr}}(\mathbf{r}_i) \tag{2.44}$$

The Bose-Hubbard model can describe a new phase, the Mott-insulator (MI). It is characterised by a complete loss of phase coherence between different lattice sites and an integer number of bosons at each lattice site. The loss of phase coherence has been shown in experiments [7]. The MI is favored if the on-site interaction dominates the

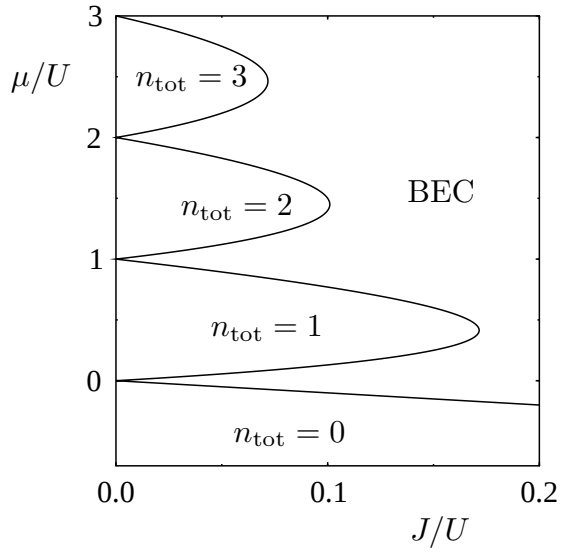

Figure 2.2: Zero temperature phase diagram of the Bose-Hubbard model calculated in mean-field theory.

kinetic energy. A self-consistent mean-field theory can be constructed by substituting

$$\hat{a}^+_{\mathbf{r}}\hat{a}_{\mathbf{r}'} \approx \langle\hat{a}^+_{\mathbf{r}}\rangle\hat{a}_{\mathbf{r}'} + \hat{a}^+_{\mathbf{r}}\langle\hat{a}_{\mathbf{r}'}\rangle - \langle\hat{a}^+_{\mathbf{r}}\rangle\langle\hat{a}_{\mathbf{r}'}\rangle = \Phi_0\left(\hat{a}^+_{\mathbf{r}} + \hat{a}_{\mathbf{r}'}\right) - \Phi_0^2 \tag{2.45}$$

into the Bose-Hubbard Hamiltonian (2.41), where $\Phi_0 = \langle\hat{a}^+_{\mathbf{r}}\rangle = \langle\hat{a}_{\mathbf{r}'}\rangle$ is identified as the condensate order parameter [35]. If the external potential is absent, this yealds the effective Hamiltonian

$$\hat{H}_{\rm BH} = -J\Phi_0\sum_{\mathbf{r}}\left(\hat{a}^+_{\mathbf{r}} + \hat{a}_{\mathbf{r}}\right) + J\Phi_0^2\mathcal{N} + \frac{U}{2}\sum_{\mathbf{r}}\hat{a}^+_{\mathbf{r}}\hat{a}^+_{\mathbf{r}}\hat{a}_{\mathbf{r}}\hat{a}_{\mathbf{r}}\ , \tag{2.46}$$

which is decoupled with respect to the lattice sites ($\mathcal{N}$ is the total number of lattice sites). In second order perturbation theory, the phase boudary between the BEC and the Mott-insulating phases is found to be given as

$$\frac{U}{J} = \frac{n_{\rm tot}+1}{n_{\rm tot} - \frac{\mu}{U}} - \frac{n_{\rm tot}}{(n_{\rm tot}-1) - \frac{\mu}{U}}\ , \tag{2.47}$$

where $n_{\rm tot}$ is the integer occupation number of the Mott lobe.

An alternative to describing an interacting Bose gas in an optical lattice by means of the Bose-Hubbard model is to use a hard-core interaction. In the hard-core model each lattice site cannot be occupied by more than one boson (or in a multi-component system: by more than one boson of each component). In contrary, the Bose-Hubbard model allows multiple occupation to the price of the interaction energy U. The larger U, the stronger multiple occupation in suppressed. Therefore many aspects of the physics

of the hard-core Bose gas agree with those of the Bose-Hubbard model in the large U limit. Some different approaches to treat the hard-core boson model shall be presented in this thesis. One reason for the choice of this model is, that it needs one parameter less than the Bose-Hubbard model, namely the interaction energy U. However, it contains a condensed phase, a non-condensed phase, and a Mott insulator, as will be discussed later. The existence of the BEC phase in three dimensions has been proven rigorously [36].

The Hamiltonian of the hard-core boson model can be written in terms of creation- and annihilation operators $\hat{a}_{\mathbf{r}}^{+}$ and $\hat{a}_{\mathbf{r}}$ with the usual bosonic commutation relations $[\hat{a}_{\mathbf{r}}, \hat{a}_{\mathbf{r}'}^{+}] = 0$ for different sites $\mathbf{r} \neq \mathbf{r}'$ but have the additional hard-core property

$$\hat{a}_{\mathbf{r}}^{2} = (\hat{a}_{\mathbf{r}}^{+})^{2} = 0 \,, \tag{2.48}$$

which limits the occupation number at lattice site $\mathbf{r}$ to 0 and 1. With those operators, the Hamiltonian is [37, 38]

$$\hat{H}_{\mathrm{hc}} = -\frac{J}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \hat{a}_{\mathbf{r}}^{+} \hat{a}_{\mathbf{r}'} + \sum_{\mathbf{r}} V_{\mathbf{r}}\, \hat{a}_{\mathbf{r}}^{+} \hat{a}_{\mathbf{r}} \,. \tag{2.49}$$

The Fock space can be written as a direct product of the Hilbert spaces of each lattice site $\mathbf{r}$, which themselves are two-dimensional (one basis vector for an empty site denoted by $|0\rangle_{\mathbf{r}}$ and one for an occupied site $|1\rangle_{\mathbf{r}}$, respectively):

$$\mathcal{F} = \prod_{\mathbf{r}} \mathcal{F}_{\mathbf{r}} \,, \quad \mathcal{F}_{\mathbf{r}} = \{c_0|0\rangle_{\mathbf{r}} + c_1|1\rangle_{\mathbf{r}};\ c_0, c_1 \text{ complex numbers}\} \,. \tag{2.50}$$

Within this two-dimensional structure, it is possible to represent the creation and annihilation operators for each lattice site as 2×2 matrices:

$$\hat{a}_{\mathbf{r}}^{+} \rightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \,, \quad \hat{a}_{\mathbf{r}} \rightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \,. \tag{2.51}$$

Using the spin matrices

$$S^{x} = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \,, \quad S^{y} = \frac{1}{2} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \,, \quad S^{z} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \,, \tag{2.52}$$

it is possible to show the well-known equivalence of this model to the spin one-half Heisenberg model [39], where the role of the external potential is played by an external magnetic field in a magnetic system:

$$\hat{H}_{\mathrm{hc}} = -\frac{J}{d} \sum_{\mathbf{r},\mathbf{r}'} (S_{\mathbf{r}}^{x} S_{\mathbf{r}'}^{x} + S_{\mathbf{r}}^{y} S_{\mathbf{r}'}^{y}) + V_{\mathbf{r}} \sum_{\mathbf{r}} \left(S_{\mathbf{r}}^{z} + \frac{1}{2} \right) \,. \tag{2.53}$$

It should be mentioned, that the hard-core Bose model is not only restricted to lattice systems. It is always possible to construct a lattice model and perform the continuum limit with the lattice constant a going to zero. A model to describe a homogeneous Bose gas via hard-core creation- and annihilation operators like above has been put forward by Siegert [40], and the way to approximate the continuum by a lattice was shown by Whitlock and Zisel [41]. A similar approach will be applied in chapter 9.

3 Functional integral representation

3.1 Grand canonical partition function as functional integral

The grand canonical partition function Z of a many-body system contains all information about the thermodynamic equilibrium properties of that system [11]. With given Hamiltonian $\hat{H}$ it is given as the trace of the density operator ρ:

$$\hat{\rho} = e^{-\beta(\hat{H}-\mu\hat{N}_{\mathrm{tot}})} , \quad Z = \mathrm{Tr}\,(\hat{\rho}) \tag{3.1}$$

Here, $\beta = 1/(k_{\mathrm{B}}T)$ is the inverse temperature, μ is the chemical potential and the particle number operator is $\hat{N}_{\mathrm{tot}} = \sum_\alpha \hat{a}_\alpha^+ \hat{a}_\alpha$. It is possible to write a grand canonical partition function in terms of a functional integral [8, 9].

Bosonic functional integral

Consider a bosonic many-body system given by the Hamiltonian $\hat{H}(\hat{a}_\alpha^+, \hat{a}_\alpha)$, where the creation and annihilation operators $\hat{a}_\alpha^+$ and $\hat{a}_\alpha$ fulfil bosonic commutation relations:

$$[\hat{a}_\alpha, \hat{a}_\beta^+]_- = \delta_{\alpha\beta} ; \quad [\hat{a}_\alpha, \hat{a}_\beta]_- = [\hat{a}_\alpha^+, \hat{a}_\beta^+]_- = 0 . \tag{3.2}$$

The index α denotes the states $|\alpha\rangle$ of an arbitrary single-particle basis, e.g. α can denote a lattice site or a wave vector. The grand canonical partition function is given as a functional integral over the complex field ϕ:

$$Z = \lim_{M\to\infty} \int e^{-A(\phi^*,\phi)} \prod_{n=1}^{M} \prod_\alpha \frac{\mathrm{d}\phi_{\alpha,n}^* \mathrm{d}\phi_{\alpha,n}}{2\pi\mathrm{i}} \tag{3.3}$$

with the action

$$A(\phi^*,\phi) = \frac{\beta}{M} \sum_{n=1}^{M} \left\{ \sum_\alpha \phi_{\alpha,n+1}^* \left[\frac{M}{\beta} (\phi_{\alpha,n+1} - \phi_{\alpha,n}) - \mu\phi_{\alpha,n} \right] + H(\phi_{\alpha,n+1}^*, \phi_{\alpha,n}) \right\} . \tag{3.4}$$

We require for bosons, that the field has periodic boundary conditions in the index n with periodicity M, i.e. $\phi_{\alpha,1} = \phi_{\alpha,M+1}$ and $\phi_{\alpha,1}^* = \phi_{\alpha,M+1}^*$. The function $H(\phi_{\alpha,n+1}^*, \phi_{\alpha,n})$ is received from the Hamiltonian $\hat{H}(\hat{a}_\alpha^+, \hat{a}_\alpha)$ by making the replacements $\hat{a}_\alpha^+ \to \phi_{\alpha,n+1}^*$

and $\hat{a}_\alpha \to \phi_{\alpha,n}$. After performing the limit $M \to \infty$, n plays the role of a continuous imaginary time variable. Using $\tau := n\hbar\beta/M$ we can write

$$Z = \int e^{-A(\phi^*,\phi)} \mathcal{D}(\phi^*(\tau)\phi(\tau)) \;, \quad \mathcal{D}(\phi^*(\tau)\phi(\tau)) := \lim_{M\to\infty} \prod_{n=1}^{M} \prod_{\alpha} \frac{\mathrm{d}\phi^*_{\alpha,n}\mathrm{d}\phi_{\alpha,n}}{2\pi\mathrm{i}} \tag{3.5}$$

and

$$A(\phi^*,\phi) = \frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \left\{ \sum_\alpha \phi^*_\alpha(\tau) \left(\hbar\frac{\partial}{\partial\tau} - \mu \right) \phi_\alpha(\tau) + H(\phi^*_\alpha(\tau), \phi^*_\alpha(\tau)) \right\} . \tag{3.6}$$

Again, we require the periodic boundary conditions $\phi_\alpha(\beta) = \phi_\alpha(0)$ and $\phi^*_\alpha(\beta) = \phi^*_\alpha(0)$.

Fermionic functional integral

In the case of a fermionic many-body Hamiltonian $\hat{H}(\hat{c}^+_\alpha, \hat{c}_\alpha)$, the creation and annihilation operators fulfil the anti-commutation relations

$$[\hat{c}_\alpha, \hat{c}^+_\beta]_+ = \delta_{\alpha\beta} \;; \quad [\hat{c}_\alpha, \hat{c}_\beta]_+ = [\hat{c}^+_\alpha, \hat{c}^+_\beta]_+ = 0 \;. \tag{3.7}$$

A functional integral of a fermionic system is given as an integral of conjugate Grassmann variables. The definition of a Grassmann algebra and of Grassmann integrals can be found in refs. [8, 9, 42]. Here it shall only be mentioned that the variables of a conjugate Grassmann field $\bar{\psi}, \psi$ are anti-commuting, i. e.

$$\psi_{\alpha,n}\psi_{\beta,m} = -\psi_{\beta,m}\psi_{\alpha,n} \;, \quad \bar{\psi}_{\alpha,n}\bar{\psi}_{\beta,m} = -\bar{\psi}_{\beta,m}\bar{\psi}_{\alpha,n} \;, \quad \bar{\psi}_{\alpha,n}\psi_{\beta,m} = -\psi_{\beta,m}\bar{\psi}_{\alpha,n} \;,$$

and a Grassmann integral gives unity only if it is performed over a full product of all variables, and zero otherwise:

$$\int \bar{\psi}_{\alpha,n}\psi_{\alpha,n}\,\mathrm{d}\psi_{\alpha,n}\mathrm{d}\bar{\psi}_{\alpha,n} = 1 \;, \tag{3.8}$$

$$\int \mathrm{d}\psi_{\alpha,n}\mathrm{d}\bar{\psi}_{\alpha,n} = \int \bar{\psi}_{\alpha,n}\,\mathrm{d}\psi_{\alpha,n}\mathrm{d}\bar{\psi}_{\alpha,n} = \int \psi_{\alpha,n}\,\mathrm{d}\psi_{\alpha,n}\mathrm{d}\bar{\psi}_{\alpha,n} = 0 \;. \tag{3.9}$$

Using these rules, the functional integral of the fermionic grand partition function can be constructed in analogy to eq. (3.3) as

$$Z = \lim_{M\to\infty} \int e^{-A(\bar{\psi},\psi)} \prod_{n=1}^{M} \prod_{\alpha} \mathrm{d}\bar{\psi}_{\alpha,n}\mathrm{d}\psi_{\alpha,n} \;, \tag{3.10}$$

where the exponential is defined as a Taylor series. In the action (3.4), the complex variables $\phi^*_{\alpha,n}, \phi_{\alpha,n}$ have to be replaced by the Grassmann variables $\bar{\psi}_{\alpha,n}, \psi_{\alpha,n}$, and

the periodic boundary conditions in the index n have to be replaced by anti-periodic boundary conditions $\psi_{\alpha,1} = -\psi_{\alpha,M+1}$ and $\bar{\psi}_{\alpha,1} = -\bar{\psi}_{\alpha,M+1}$. The same replacements can be done in the imaginary time functional integral defined by eqs. (3.5) and (3.6), when the integration measure in (3.5) is replaced by

$$\mathcal{D}(\bar{\psi}(\tau)\psi(\tau)) := \lim_{M\to\infty} \prod_{n=1}^{M} \prod_{\alpha} \mathrm{d}\bar{\psi}_{\alpha,n} \mathrm{d}\psi_{\alpha,n} \tag{3.11}$$

for the Grassmann field. For the construction of the functional integral for bosons and fermions (and hard-core boson operators with the additional property (2.48)) see Appendix C.

3.2 Correlation functions

Thermodynamic functions can be written in terms of expectation values. The expectation value of an arbitrary operator $\hat{X}$ is given by the relation

$$\langle \hat{X} \rangle = \frac{1}{Z} \mathrm{Tr} \left(\hat{X}\, \hat{\rho} \right) \tag{3.12}$$

with the density operator (3.1). A general static n-particle correlation function (CF) is defined as a product of n creation and n annihilation operators:

$$C_n(\alpha_1, \ldots, \alpha_n; \beta_n, \ldots, \beta_1) := \langle \hat{a}^+_{\alpha_1} \cdots \hat{a}^+_{\alpha_n} \hat{a}_{\beta_n} \cdots \hat{a}_{\beta_1} \rangle \,. \tag{3.13}$$

In the functional integral representation of a bosonic system, an expectation value of some function $f(\phi^*, \phi)$, which depends on the complex field variables, is defined as

$$\langle f(\phi^*, \phi) \rangle = \frac{1}{Z} \int f(\phi^*, \phi)\, e^{-A(\phi^*,\phi)} \mathcal{D}(\phi^*(\tau)\phi(\tau)) \,. \tag{3.14}$$

To translate the static CF (3.13) to an expectation value in terms of a functional integral, it is at first necessary to introduce a dynamic n-particle CF, which depends on the imaginary time variable τ. Therefore we introduce the imaginary time Heisenberg representation of the bosonic creation and annihilation operators $\hat{a}^+_\alpha$ and $\hat{a}_\alpha$:

$$\hat{a}^+_\alpha(\tau) = e^{\tau(\hat{H}-\mu\hat{N}_{\mathrm{tot}})/\hbar} \hat{a}^+_\alpha \mathrm{e}^{-\tau(\hat{H}-\mu\hat{N}_{\mathrm{tot}})/\hbar} \tag{3.15}$$

$$\hat{a}_\alpha(\tau) = e^{\tau(\hat{H}-\mu\hat{N}_{\mathrm{tot}})/\hbar} \hat{a}_\alpha \mathrm{e}^{-\tau(\hat{H}-\mu\hat{N}_{\mathrm{tot}})/\hbar} \,. \tag{3.16}$$

The dynamic n-particle CF can now be defined as

$$C_n(\alpha_1\tau_1, \ldots, \alpha_n\tau_n; \beta_n\tau_{n+1}, \ldots, \beta_1\tau_{2n}) := \langle \hat{a}^+_{\alpha_1}(\tau_1) \cdots \hat{a}^+_{\alpha_n}(\tau_n) \hat{a}_{\beta_n}(\tau_{n+1}) \cdots \hat{a}_{\beta_1}(\tau_{2n}) \rangle \,. \tag{3.17}$$

An expectation value of the complex field variables is given as an expectation value of a time ordered product of the creation and annihilation operators in the Heisenberg representation [9]. The time ordering in the imaginary time variable is indicated by the time ordering operator $\hat{T}$. The ordering begins with the largest imaginary time and ends with the smallest. The rule for a translation of an expectation value of a time ordered product of operators into an expectation value of a product of complex field variables is simply

$$\begin{aligned}&\langle \phi^*_{\alpha_1}(\tau_1)\cdots\phi^*_{\alpha_n}(\tau_n)\phi_{\alpha_{n+1}}(\tau_{n+1})\cdots\phi_{\alpha_{2n}}(\tau_{2n})\rangle = \\ &\langle \hat{T}\hat{a}^+_{\alpha_1}(\tau_1)\cdots\hat{a}^+_{\alpha_n}(\tau_n)\hat{a}_{\alpha_{n+1}}(\tau_{n+1})\cdots\hat{a}_{\alpha_{2n}}(\tau_{2n})\rangle\ .\end{aligned} \tag{3.18}$$

Introducing a time-slice $\varepsilon > 0$, the static n-particle CF (3.13) can thus be constructed by

$$\begin{aligned}&C_n(\alpha_1,\ldots,\alpha_n;\beta_n,\ldots,\beta_1) = \\ &\lim_{\varepsilon\to 0}\langle \hat{a}^+_{\alpha_1}(\tau+(2n-1)\varepsilon)\cdots\hat{a}^+_{\alpha_n}(\tau+n\varepsilon)\hat{a}_{\beta_n}(\tau+(n-1)\varepsilon)\cdots\hat{a}_{\beta_1}(\tau)\rangle = \\ &\lim_{\varepsilon\to 0}\langle \phi^*_{\alpha_1}(\tau+(2n-1)\varepsilon)\cdots\phi^*_{\alpha_n}(\tau+n\varepsilon)\phi_{\beta_n}(\tau+(n-1)\varepsilon)\cdots\phi_{\beta_1}(\tau)\rangle\end{aligned} \tag{3.19}$$

Note that this expression is independent of τ. Because the imaginary time is periodic with periodicity $\hbar\beta$, it does not matter which point τ is regarded as the beginning of a period, thus in particular we can assume $\tau = 0$. In general, it is not possible to replace the limit $\varepsilon \to 0$ simply by putting $\varepsilon = 0$, because the limits for $\varepsilon > 0$ and $\varepsilon < 0$ are not necessarily the same. This feature reflects the fact that the creation and annihilation operators do not commute in the operator formalism.

Some relevant physical quantities which can be calculated from correlation functions shall be mentioned here:

Total particle number

The total particle number is derived from the grand canonical partition function by [11]

$$N_{\text{tot}} = \frac{1}{\beta}\frac{\partial}{\partial\mu}\log Z \tag{3.20}$$

Applying eq. (3.20) to Z as it is given in eqs. (3.5) and (3.6), we get

$$N_{\text{tot}} = \lim_{\varepsilon\to 0}\frac{1}{\beta}\frac{1}{Z}\int\left[\sum_\alpha\int_0^{\hbar\beta}\phi^*_\alpha(\tau+\varepsilon)\phi_\alpha(\tau)\mathrm{d}\tau\right]e^{-A(\phi^*,\phi)}\mathcal{D}(\phi^*(\tau)\phi(\tau))\ .$$

Because of the independence of the CFs of τ, we have

$$N_{\text{tot}} = \lim_{\varepsilon\to 0}\sum_\alpha\langle\phi^*_\alpha(\varepsilon)\phi_\alpha(0)\rangle\ . \tag{3.21}$$

The particle occupation number in state α is

$$n_\alpha = \lim_{\varepsilon \to 0} \langle \phi^*_\alpha(\varepsilon)\phi_\alpha(0)\rangle \ . \tag{3.22}$$

In the case that α denotes a position in space or a lattice site, n_α is a local particle density, if α is a momentum index, n_α is the momentum distribution of particles.

As has been mentioned before, it is not allowed to put the time-slice $\varepsilon = 0$ in general. The reason is, that in the discrete-time definition of the action (3.4), the μ-dependent term is given by

$$-\frac{\beta}{M}\sum_{n=0}^{M-1}\sum_{\alpha}\mu\phi^*_{\alpha,n+1}\phi_{\alpha,n} \tag{3.23}$$

and therefore occupies the off-diagonal matrix elements in the imaginary time index. It should be noted here, that it is also possible to construct the functional integral with the μ-dependent term being on the diagonal matrix elements, i. e.

$$-\frac{\beta}{M}\sum_{n=0}^{M-1}\sum_{\alpha}\mu\phi^*_{\alpha,n}\phi_{\alpha,n} \ . \tag{3.24}$$

In this case the occupation number would be $n_\alpha = \langle \phi^*_\alpha(0)\phi_\alpha(0)\rangle$, which means that the expressions for the physical quantities significantly depend on the definition of the functional integral, which in some cases might be more convenient. However, in this chapter we will keep the off-diagonal representation given in (3.23).

Condensate density

The condensate density of a BEC is a measure for the off-diagonal long range order of the one-particle CF and is defined by eq. (2.6). It has to do with the spacial range of the one-particle CF and thus α should denote a position vector (in a continuous system) or a lattice site (in an optical lattice). In terms of complex variables, the definition of the condensate density is

$$n_0 := \lim_{\varepsilon \to 0}\lim_{\mathbf{r}-\mathbf{r}'\to\infty} \langle \phi^*_{\mathbf{r}}(\varepsilon)\phi_{\mathbf{r}'}(0)\rangle \ . \tag{3.25}$$

Density-density correlation function

The density-density CF is a two-particle CF. It describes the spacial behaviour of density correlations, which means that here α denotes a position index as well. In terms of field operators it is defined as

$$D(\mathbf{r}-\mathbf{r}') = \langle \hat{n}_{\mathbf{r}}\hat{n}_{\mathbf{r}'}\rangle = \langle \hat{\psi}^+_{\mathbf{r}}\hat{\psi}_{\mathbf{r}}\hat{\psi}^+_{\mathbf{r}'}\hat{\psi}_{\mathbf{r}'}\rangle \, , \tag{3.26}$$

and in terms of complex field variables it is given as

$$\begin{aligned} D(\mathbf{r}-\mathbf{r}') &= \lim_{\varepsilon\to 0}\langle\phi^*_{\mathbf{r}}(3\varepsilon)\phi_{\mathbf{r}}(2\varepsilon)\phi^*_{\mathbf{r}'}(\varepsilon)\phi_{\mathbf{r}'}(0)\rangle \\ &= \lim_{\epsilon\to 0}\langle\phi^*_{\mathbf{r}}(\varepsilon)\phi_{\mathbf{r}}(0)\phi^*_{\mathbf{r}'}(\varepsilon)\phi_{\mathbf{r}'}(0)\rangle \end{aligned} \tag{3.27}$$

A good physical quantity to describe correlations of density fluctuations is the truncated density-density CF

$$D_{\text{trunc}}(\mathbf{r}-\mathbf{r}') = \langle\hat{n}_{\mathbf{r}}\hat{n}_{\mathbf{r}'}\rangle - \langle\hat{n}_{\mathbf{r}}\rangle\langle\hat{n}_{\mathbf{r}'}\rangle\ . \tag{3.28}$$

The Fourier transform of the density-density CF is the static structure factor given in eq. (2.31).

4 Ideal Bose gas

4.1 The Hamiltonian

In this chapter we will survey the basic results of the previously mentioned quantities for an ideal Bose gas. This seems to be reasonable, because it allows us to introduce the methods we will apply for the interacting hard-core Bose gas as well. In contrary to the interacting system, exact analytic results can be found for the non-interacting case of the ideal Bose gas.

A non-interacting Bose gas is given by the Hamiltonian in momentum space

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \, \hat{a}^{+}_{\mathbf{k}} \hat{a}_{\mathbf{k}} \, . \tag{4.1}$$

Its eigenstates and eigenenergies are

$$|n\rangle = |\{n_{\mathbf{k}}\}\rangle = \frac{1}{\sqrt{\prod_{\mathbf{k}} n_{\mathbf{k}}!}} \left(\hat{a}^{+}_{\mathbf{k}}\right)^{n_{\mathbf{k}}} |0\rangle \ , \tag{4.2}$$

$$E_n = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \, n_{\mathbf{k}} \ , \tag{4.3}$$

and $|n\rangle$ are pure number states. In the case of a homogeneous system, i. e.

$$\hat{H} = \int \mathrm{d}^3 r \, \hat{\psi}^{+}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \hat{\psi}(\mathbf{r}) \tag{4.4}$$

the dispersion relation is given as

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m} \ , \tag{4.5}$$

and for a system on a d-dimensional cubic lattice with nearest-neighbour hopping and lattice constant a given by the Hamiltonian

$$\hat{H} = J - \frac{J}{2d} \sum_{\langle \mathbf{r}_i, \mathbf{r}_j \rangle} \hat{a}^{+}_{\mathbf{r}_i} \hat{a}_{\mathbf{r}_j} \tag{4.6}$$

it is given by

$$\epsilon_{\mathbf{k}} = J - \frac{J}{d} \sum_{\nu=1}^{d} \cos(a k_\nu) \ , \tag{4.7}$$

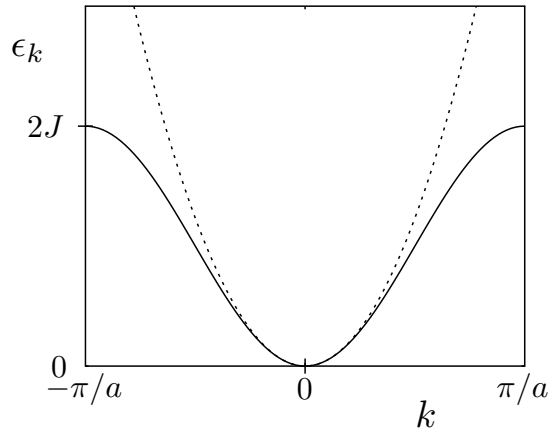

Figure 4.1: Lattice dispersion (solid line) from eq. (4.7) and free-particle dispersion (dashed line) from eq. (4.8) in one dimension.

where k_ν is the ν-th component of the d-dimensional wave vector $\mathbf{k}$. Note that the sum over nearest neighbours $\langle \mathbf{r}_i, \mathbf{r}_j \rangle$ means, that the index i runs over the entire lattice and the index j runs over all sites, which are nearest neighbours of j. This means, that each bond appears twice in the sum, once with a hopping process from site i to site j and vice versa. For small wave vectors $\mathbf{k}$, the lattice dispersion can be approximated by

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m^*} + \mathcal{O}(\mathbf{k}^4) \,, \quad m^* := \frac{d\hbar^2}{Ja^2} \,, \tag{4.8}$$

where m^* is the band-mass, see fig. 4.1.

4.2 Green's function and partition function

According to eq. (3.6), the action of the imaginary time functional integral representation is

$$A = \frac{1}{\hbar} \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{\mathbf{k}} \phi^*_{\mathbf{k}}(\tau) \left[\left(\hbar \frac{\partial}{\partial \tau} - \mu \right) + \epsilon_{\mathbf{k}} \right] \phi_{\mathbf{k}}(\tau) \,. \tag{4.9}$$

Because of the periodicity in the imaginary time variable we can expand the complex fields in a Fourier series

$$\phi_{\mathbf{k}}(\tau) = \sum_n \phi_{\mathbf{k},\omega_n} \, e^{\mathrm{i}\omega_n \tau} \,, \quad \phi^*_{\mathbf{k}}(\tau) = \sum_n \phi^*_{\mathbf{k},\omega_n} \, e^{-\mathrm{i}\omega_n \tau} \,, \tag{4.10}$$

with the Matsubara frequencies for bosons

$$\omega_n = \frac{2\pi}{\hbar\beta} \, n \,, \quad n = \ldots, -2, -1, 0, 1, 2, \ldots \tag{4.11}$$

such that the Matsubara representation of the action is

$$A = \beta \sum_{\mathbf{k}} \phi^*_{\mathbf{k},\omega_\mathbf{n}} \left(\mathrm{i}\hbar\omega_n - \mu + \epsilon_\mathbf{k} \right) \phi_{\mathbf{k},\omega_\mathbf{n}} \ . \tag{4.12}$$

From this action we get the correct Green's function of the ideal Bose gas in the Matsubara formalism according to ref. [8] as

$$G_0(\mathbf{k}, \omega_n) = \frac{1}{\mathrm{i}\hbar\omega_n - \mu + \epsilon_\mathbf{k}} \tag{4.13}$$

but it is inappropriate to get the grand canonical partition function. Therefore it seems to be necessary to go back to the discrete time action given in eq. (3.4) and perform the limit $M \to \infty$ at the very end. It is possible to write the functional integral (3.4) in the form

$$Z = \lim_{M\to\infty} \int \exp\left[-\sum_{\mathbf{k}} \sum_{n,m=1}^{M} \phi^*_{\mathbf{k},n} \hat{A}^{(\mathbf{k})}_{nm} \phi_{\mathbf{k},m} \right] \prod_{\mathbf{k}} \prod_{n=1}^{M} d\phi^*_{\mathbf{k},n} d\phi_{\mathbf{k},n} \ , \tag{4.14}$$

where the matrix elements of $\hat{A}^{(\mathbf{k})}$ represent the structure of the discrete imaginary time variable:

$$\hat{A}^{(\mathbf{k})} = \begin{bmatrix} 1 & 0 & & \cdots & 0 & -b_\mathbf{k} \\ -b_\mathbf{k} & 1 & 0 & & & \\ 0 & -b_\mathbf{k} & 1 & \ddots & & \vdots \\ & 0 & -b_\mathbf{k} & \ddots & 0 & \\ \vdots & & 0 & \ddots & 1 & 0 \\ 0 & & & \cdots & -b_\mathbf{k} & 1 \end{bmatrix} , \quad b_\mathbf{k} = 1 - \frac{\beta}{M}(\epsilon_\mathbf{k} - \mu) \ . \tag{4.15}$$

The entry in the upper right corner is necessary to realise the periodic boundary conditions. The Gaussian integral can be integrated out and gives a determinant:

$$Z = \lim_{M\to\infty} \prod_{\mathbf{k}} \det \hat{A}^{(\mathbf{k})} = \lim_{M\to\infty} \prod_{\mathbf{k}} \left[1 - \left(1 - \frac{\beta(\epsilon_\mathbf{k} - \mu)}{M} \right)^M \right]^{-1}$$

If we now, as a final step, perform the limit $M \to \infty$, we get the correct form of the grand canonical partition function of an ideal Bose gas [9]:

$$Z = \prod_{\mathbf{k}} \left[1 - e^{-\beta(\epsilon_\mathbf{k} - \mu)} \right]^{-1} \ . \tag{4.16}$$

4.3 One-particle correlation function

As already discussed in section 3.2, the momentum distribution and the condensate density in a Bose gas can both be described by the one-particle correlation function, cf. eqs. (3.21) and (3.25). Thus we should at first calculate the one-particle CF for the ideal Bose gas in general to determine those quantities. To achieve this we again start with the discrete time functional integral and take the limit $M \to \infty$ in the final step. In this sense, we define the imaginary time dependent one-particle CF in momentum space as

$$C(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = \langle \phi^*_{\mathbf{k}_1, n_1} \phi_{\mathbf{k}_2, n_2} \rangle =$$

$$\lim_{M\to\infty} \frac{1}{Z} \int \phi^*_{\mathbf{k}_1,n_1} \phi_{\mathbf{k}_2,n_2} \exp\left[- \sum_{\mathbf{k}} \sum_{n,m=1}^{M} \phi^*_{\mathbf{k},n} \hat{A}^{(\mathbf{k})}_{nm} \phi_{\mathbf{k},m} \right] \prod_{\mathbf{k}} \prod_{n=1}^{M} d\phi^*_{\mathbf{k},n} d\phi_{\mathbf{k},n} \ , \tag{4.17}$$

where the indices n_1, n_2 are defined such that

$$\frac{\beta}{M}(n_{1,2} - 1) < \tau_{1,2} < \frac{\beta}{M} n_{1,2} \ . \tag{4.18}$$

The Gaussian integral (4.17) picks out a matrix element of the inverse matrix $\hat{A}^{-1}$ (see Appendix B.2):

$$C(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = \lim_{M\to\infty} (\hat{A}^{(\mathbf{k}_1)})^{-1}_{n_2,n_1} \, \delta_{\mathbf{k}_1,\mathbf{k}_2} \ . \tag{4.19}$$

Therefore it is necessary to determine the matrix elements of $\hat{A}^{-1}$. This is achieved by a Fourier transformation with the unitary transformation matrices

$$U_{nm} = \frac{1}{\sqrt{M}} e^{\frac{2\pi \mathrm{i}}{M} nm} \ , \quad U^+_{nm} = \frac{1}{\sqrt{M}} e^{-\frac{2\pi \mathrm{i}}{M} nm} \ , \tag{4.20}$$

with which we can diagonalise the matrix:

$$(U \hat{A}^{(\mathbf{k})} U^+)_{kn} = \frac{1}{M} \sum_{l,m=1}^{M} e^{\frac{2\pi \mathrm{i}}{M}(jl - mn)} \hat{A}_{lm} = \delta_{jn} \left(1 - b_{\mathbf{k}} e^{\frac{2\pi \mathrm{i}}{M} n} \right) \ .$$

The inversion and back transformation of this diagonal matrix leads to

$$(U(\hat{A}^{(\mathbf{k})})^{-1} U^+)_{jn} = \frac{\delta_{jn}}{1 - b_{\mathbf{k}} e^{\frac{2\pi \mathrm{i}}{M} n}} \ ,$$

$$(\hat{A}^{(\mathbf{k})})^{-1}_{jn} = [U^+(U(\hat{A}^{(\mathbf{k})})^{-1} U^+) U]_{jn} = \sum_{l=1}^{M} \frac{1}{M} \frac{e^{-\frac{2\pi \mathrm{i}}{M} l(j-n)}}{1 - b_{\mathbf{k}} e^{\frac{2\pi \mathrm{i}}{M} l}} \ .$$

This sum is of the type as given in eq. (A.3) and is calculated in the Appendix. The result is

$$(\hat{A}^{(\mathbf{k})})^{-1}_{jn} = \frac{1}{1-b_{\mathbf{k}}^M} \times \begin{cases} b_{\mathbf{k}}^{j-n} & \text{if} \quad j \geq n \\ b_{\mathbf{k}}^{M+n-j} & \text{if} \quad j < n \end{cases} . \tag{4.21}$$

Thus we find the result for the imaginary time CF (4.19) as

$$C(\mathbf{k}_1,\tau_1;\mathbf{k}_2,\tau_2) = \delta_{\mathbf{k}_1,\mathbf{k}_2} \lim_{M\to\infty} \frac{1}{1-b_{\mathbf{k}}^M} \times \begin{cases} b_{\mathbf{k}}^{n_2-n_1} & \text{if} \quad n_2 \geq n_1 \\ b_{\mathbf{k}}^{M+n_1-n_2} & \text{if} \quad n_2 < n_1 \end{cases} .$$

Performing the limit $M \to \infty$ in (4.18) and using the results

$$\lim_{M\to\infty} b_{\mathbf{k}}^M = e^{-\beta(\epsilon_{\mathbf{k}}-\mu)} , \quad \lim_{M\to\infty} b_{\mathbf{k}}^{n_2-n_1} = e^{(\tau_1-\tau_2)(\epsilon_{\mathbf{k}}-\mu)}$$

we yield

$$C(\mathbf{k}_1,\tau_1;\mathbf{k}_2,\tau_2) = \frac{\delta_{\mathbf{k}_1,\mathbf{k}_2}}{1-e^{-\beta(\epsilon_{\mathbf{k}}-\mu)}} \times \begin{cases} e^{(\tau_2-\tau_1)(\epsilon_{\mathbf{k}}-\mu)/\hbar} & \text{if} \quad \tau_1 \geq \tau_2 \\ e^{(\tau_1-\tau_2-\hbar\beta)(\epsilon_{\mathbf{k}}-\mu)/\hbar} & \text{if} \quad \tau_1 < \tau_2 \end{cases} . \tag{4.22}$$

Using this result and the definition (3.19), the one-particle CF in momentum space for the ideal Bose gas is

$$C_1(\mathbf{k};\mathbf{k}') = \lim_{\epsilon\to 0} \langle \phi_{\mathbf{k}}^*(\epsilon)\phi_{\mathbf{k}'}(0)\rangle = \frac{\delta_{\mathbf{k},\mathbf{k}'}}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)}-1} . \tag{4.23}$$

Thus we find the usual momentum distribution of the ideal Bose gas

$$n_{\mathbf{k}} = C(\mathbf{k};\mathbf{k}) = C(\mathbf{k},\tau;\mathbf{k},\tau) = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)}-1} . \tag{4.24}$$

In the condensed phase, where the chemical potential takes the value $\mu = 0$, the momentum distribution function diverges at $\mathbf{k} = 0$. In this case, the lowest momentum state $\mathbf{k} = 0$ is macroscopically occupied and builds the condensate. The condensate density in this case is given as

$$n_0 = \frac{n_{\mathbf{k}=0}}{V} . \tag{4.25}$$

The normalisation with the volume of the Bose gas V is necessary, because in the BEC phase the ground state is the only macroscopically occupied state, whereas all other occupation numbers are of the order of unity. The total particle density in the condensed phase is the sum of the condensate density and the particle density of all excited states:

$$n_{\text{tot}} = n_0 + \frac{1}{V}\int n_{\mathbf{k}}\, \mathrm{d}^3k . \tag{4.26}$$

It should be noted here, that in one and two dimensions a condensate cannot exist. The reason is, that the integral (4.26) is divergent in these cases if $\mu = 0$, because $n_{\mathbf{k}}$ behaves like k^{-2} for small momenta.

This definition of the condensate density in an ideal Bose gas is also compatible with the more general definition via off-diagonal long range order given in eq. (3.25):

$$\lim_{\epsilon\to 0}\lim_{\mathbf{r}-\mathbf{r}'\to\infty}\langle\phi^*_{\mathbf{r}}(\epsilon)\phi_{\mathbf{r}'}(0)\rangle = \lim_{\mathbf{r}-\mathbf{r}'\to\infty} C(\mathbf{r};\mathbf{r}') = \lim_{\mathbf{r}-\mathbf{r}'\to\infty}\frac{1}{V}\sum_{\mathbf{k}}\underbrace{C(\mathbf{k};\mathbf{k})}_{=n_{\mathbf{k}}}\, e^{\mathrm{i}\mathbf{k}(\mathbf{r}-\mathbf{r}')}$$

$$= n_0 + \underbrace{\lim_{\mathbf{r}-\mathbf{r}'\to\infty}\frac{1}{V}\int n_{\mathbf{k}}\, e^{\mathrm{i}\mathbf{k}(\mathbf{r}-\mathbf{r}')}\,\mathrm{d}^3k}_{=0}\ .$$

4.4 Structure factor

It is possible to calculate the dynamic structure factor of the ideal Bose gas with eigenstates and eigenenergies as given in eqs. (4.2) and (4.3). We write

$$|n\rangle = |n_0, n_1, \ldots, n_{\mathbf{k}}, \ldots\rangle\ , \quad |m\rangle = |m_0, m_1, \ldots, m_{\mathbf{k}}, \ldots\rangle$$

and calculate the matrix elements of the density matrix:

$$\langle n|\hat{\rho}^+_{\mathbf{q}}|m\rangle = \sum_{\mathbf{k}}\langle n|\hat{a}^+_{\mathbf{k}+\mathbf{q}}\hat{a}_{\mathbf{k}}|m\rangle =$$

$$\sum_{\mathbf{k}}\sqrt{m_{\mathbf{k}}(m_{\mathbf{k}+\mathbf{q}}+1)}\,\delta_{n_0,m_0}\cdots\delta_{n_{\mathbf{k}},m_{\mathbf{k}}-1}\cdots\delta_{n_{\mathbf{k}+\mathbf{q}},m_{\mathbf{k}+\mathbf{q}}+1}\,, \tag{4.27}$$

which means, that

$$\left|\langle n|\hat{\rho}^+_{\mathbf{q}}|m\rangle\right|^2 = \sum_{\mathbf{k}} m_{\mathbf{k}}(m_{\mathbf{k}+\mathbf{q}}+1)\,\delta_{n_0,m_0}\cdots\delta_{n_{\mathbf{k}},m_{\mathbf{k}}-1}\cdots\delta_{n_{\mathbf{k}+\mathbf{q}},m_{\mathbf{k}+\mathbf{q}}+1}\,. \tag{4.28}$$

The δ-functions mean, that the states $|n\rangle$ are determined by the states $|m\rangle$. The energy difference can be calculated as

$$\hbar\omega_{nm} = \sum_{\mathbf{k}'}\epsilon_{\mathbf{k}'}(m_{\mathbf{k}'} - n_{\mathbf{k}'}) = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} \tag{4.29}$$

After inserting this into (2.30), we can perform the sum over the states $|n\rangle$ and get

$$S(\mathbf{q},\omega) = \frac{1}{ZN_{\mathrm{tot}}}\sum_{|m\rangle}\mathrm{e}^{-\beta E_m}\sum_{\mathbf{k}} m_{\mathbf{k}}(m_{\mathbf{k}+\mathbf{q}}+1)\,\delta(\omega - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})/\hbar) =$$

$$\sum_{\mathbf{k}}\langle m_{\mathbf{k}}\rangle(\langle m_{\mathbf{k}+\mathbf{q}}\rangle + 1)\,\delta(\omega - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})/\hbar) \tag{4.30}$$

for the dynamic structure factor, and the static structure factor is then given as

$$S(\mathbf{q}) = \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k}} \langle m_{\mathbf{k}} \rangle (\langle m_{\mathbf{k}+\mathbf{q}} \rangle + 1) = 1 + \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k}} \langle m_{\mathbf{k}} \rangle \langle m_{\mathbf{k}+\mathbf{q}} \rangle \,, \tag{4.31}$$

where N_{tot} is the total particle number. The expectation values are given by the Bose distribution function as calculated before:

$$m_{\mathbf{k}} := \langle m_{\mathbf{k}} \rangle = \frac{1}{\mathrm{e}^{\beta(\epsilon_{\mathbf{k}} - \mu)} - 1} \,. \tag{4.32}$$

For **zero temperature** we have

$$m_{\mathbf{k}} = \begin{cases} N_{\text{tot}} & \text{if } \mathbf{k} = 0 \\ 0 & \text{if } \mathbf{k} \neq 0 \end{cases} \,. \tag{4.33}$$

Then from eq. (4.31) we get

$$S(\mathbf{q}) = \begin{cases} 1 + N_{\text{tot}} & \text{if } \mathbf{q} = 0 \\ 1 & \text{if } \mathbf{q} \neq 0 \end{cases} \,, \tag{4.34}$$

i.e. we have a δ-function with peak at $\mathbf{q} = 0$. The same result for the static structure factor we get from the functional integral formalism as well. From (2.25) we have

$$S(\mathbf{q}) = S(\mathbf{q}, 0) = \frac{1}{N_{\text{tot}}} \langle \hat{\rho}_{\mathbf{q}} \hat{\rho}_{\mathbf{q}}^{+} \rangle = \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k},\mathbf{k}'} \left\langle \hat{a}_{\mathbf{k}}^{+} \hat{a}_{\mathbf{k}+\mathbf{q}} \hat{a}_{\mathbf{k}'+\mathbf{q}}^{+} \hat{a}_{\mathbf{k}'} \right\rangle =$$

$$\lim_{\varepsilon \to 0} \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k},\mathbf{k}'} \left\langle \phi_{\mathbf{k}}^{*}(3\varepsilon) \phi_{\mathbf{k}'+\mathbf{q}}^{*}(\varepsilon) \phi_{\mathbf{k}+\mathbf{q}}(2\varepsilon) \phi_{\mathbf{k}'}(0) \right\rangle \,. \tag{4.35}$$

This forth-order correlation function can be calculated using Wick's theorem (see Appendix B.2):

$$\lim_{\varepsilon \to 0} \left\langle \phi_{\mathbf{k}}^{*}(3\varepsilon) \phi_{\mathbf{k}'+\mathbf{q}}^{*}(\varepsilon) \phi_{\mathbf{k}+\mathbf{q}}(2\varepsilon) \phi_{\mathbf{k}'}(0) \right\rangle =$$

$$\lim_{\varepsilon \to 0} [\langle \phi_{\mathbf{k}}^{*}(3\varepsilon) \phi_{\mathbf{k}+\mathbf{q}}(2\varepsilon) \rangle \langle \phi_{\mathbf{k}'+\mathbf{q}}^{*}(\varepsilon) \phi_{\mathbf{k}'}(0) \rangle + \langle \phi_{\mathbf{k}}^{*}(3\varepsilon) \phi_{\mathbf{k}'}(0) \rangle \langle \phi_{\mathbf{k}'+\mathbf{q}}^{*}(\varepsilon) \phi_{\mathbf{k}+\mathbf{q}}(2\varepsilon) \rangle] =$$

$$n_{\mathbf{k}} \delta_{\mathbf{k},\mathbf{k}+\mathbf{q}} n_{\mathbf{k}'} \delta_{\mathbf{k}'+\mathbf{q},\mathbf{k}'} + n_{\mathbf{k}} \delta_{\mathbf{k},\mathbf{k}'} \left(n_{\mathbf{k}+\mathbf{q}} + 1\right) \delta_{\mathbf{k}'+\mathbf{q},\mathbf{k}+\mathbf{q}} \,.$$

For $\mathbf{q} \neq 0$, the first term vanishes. Thus we find the result

$$S(\mathbf{q}) = \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k}} n_{\mathbf{k}} (n_{\mathbf{k}+\mathbf{q}} + 1) \tag{4.36}$$

for the static structure factor, in agreement with eq. (4.31). In the condensed phase we again have to separate the ground state and the excited states. We use the definition of the condensate density given in eq. (4.25) and assume $n_{\mathbf{q}} = n_{-\mathbf{q}}$. We get:

$$S(\mathbf{q}) = 1 + 2 \frac{N_0}{N_{\text{tot}}} n_{\mathbf{q}} + \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k} \neq \{0, -\mathbf{q}\}} n_{\mathbf{k}} n_{\mathbf{k}+\mathbf{q}} \,. \tag{4.37}$$

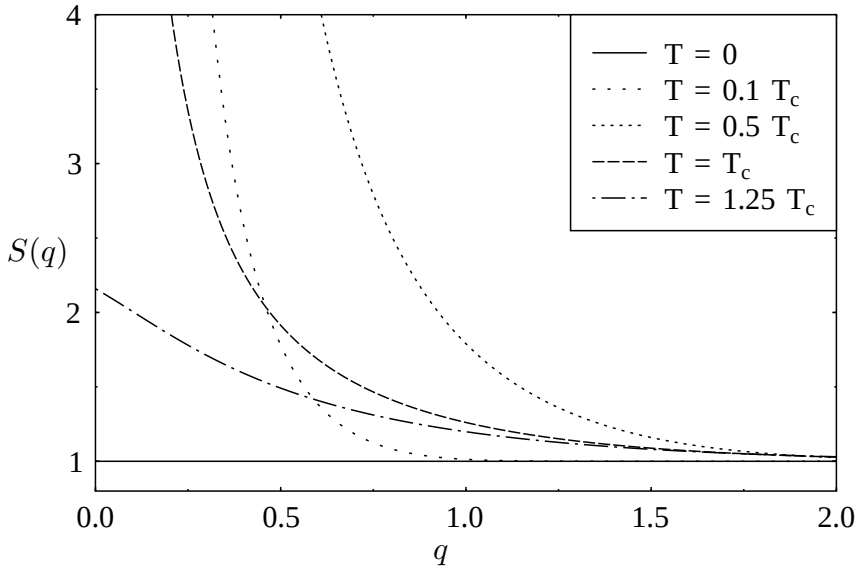

Figure 4.2: Static structure factor of an ideal Bose gas of free particles. At $T = 0$, S is constantly unity and has a δ-peak at $q = 0$. At $0 < T < T_c$ it diverges, and at $T > T_c$ it reaches a constant near $q = 0$. All cases are characterised by the relation $\lim_{q\to\infty} S(q) = 1$.

Note that this expression in also valid in the non-condensed phase where $n_0 = 0$ and the contribution of the ground state $\mathbf{k} = 0$ to $S(\mathbf{q})$ can be neglected compared to the contribution of all excited states. Instead of eq. (4.35) one can use the more convenient definition in terms of expectation values without time slices

$$S(\mathbf{q}) = 1 + \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k},\mathbf{k}'} \left\langle \phi^*_{\mathbf{k}}(0)\phi^*_{\mathbf{k}'+\mathbf{q}}(0)\phi_{\mathbf{k}+\mathbf{q}}(0)\phi_{\mathbf{k}'}(0)\right\rangle \ , \tag{4.38}$$

which leads to eq. (4.37) as well.

Considering a three-dimensional ideal Bose gas with the free-particle dispersion relation $\epsilon(\mathbf{k}) = k^2/2m$, we have to perform the integral

$$\frac{1}{V} \sum_{\mathbf{k}\neq\{0,\mathbf{q}\}} n_{\mathbf{k}} n_{\mathbf{k}+\mathbf{q}} =$$

$$\frac{1}{(2\pi)^2} \int_0^\infty \mathrm{d}k\, k^2 \int_0^1 \mathrm{d}x \left(e^{\beta\left(\frac{k^2+q^2}{2m}-\mu\right)} - 1 \right)^{-1} \left(e^{\beta\left(\frac{k^2+q^2}{2m}+\frac{kq}{m}x-\mu\right)} - 1 \right)^{-1} .$$

Note that $S(\mathbf{q})$ only depends on the modulus $q = |\mathbf{q}|$ in this case. Graphs for different temperature regimes are shown in fig. 4.2.

4.5 Random walk expansion and world-lines

In this section a very intuitive method of diagrammatically visualising a grand canonical partition function shall be introduced for an ideal Bose gas in an optical lattice, namely the random walk expansion [43, 44]. We will perform the same expansion in the following chapters for a system of hard-core bosons, in order to demonstrate the effect of the hard-core condition.

The grand canonical partition function of an ideal Bose gas in a d-dimensional cubic lattice is given by the functional integral

$$Z = \lim_{M\to\infty} \int \exp\left[-\sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m=1}^{M} \phi^*_{\mathbf{r},n} \hat{A}_{\mathbf{r}\mathbf{r}';nm} \phi_{\mathbf{r}',m} \right] \prod_{\mathbf{r}} \prod_{n=1}^{M} \mathrm{d}\phi^*_{\mathbf{r},n} \mathrm{d}\phi_{\mathbf{r},n} \tag{4.39}$$

It is identical to the partition function (4.14) together with the lattice dispersion relation (4.7), but here we use the real-space representation, where $\mathbf{r}, \mathbf{r}'$ are lattice sites. The time structure of the matrix $\hat{A}$ is the same as in eq. (4.15), but instead of the dispersion relation $\epsilon_{\mathbf{k}}$ we use the hopping matrix

$$\hat{J}_{\mathbf{r}\mathbf{r}'} := \begin{cases} -J/2d & \text{if } \mathbf{r}, \mathbf{r}' \text{ nearest neighbours} \\ 0 & \text{otherwise} \end{cases} , \tag{4.40}$$

which establishes the spacial structure of $\hat{A}$, and make use of

$$\hat{\epsilon}_{\mathbf{r}\mathbf{r}'} := \hat{J}_{\mathbf{r}\mathbf{r}'} + J\,\delta_{\mathbf{r}\mathbf{r}'} . \tag{4.41}$$

Thus we can write

$$\hat{A}_{\mathbf{r}\mathbf{r}';nm} := \delta_{nm}\delta_{\mathbf{r}\mathbf{r}'} - (\delta_{n,m+1} + \delta_{n1}\delta_{mM}) \left[\delta_{\mathbf{r}\mathbf{r}'} - \frac{\beta}{M} (\hat{\epsilon}_{\mathbf{r}\mathbf{r}'} - \mu\,\delta_{\mathbf{r}\mathbf{r}'}) \right] , \tag{4.42}$$

where the term $\delta_{n1}\delta_{mM}$ accounts for the upper right matrix element in (4.15) which arises from the periodicity in imaginary time.

The idea of the random walk expansion is to expand the off-diagonal part of the exponential in the functional integral expression in terms of the field variables:

$$\exp\left[-\sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m=1}^{M} \phi^*_{\mathbf{r},n} \hat{A}_{\mathbf{r}\mathbf{r}';nm} \phi_{\mathbf{r}',m} \right] =$$

$$\exp\left[-\sum_{\mathbf{r}} \sum_{n=1}^{M} \phi^*_{\mathbf{r},n} \phi_{\mathbf{r},n} \right] \sum_{\{l_{\mathbf{r}\mathbf{r}',n} \geq 0\}} \frac{1}{l_{\mathbf{r}\mathbf{r}',n}!} \left[\prod_{\mathbf{r},\mathbf{r}',n} \phi^*_{\mathbf{r},n} \underbrace{\left(\delta_{\mathbf{r}\mathbf{r}'} - \frac{\beta}{M} \left(\hat{\epsilon}_{\mathbf{r}\mathbf{r}'} - \mu\delta_{\mathbf{r}\mathbf{r}'} \right) \right)}_{=:\,\hat{u}_{\mathbf{r}\mathbf{r}'}} \phi_{\mathbf{r},n-1} \right]^{l_{\mathbf{r}\mathbf{r}',n}}$$

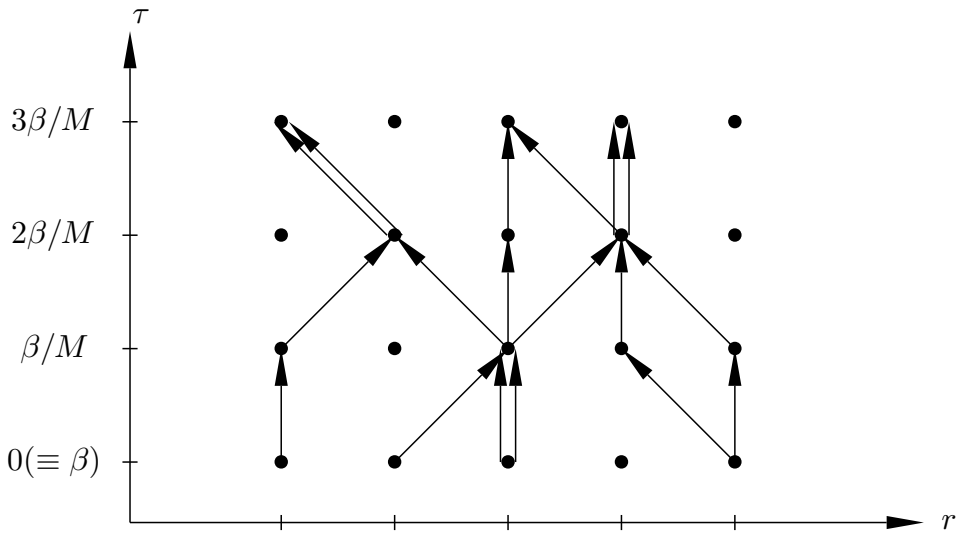

Figure 4.3: Random walk expansion of an ideal Bose gas; world-line diagram.

The abbreviation $\hat{u}_{\mathbf{r}\mathbf{r}'}$ has been introduced for convenience. After substitution into the expression (4.39) the functional integral can be solved by using the identities

$$\prod_{\mathbf{r},\mathbf{r}',n} \left(\phi^*_{\mathbf{r},n}\phi_{\mathbf{r},n-1}\right)^{l_{\mathbf{r}\mathbf{r}',n}} = \prod_{\mathbf{r},n} \left[(\phi^*_{\mathbf{r},n})^{m_{\mathbf{r},n}} (\phi_{\mathbf{r},n})^{m'_{\mathbf{r},n}}\right] , \tag{4.43}$$

$$\text{where } m_{\mathbf{r},n} := \sum_{\mathbf{r}'} l_{\mathbf{r}\mathbf{r}',n} \text{ and } m'_{\mathbf{r},n} := \sum_{\mathbf{r}'} l_{\mathbf{r}'\mathbf{r},n+1}$$

and

$$\int (\phi^*)^m \phi^{m'} \, e^{-\phi^*\phi} \, \frac{\mathrm{d}\phi^*\mathrm{d}\phi}{2\pi\mathrm{i}} = m!\, \delta_{mm'} \, . \tag{4.44}$$

This results in the following form of the grand canonical partition function as a sum over all indices $l_{\mathbf{r}\mathbf{r}',n}$:

$$Z = \sum_{\{l_{\mathbf{r}\mathbf{r}',n} \geq 0\}} \prod_{\mathbf{r},n} \left(m_{\mathbf{r},n}!\, \delta_{m_{\mathbf{r},n},m'_{\mathbf{r},n}} \right) \prod_{\mathbf{r},\mathbf{r}',n} \left[\frac{(\hat{u}_{\mathbf{r}\mathbf{r}'})^{l_{\mathbf{r}\mathbf{r}',n}}}{l_{\mathbf{r}\mathbf{r}',n}!} \right] . \tag{4.45}$$

Note that it is necessary to define $(\hat{u}_{\mathbf{r}\mathbf{r}'})^0 \equiv 1$ here, even for the vanishing matrix elements of $\hat{u}$.

One possible interpretation of this expression is as follows: Each term of the sum can be represented by a diagram, where a particle propagation from site $\mathbf{r}$ at imaginary time

τ to site $\mathbf{r}'$ at time $\tau + \hbar\beta/M$ is indicated by an arrow. So each particle is characterised by a "world-line" showing its movement through the lattice in imaginary time. The contribution of a certain diagram is defined by the following properties:

- The number of particles (arrows) propagated from site $\mathbf{r}'$ at time $(n-1)\hbar\beta/M$ to site $\mathbf{r}$ at time $n\hbar\beta/M$ is given by $l_{\mathbf{r}\mathbf{r}',n}$. In the case of nearest neighbour hopping, particle propagation in one time step $\hbar\beta/M$ is only possible between neighbouring sites, or the particle stays at the same site.
- The number of particles (arrows) which are propagated to site $\mathbf{r}$ at time $n\hbar\beta/M$ from the previous time step is $m_{\mathbf{r},n}$.
- The number of particles (arrows) propagating from site r at time $n\hbar\beta/M$ to the next time step is $m'_{\mathbf{r},n}$.
- Particle conservation is assured by the δ-function in eq. (4.45), such that $m_{\mathbf{r},n} = m'_{\mathbf{r},n}$ is equal to the number of particles at site $\mathbf{r}$ and time $n\hbar\beta/M$.
- There is a periodicity in imaginary time: Time $\tau = \hbar\beta$ is equivalent to time $\tau = 0$, so the diagrams have to be periodic in time.

Note that in the ideal Bose gas $m_{\mathrm{r},n} > 1$ is possible, i.e. more than one particle can occupy the same lattice site at the same time. This will be excluded to establish the hard-core interaction in a Bose gas.

5 Bogoliubov theory

5.1 Bogoliubov transformation

Before discussing an interacting Bose gas in an optical lattice, we begin with the derivation of the Bogoliubov approximation for a dilute homogeneous Bose gas. However, the Bogoliubov theory can also be applied for bosons in a lattice potential, but a Mott-insulating phase is not found within this approximation [35]. Many aspects of the physics discussed in this chapter show up in the hard-core Bose gases in optical lattices as well.

The idea of Bogoliubov theory is to treat a weakly interacting Bose gas ($n_{\mathrm{tot}} a_s^3 \ll 1$) by an order parameter which describes the condensate and quasiparticle excitations, where the quasiparticles are regarded as non-interacting bosons. This assumption is valid, if a large fraction of particles occupies the condensate, i.e. if the temperature is small compared to the transition temperature. The Hamiltonian of the interacting system is given by eq. (2.5). For simplicity we assume, that a lattice potential is absent, i. e. $V_{\mathrm{latt}}(\mathbf{r}) \equiv 0$. After a Fourier transformation of the field operators by

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{2\pi V}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}\, e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \;, \quad \hat{\psi}^{+}(\mathbf{r}) = \frac{1}{\sqrt{2\pi V}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{+}\, e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \;,$$

the Hamiltonian has the form [45]

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{+} \hat{a}_{\mathbf{k}} + \frac{g}{2V} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \hat{a}_{\mathbf{k}_1}^{+} \hat{a}_{\mathbf{k}_2}^{+} \hat{a}_{\mathbf{k}_3} \hat{a}_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3} \;. \tag{5.1}$$

Like in the non-interacting system, the dispersion relation $\epsilon_{\mathbf{k}}$ is given by eq. (4.5) for a homogeneous system and by eq. (4.7) for a lattice with nearest-neighbour hopping.

In the Bogoliubov approximation, the zero-momentum operators are replaced by their expectation value plus a fluctuation

$$\hat{a}_0^{+} \longrightarrow V^{\frac{1}{2}} \Phi_0 + \delta\hat{a}_0^{+} \;, \quad \hat{a}_0 \longrightarrow V^{\frac{1}{2}} \Phi_0^{*} + \delta\hat{a}_0 \;, \tag{5.2}$$

where the condensate density can be identified by $|\Phi_0|^2$. This identification is justified if the zero-momentum level is macroscopically occupied, because the states with one particle more and one particle less in the zero-momentum level have almost no overlap with the original state. After performing this replacement in the interaction term, all terms which are of higher than second order in the field operators are neglected:

$$\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \hat{a}^+_{\mathbf{k}_1}\hat{a}^+_{\mathbf{k}_2}\hat{a}_{\mathbf{k}_3}\hat{a}_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3} \approx$$

$$V^2|\Phi_0|^4 + V{\sum_{\mathbf{k}}}' \left((\Phi_0^*)^2\hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}} + \Phi_0^2\hat{a}^+_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}} + 2|\Phi_0|^2(\hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}^+_{-\mathbf{k}}\hat{a}_{-\mathbf{k}})\right)$$

The prime in ${\sum_{\mathbf{k}}}'$ omits the term $\mathbf{k} = 0$ and the total number of particles in the condensate is $N_0 = V|\Phi_0|^2$. Thus, the effective Bogoliubov Hamiltonian is given by

$$\hat{H}_{\mathrm{B}} = \frac{gN_0^2}{2V} + \frac{1}{2}{\sum_{\mathbf{k}}}' \left[\left(\epsilon(\mathbf{k}) + 2g|\Phi_0|^2\right)(\hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}^+_{-\mathbf{k}}\hat{a}_{-\mathbf{k}}) + g\,(\Phi_0^*)^2\hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}} + g\,\Phi_0^2\,\hat{a}^+_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}}\right] . \tag{5.3}$$

Note that this effective Hamiltonian has a broken $U(1)$-symmetry because it changes if the replacement $\Phi_0 \to e^{\mathrm{i}\alpha}\Phi_0$ is performed. This reflects the fact that the BEC phase of an interacting Bose gas has a broken $U(1)$ symmetry. For simplicity, the phase α may be chosen here such that Φ_0 is real and $(\Phi_0^*)^2 = \Phi_0^2 = N_0/V = n_0$. We now eliminate the condensate particle number N_0 by the total particle number, which is given by the *operator*

$$\hat{N}_{\mathrm{tot}} = N_0 + \frac{1}{2}{\sum_{\mathbf{k}}}'(\hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}^+_{-\mathbf{k}}\hat{a}_{-\mathbf{k}}) . \tag{5.4}$$

The problem here is, that $\hat{N}_{\mathrm{tot}}$ does not commute with $\hat{H}_{\mathrm{B}}$, so the particle number conservation is violated. This is known to be the case in systems with a broken global gauge symmetry, which is discussed in detail in ref. [46]. There are two ways to deal with this problem:

- The first way is to eliminate N_0 by replacing the operator $\hat{N}_{\mathrm{tot}}$ by its expectation value $N_{\mathrm{tot}} = \langle\hat{N}_{\mathrm{tot}}\rangle$ after substituting eq. (5.4) into eq. (5.3). In the Bogoliubov approximation we assume that almost all particles occupy the condensate, i.e. $N_{\mathrm{tot}} - N_0 \ll N_{\mathrm{tot}}$. Therefore we can neglect terms of the order $({\sum_{\mathbf{k}}}'\hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}})^2$ such that in the first term we substitute

$$N_0^2 \approx N_{\mathrm{tot}}^2 - N_{\mathrm{tot}}{\sum_{\mathbf{k}}}'(\hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}^+_{-\mathbf{k}}\hat{a}_{-\mathbf{k}}) ,$$

and in all the other terms we just substitute $N_0 \to N_{\text{tot}}$. Then the the Bogoliubov-Hamiltonian is given in the form [45]

$$\hat{H}_{\text{B}} = \frac{1}{2} V g n_{\text{tot}}^2 + \frac{1}{2}{\sum_{\mathbf{k}}}' \left[(\epsilon_{\mathbf{k}} + g n_{\text{tot}}) \left(\hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^+ \hat{a}_{-\mathbf{k}} \right) + g n_{\text{tot}} (\hat{a}_{\mathbf{k}}^+ \hat{a}_{-\mathbf{k}}^+ + \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}}) \right] , \tag{5.5}$$

and depends explicitly on the total particle density $n_{\text{tot}} = N_{\text{tot}}/V$. This means, that the system is given as a canonical ensemble (i.e. n_{tot} is fixed).

- The second way is to consider a grand canonical ensemble by performing a Legendre transformation

$$\hat{K}_{\text{B}} = \hat{H}_{\text{B}} - \mu \hat{N}_{\text{tot}}$$

and eliminating the chemical potential μ. This is done by the requirement that the term which is of the first order in the zero-momentum fluctuations $\delta\hat{a}_0^+$, $\delta\hat{a}_0^+$ should vanish (this is done e.g. in ref. [35] for the Bose-Hubbard model):

$$V^{\frac{1}{2}} \left(\epsilon_0 - \mu + g |\Phi_0|^2 \right) = 0 \, .$$

This yields

$$\mu = g |\Phi_0|^2 = g n_0 \, , \tag{5.6}$$

which is the solution of the Gross-Pitaevskii equation (2.12) in the case of a homogeneous condensate. Thus the Bogoliubov-Hamiltonian can be written as

$$\hat{H}_{\text{B}} = \frac{1}{2} V g n_0^2 + \frac{1}{2}{\sum_{\mathbf{k}}}' \left[(\epsilon_{\mathbf{k}} + g n_0) \left(\hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^+ \hat{a}_{-\mathbf{k}} \right) + g n_0 (\hat{a}_{\mathbf{k}}^+ \hat{a}_{-\mathbf{k}}^+ + \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}}) \right] \, . \tag{5.7}$$

Note that the Hamiltonian (5.7) which is derived form a grand canonical ensemble, has exactly the same form as the Hamiltonian (5.5) which is derived from a canonical ensemble, except that the total particle density n_{tot} is replaced by the condensate density n_0. This means that the two approximations are not exactly the same. However, both of them are valid if the assumption $(n_{\text{tot}} - n_0)/n_{\text{tot}} \ll 1$ is fulfilled. In the following, we will use the form of the Hamiltonian which given in eq. (5.7).

This Hamiltonian can be solved exactly because it is of second order in the creation and annihilation operators. It can be diagonalised by introducing new creation and annihilation operators $\hat{\alpha}_{\mathbf{k}}^+$ and $\hat{\alpha}_{\mathbf{k}}$ by the transformation

$$\hat{a}_{\mathbf{k}} = u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} - v_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}^+ \, , \quad \hat{a}_{-\mathbf{k}}^+ = u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^+ - v_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}} \, , \tag{5.8}$$

where the coefficients have to be chosen such that the anomalous terms proportional to $\hat{\alpha}_{\mathbf{k}}^+ \hat{\alpha}_{-\mathbf{k}}^+$ and $\hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}$ vanish, and that $\hat{\alpha}_{\mathbf{k}}^+$ and $\hat{\alpha}_{\mathbf{k}}$ fulfill bosonic commutation relations. This is achieved by the choice

$$u_{\mathbf{k}} = \cosh \varphi_{\mathbf{k}} \, , \quad v_{\mathbf{k}} = \sinh \varphi_{\mathbf{k}} \, , \quad \tanh(2\varphi_{\mathbf{k}}) = \frac{g n_0}{\epsilon_{\mathbf{k}} + g n_0} \, . \tag{5.9}$$

This transformation is known as the Bogoliubov transformation. After substituting it into eq. (5.7), the Bogoliubov-Hamiltonian takes the form

$$\hat{H}_{\mathrm{B}} = \frac{1}{2} V g n_0^2 + \frac{1}{2}{\sum_{\mathbf{k}}}' (\epsilon_{\mathbf{k}} + g n_0 - E_{\mathbf{k}}) + \frac{1}{2}{\sum_{\mathbf{k}}}' E_{\mathbf{k}} \left(\hat{\alpha}^+_{\mathbf{k}} \alpha_{\mathbf{k}} + \hat{\alpha}^+_{-\mathbf{k}} \alpha_{-\mathbf{k}}\right) , \tag{5.10}$$

where $E_{\mathbf{k}}$ is the dispersion relation of the quasiparticles which is called the Bogoliubov spectrum:

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} \left(2 g n_0 + \epsilon_{\mathbf{k}}\right)} . \tag{5.11}$$

Again, it should be mentioned that if one chooses the Hamiltonian (5.5) which was derived from a canonical ensemble, the Bogoliubov spectrum contains the total density n_{tot} instead of n_0. If $\epsilon_{\mathbf{k}}$ is the free-particle dispersion, it is identical to eq. (2.8). For small wave vectors $|k| \ll \sqrt{a_s n_0}$, the spectrum is linear like a phonon spectrum:

$$E_{\mathbf{k}} = \hbar c^{\mathrm{qp}} |\mathbf{k}| , \quad c^{\mathrm{qp}} = \left(\frac{4\pi a_s n_0 \hbar^2}{m^2}\right)^{\frac{1}{2}} , \tag{5.12}$$

where c^{qp} is the sound velocity. In the case of a lattice dispersion relation, m is given by the band-mass m^* in eq. (4.8). The operators $\hat{\alpha}^+_{\mathbf{k}}$ and $\hat{\alpha}_{\mathbf{k}}$ can be regarded as creation- and annihilation operators of quasiparticles.

5.2 Bogoliubov ground state

In Bogoliubov theory, quasiparticles are non-interacting, therefore the elementary excitations are given by the Bose distribution:

$$n^{\mathrm{qp}}_{\mathbf{k}} = \frac{1}{e^{\beta E_{\mathbf{k}}} - 1} . \tag{5.13}$$

In the ground state, there are no quasiparticle excitations. Therefore the ground state $|\mathbf{O}\rangle$ of the system is given by the condition

$$\hat{\alpha}_{\mathbf{k}} |\mathbf{O}\rangle = 0 \quad \text{for all} \quad \mathbf{k} \neq 0 . \tag{5.14}$$

One might suppose that the ground state energy is simply

$$E_0 = \langle \mathbf{O} | \hat{H}_{\mathrm{B}} | \mathbf{O} \rangle = \frac{1}{2} V g n_0^2 + \frac{1}{2}{\sum_{\mathbf{k}}}' (\epsilon_{\mathbf{k}} + g n_0 - E_{\mathbf{k}}) ,$$

but in the case of a free-particle dispersion relation the sum is divergent in three dimensions like $\sum'_{\mathbf{k}} k^{-2}$. Therefore it is necessary to renormalise the sum by adding the term [12, 47]

$$\frac{1}{2}{\sum_{\mathbf{k}}}' \frac{(g n_0)^2}{2\epsilon_{\mathbf{k}}}$$

such that the ground state energy is given by the convergent integral

$$E_0 = \frac{V}{2} g n_0^2 + \frac{V}{2} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \left(E_{\mathbf{k}} - \epsilon_{\mathbf{k}} - 1 + \frac{(g n_0)^2}{2\epsilon_{\mathbf{k}}} \right) . \tag{5.15}$$

For the free-particle dispersion

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}$$

the result is

$$E_0 = \frac{V}{2} g n_0^2 \left[1 + \frac{128}{15} \left(\frac{a_s^3 n_0}{\pi} \right)^{\frac{1}{2}} \right] , \tag{5.16}$$

where a_s is the s-wave scattering length which is related to g by eq. (2.4).

Another interesting quantity is the ground state depletion. While in an ideal Bose gas all particles occupy the lowest momentum state (i.e. the condensate) at zero temperature, this is not the case in an interacting system. While the condensate occupation number is given as

$$N_0 = n_0 V = \langle \mathbf{O} | \hat{a}_0^+ \hat{a}_0 | \mathbf{O} \rangle , \tag{5.17}$$

the particles out of the condensate in the ground state with momentum $\mathbf{k} \neq 0$ are given by the distribution function

$$\langle n_{\mathbf{k}} \rangle = \langle \mathbf{O} | \hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}} | \mathbf{O} \rangle = v_{\mathbf{k}}^2 \langle \mathbf{O} | \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^+ | \mathbf{O} \rangle = v_{\mathbf{k}}^2 , \tag{5.18}$$

where we have used the Bogoliubov transformation (5.8), the ground state condition (5.14), and the bosonic commutation relations of the operators $\hat{\alpha}_{\mathbf{k}}^+$ and $\hat{\alpha}_{\mathbf{k}}$. Thus the condensate depletion of the Bogoliubov ground state is

$$\frac{N_{\mathrm{tot}} - N_0}{N_{\mathrm{tot}}} = \frac{1}{N_{\mathrm{tot}}} {\sum_{\mathbf{k}}}' v_{\mathbf{k}}^2 = \frac{1}{n_{\mathrm{tot}}} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} v_{\mathbf{k}}^2 .$$

or

$$\frac{N_{\mathrm{tot}} - N_0}{N_{\mathrm{tot}}} = \frac{1}{n_0} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} v_{\mathbf{k}}^2 + \mathcal{O}(n_{\mathrm{tot}} - n_0) , \tag{5.19}$$

where the term of the order $n_{\mathrm{tot}} - n_0$ can be neglected. The result for bosons with a free-particle dispersion is

$$\frac{N_{\mathrm{tot}} - N_0}{N_{\mathrm{tot}}} = \frac{8}{3} \left(\frac{a_s^3 n_0}{\pi} \right)^{\frac{1}{2}} . \tag{5.20}$$

In typical experiments with sodium BECs, the interparticle distance is $n^{-1/3} \sim 200\mathrm{nm}$ and the scattering length is $a_s \sim 3\mathrm{nm}$ [48]. This yields a ground-state depletion of $\sim 10^{-3} \ll 1$ such that Bogoliubov theory is a good approximation here.

5.3 Thermal excitations

In Bogoliubov theory, thermal excitations are described as quasiparticle excitations out of the ground state. An excited state with $n_{\mathbf{k}}$ quasiparticles with momentum $\mathbf{k} \neq 0$ can be constructed as

$$|n\rangle_{\mathrm{B}} = |\{n_{\mathbf{k}}\}\rangle = \frac{1}{\sqrt{\prod_{\mathbf{k}} n_{\mathbf{k}}!}} \left(\hat{\alpha}_{\mathbf{k}}^{+}\right)^{n_{\mathbf{k}}} |\mathbf{O}\rangle \ . \tag{5.21}$$

These are pure number states similar to the states given in eq. (4.2), except that here we have number states of quasiparticles created by the operators $\hat{\alpha}_{\mathbf{k}}^{+}$, and the ground state is now not the vacuum state which contains no particles but the Bogoliubov ground state, which is defined by the property (5.14). These number states are also the eigenstates of the Bogoliubov Hamiltonian (5.10), because it is diagonal with respect to the quasiparticle numbers. To find the average number of particles with momentum $\mathbf{k} \neq 0$ at finite temperature, instead of the ground state expectation value (5.18), we have to calculate the finite temperature expectation value

$$\langle n_{\mathbf{k}} \rangle = \frac{1}{Z_{\mathrm{can}}} \mathrm{Tr} \left(e^{-\beta \hat{H}_{\mathrm{B}}} \hat{a}_{\mathbf{k}}^{+} \hat{a}_{\mathbf{k}} \right) \ , \tag{5.22}$$

where $Z_{\mathrm{can}} = \mathrm{Tr}\, e^{-\beta \hat{H}_{\mathrm{B}}}$ is the *canonical* partition function ($\hat{H}_{\mathrm{B}}$ depends explicitly on n_{tot}, and the chemical potential μ has been eliminated). The expectation value can be calculated by substituting the Bogoliubov transformation (5.8) and evaluating the trace in the basis of the quasiparticle number states:

$$\langle n_{\mathbf{k}} \rangle = \frac{1}{Z_{\mathrm{can}}} \sum_{\{n_{\mathbf{k}'}\}} \langle \{n_{\mathbf{k}'}\} | e^{-\beta \hat{H}_{\mathrm{B}}} (u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{+} - v_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}) (u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} - v_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}^{+}) | \{n_{\mathbf{k}'}\} \rangle \tag{5.23}$$

Because of the fact that all pure number states are orthogonal to each other, and that they are the eigenstates of the Hamiltonian, the two terms which are proportional to $-u_{\mathbf{k}} v_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{+} \hat{\alpha}_{-\mathbf{k}}^{+}$ and $-u_{\mathbf{k}} v_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}$ vanish and we have

$$\langle n_{\mathbf{k}} \rangle = \frac{1}{Z_{\mathrm{can}}} \sum_{\{n_{\mathbf{k}'}\}} \left[u_{\mathbf{k}}^2 \langle \{n_{\mathbf{k}}\} | e^{-\beta \hat{H}_{\mathrm{B}}} \hat{\alpha}_{\mathbf{k}}^{+} \hat{\alpha}_{\mathbf{k}} | \{n_{\mathbf{k}'}\} \rangle + v_{\mathbf{k}}^2 \langle \{n_{\mathbf{k}'}\} | e^{-\beta \hat{H}_{\mathrm{B}}} \hat{\alpha}_{-\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}^{+} | \{n_{\mathbf{k}'}\} \rangle \right] \ . \tag{5.24}$$

After substituting the commutation relation $\hat{\alpha}_{-\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}^{+} = \hat{\alpha}_{-\mathbf{k}}^{+} \hat{\alpha}_{-\mathbf{k}} + 1$ and the Bose distribution (5.13), we find the result

$$\langle n_{\mathbf{k}} \rangle = v_{\mathbf{k}}^2 + \frac{u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2}{e^{\beta E_{\mathbf{k}}} - 1} \tag{5.25}$$

with the Bogoliubov spectrum $E_{\mathbf{k}}$ given in eq. (5.11). In this expression, the first term is identical to the ground state depletion given in (5.18), and the second term describes

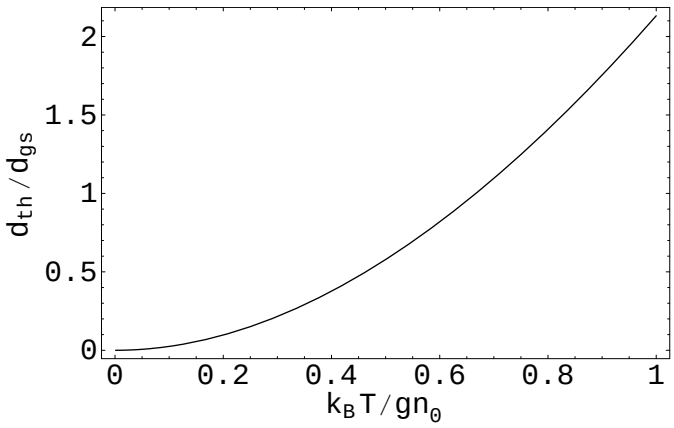

Figure 5.1: The ratio $d_{\mathrm{th}}/d_{\mathrm{gs}}$ plotted against $k_{\mathrm{B}}T/gn_0$. The ratio is unity at $k_{\mathrm{B}}T/gn_0 \approx 0.67$. With the experimental parameters given below eq. (5.20), $k_{\mathrm{B}}T/gn_0 = 1$ corresponds to a temperature ~ 100nK.

the thermal excitations. Note that at zero temperature where $\beta \to \infty$, the second term vanishes because the Bose distribution then vanishes for all $\mathbf{k} \neq 0$, such that the expression reduces to the ground state result (5.18). We also mention that in the case of vanishing interparticle interaction where $g = 0$, we find $u_{\mathbf{k}} = 1$, $v_{\mathbf{k}} = 0$ and $E_{\mathbf{k}} = \epsilon_{\mathbf{k}}$, and the distribution function (5.25) reduces to the ordinary Bose distribution (4.24).

Analogous to eq. (5.19), the ratio of particles out of the condensate is given as the integral over all finite momenta:

$$\frac{N_{\mathrm{tot}} - N_0}{N_{\mathrm{tot}}} = \underbrace{\frac{1}{n_{\mathrm{tot}}} \int \frac{\mathrm{d}^3 k}{(2\pi)^3}\, v_{\mathbf{k}}^2}_{:= d_{\mathrm{gs}}} + \underbrace{\frac{1}{n_{\mathrm{tot}}} \int \frac{\mathrm{d}^3 k}{(2\pi)^3}\, \frac{u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2}{e^{\beta E_{\mathbf{k}}} - 1}}_{:= d_{\mathrm{th}}} \tag{5.26}$$

Here, d_{gs} is the ground state depletion and d_{th} is the depletion which is induced by thermal fluctuations. In fig. 5.1 the ratio between these two quantities is plotted against temperature. It can be seen that the thermal depletion begins to dominate if $k_{\mathrm{B}}T$ is of the order of gn_0.

5.4 Static structure factor

In eqs. (2.25) and (2.31) we have given the definition of the static structure factor as the expectation value

$$S(\mathbf{q}) = \frac{1}{N_{\mathrm{tot}}} \left\langle \hat{\rho}_{\mathbf{q}} \hat{\rho}_{\mathbf{q}}^{+} \right\rangle \ . \tag{5.27}$$

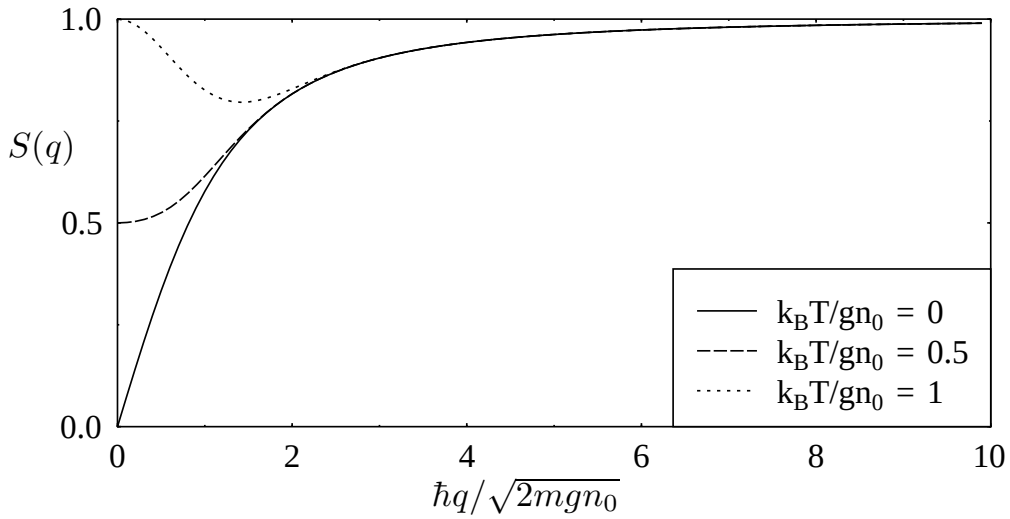

Figure 5.2: Static structure factor of a homogeneous Bose gas in Bogoliubov approximation for zero temperature and non-zero temperatures.

This means, for the Bogoliubov ground state we calculate for $\mathbf{q} \neq 0$:

$$S(\mathbf{q}) = \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k},\mathbf{k}'} \langle \mathbf{O} | \hat{a}^+_{\mathbf{k}-\mathbf{q}} \hat{a}_{\mathbf{k}} \hat{a}^+_{\mathbf{k}'+\mathbf{q}} \hat{a}_{\mathbf{k}'} | \mathbf{O} \rangle$$

By applying the replacement (5.2) and the transformation (5.9) we get

$$\sum_{\mathbf{k}} \hat{a}^+_{\mathbf{k}+\mathbf{q}} \hat{a}_{\mathbf{k}} |\mathbf{O}\rangle = \sqrt{N_0} \left(\hat{a}^+_{\mathbf{q}} + \hat{a}_{-\mathbf{q}} \right) |\mathbf{O}\rangle + \sum_{\mathbf{k} \neq 0, -\mathbf{q}} \hat{a}^+_{\mathbf{k}+\mathbf{q}} \hat{a}_{\mathbf{k}} |\mathbf{O}\rangle =$$

$$\sqrt{N_0} \left(u_{\mathbf{q}} - v_{\mathbf{q}} \right) \hat{\alpha}^+_{\mathbf{q}} + \mathcal{O}(N_0^0) \; ,$$

where the latter term can be neglected in the thermodynamic limit. As a result, we find for the static structure factor the result

$$S(\mathbf{q}) = \frac{N_0}{N_{\text{tot}}} (u_{\mathbf{q}} - v_{\mathbf{q}})^2 = \frac{N_0}{N_{\text{tot}}} \frac{\epsilon_{\mathbf{q}}}{E_{\mathbf{q}}} \; , \tag{5.28}$$

where we can approximate $N_0/N_{\text{tot}} \approx 1$. For a free-particle dispersion relation this result is identical to the Feynman relation (2.37).

We can extend the calculation to finite temperature the same way as it was performed for the total particle number in section 5.3. As before, the forth order term can be neglected and we have to calculate

$$S(\mathbf{q}) = \frac{N_0}{N_{\text{tot}}} \left\langle \left(\hat{a}^+_{\mathbf{q}} + \hat{a}_{-\mathbf{q}} \right) \left(\hat{a}_{\mathbf{q}} + \hat{a}^+_{-\mathbf{q}} \right) \right\rangle \; ,$$

where the expectation value is now a thermal expectation value. Substituting the Bogoliubov transformation and the Bose distribution of quasiparticle excitations, we find

$$S(\mathbf{q}) = \frac{N_0}{N_{\text{tot}}}(u_{\mathbf{q}} - v_{\mathbf{q}})^2 \left\langle \left(\hat{\alpha}_{\mathbf{q}} - \hat{\alpha}^+_{-\mathbf{q}}\right)\left(\hat{\alpha}^+_{\mathbf{q}} - \hat{\alpha}_{-\mathbf{q}}\right)\right\rangle =$$

$$\frac{N_0}{N_{\text{tot}}}\frac{\epsilon_{\mathbf{q}}}{E_{\mathbf{q}}}\left(1 + \frac{2}{e^{\beta E_{\mathbf{q}}} - 1}\right) , \tag{5.29}$$

which reduces to the ground-state result (5.28) for zero temperature. Like in the non-interacting system, $S(\mathbf{q})$ has a δ-peak at $\mathbf{q} = 0$, i.e. the value of $S(0)$ is of the order of N_{tot}. For both zero and finite temperature we calculate its weight:

$$S(0) = \frac{1}{N_{\text{tot}}}\sum_{\mathbf{k},\mathbf{k}'}\left\langle \hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}}\hat{a}^+_{\mathbf{k}'}\hat{a}_{\mathbf{k}'}\right\rangle =$$

$$\frac{N_0^2}{N_{\text{tot}}} + 2\frac{N_0}{N_{\text{tot}}}\sum_{\mathbf{k}\neq 0}\langle n_{\mathbf{k}}\rangle + \frac{1}{N_{\text{tot}}}\sum_{\mathbf{k},\mathbf{k}'\neq 0}\left\langle \hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}}\hat{a}^+_{\mathbf{k}'}\hat{a}_{\mathbf{k}'}\right\rangle =$$

$$\frac{N_0^2}{N_{\text{tot}}} + 2\frac{N_0}{N_{\text{tot}}}(N_{\text{tot}} - N_0) + \mathcal{O}(N_0^0) . \tag{5.30}$$

Again, we can approximate $N_0/N_{\text{tot}} \approx 1$ in eqs. (5.29) and (5.30). The static structure factor is plotted in fig. 5.2. We find the temperature dependent asymptotic behavior

$$\lim_{\mathbf{q}\to 0} S(\mathbf{q}) = \frac{k_{\text{B}}T}{gn_0} . \tag{5.31}$$

For large wave vectors $\mathbf{q}$ the static structure factor approaches unity.

5.5 Derivation from saddle point approximation

The models which shall be presented in the following are treated within the functional integral formalism. Therefore it might be interesting to derive the results from Bogoliubov theory, which were shown in the previous sections of this chapter, from the functional integral point of view. The method which will be used here and in the following chapters is the saddle point approximation (or: stationary phase approximation, Gaussian approximation) [9, 16, 49]. It allows to find a mean-field solution plus fluctuations around the mean-field result. The mean-field solution is connected to the condensate order parameter, while the fluctuations contain the information about the quasiparticles and their spectrum. The saddle-point approximation is good as long as these fluctuations are small.

The main idea of a saddle point approximation is to expand the action of the system around its minimum up to second order in the field variables. This leads to a Gaussian

integral which can be performed. The action of a bosonic system is given in eq. (3.6), where in this case the index α shall denote the position vector $\mathbf{r}$. Together with the Hamiltonian (2.5) of the interacting Bose gas we have

$$A(\phi^*,\phi) = \frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \int \mathrm{d}^3 r \Bigg\{ \phi^*(\mathbf{r},\tau) \left[\left(\hbar\frac{\partial}{\partial\tau} - \mu \right) - \frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) \right] \phi(\mathbf{r},\tau) + \frac{g}{2} \left|\phi(\mathbf{r},\tau)\right|^4 \Bigg\} . \tag{5.32}$$

The minimum of the action is found by the condition, that its variation with respect to the complex field variables should vanish:

$$\delta A = 0 .$$

The result leads to a mean-field equation for the condensate order parameter $\Phi_0(\mathbf{r},\tau)$:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) + g\left|\Phi_0(\mathbf{r},\tau)\right|^2 \right) \Phi_0(\mathbf{r},\tau) = -\left(\frac{\partial}{\partial\tau} - \mu \right) \Phi_0(\mathbf{r},\tau) . \tag{5.33}$$

After performing the analytic continuation

$$\frac{\partial}{\partial\tau} \longrightarrow -i\hbar\frac{\partial}{\partial t}$$

and omitting the chemical potential term, this is identical to the time-dependent Gross-Pitaevskii equation (2.12). We recall that the invariance of the mean-field solution under the gauge transformation (2.9) with the global phase α reflects the broken global $U(1)$ symmetry of the BEC phase.

To find the results from the previous sections in this chapter, we assume a homogeneous system, i.e. $V_{\mathrm{ext}}(\mathbf{r}) \equiv 0$ in the action (5.32). Further we assume that the mean-field solution is constant in space and imaginary time: $\Phi_0(\mathbf{r},\tau) \equiv \Phi_0$. In this case, the solution of eq. (5.33) is

$$\left|\Phi_0\right|^2 = n_0 = \frac{\mu}{g} , \tag{5.34}$$

in agreement with eq. (5.6). We now write the complex field as the sum of the mean-field solution plus fluctuations

$$\phi(\mathbf{r},\tau) = \Phi_0 + \delta\phi(\mathbf{r},\tau) , \quad \phi^*(\mathbf{r},\tau) = \Phi_0^* + \delta\phi^*(\mathbf{r},\tau) , \tag{5.35}$$

where the complex field of fluctuations $\delta\phi$ is considered to be small, such that those terms in the action which are of higher than second order in the fluctuations, can be

neglected. The expansion yields (for simplicity we write $\delta\phi(\mathbf{r},\tau)=\delta\phi$, $\delta\phi^*(\mathbf{r},\tau)=\delta\phi^*$)

$$\begin{aligned} A &= A_0+\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\int\mathrm{d}^3r\Bigg\{\delta\phi^*\left[\left(\hbar\frac{\partial}{\partial\tau}-\mu\right)-\frac{\hbar^2}{2m}\nabla^2\right]\delta\phi+ \\ &\qquad \frac{g}{2}|\Phi_0|^2\left(\delta\phi^2+(\delta\phi^*)^2+4\delta\phi\,\delta\phi^*\right)\Bigg\}+\mathcal{O}(|\delta\phi|^3) \end{aligned} \tag{5.36}$$

$$\approx A_0+\frac{1}{2\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\int\mathrm{d}^3r\begin{pmatrix}\delta\phi\\ \delta\phi^*\end{pmatrix}\cdot\begin{pmatrix}-\frac{\hbar^2}{2m}\nabla^2+\mu+\hbar\frac{\partial}{\partial\tau} & \mu\\ \mu & -\frac{\hbar^2}{2m}\nabla^2+\mu-\hbar\frac{\partial}{\partial\tau}\end{pmatrix}\begin{pmatrix}\delta\phi^*\\ \delta\phi\end{pmatrix},$$

where we have eliminated the condensate order parameter by eq. (5.34) in the second step, and the zeroth-order part of the action is

$$A_0=\beta V\left(-\mu|\Phi_0|^2+\frac{g}{2}|\Phi_0|^4\right)=-\frac{\beta V\mu^2}{2g}\,. \tag{5.37}$$

Because A_0 does not depend on the field fluctuations, and the second term is of second order in $\delta\phi$ and $\delta\phi^*$, the functional integral for the grand canonical partition function

$$Z=\int e^{-A(\delta\phi^*,\delta\phi)}\mathcal{D}(\delta\phi^*(\mathbf{r},\tau)\delta\phi(\mathbf{r},\tau)) \tag{5.38}$$

can be solved. We now split the quasiparticle field into its real and imaginary part:

$$\delta\phi=\delta\phi'+\mathrm{i}\delta\phi''\qquad\delta\phi^*=\delta\phi'-\mathrm{i}\delta\phi''\,, \tag{5.39}$$

such that instead of eq. (5.36) we get

$$A=A_0+\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\int\mathrm{d}^3r\begin{pmatrix}\delta\phi'\\ \delta\phi''\end{pmatrix}\cdot\begin{pmatrix}-\frac{\hbar^2}{2m}\nabla^2 & -\mathrm{i}\,\hbar\frac{\partial}{\partial\tau}\\ \mathrm{i}\hbar\frac{\partial}{\partial\tau} & -\frac{\hbar^2}{2m}\nabla^2+2\mu\end{pmatrix}\begin{pmatrix}\delta\phi'\\ \delta\phi''\end{pmatrix}\,. \tag{5.40}$$

We Fourier transform the field of fluctuations with respect to the spacial coordinate like

$$\delta\phi'(\mathbf{r},\tau) = \frac{1}{\sqrt{2\pi V}}\sum_{\mathbf{k}}\delta\phi'_{\mathbf{k}}(\tau)\cos(\mathbf{kr}) \tag{5.41}$$

$$\delta\phi''(\mathbf{r},\tau) = \frac{1}{\sqrt{2\pi V}}\sum_{\mathbf{k}}\delta\phi''_{\mathbf{k}}(\tau)\cos(\mathbf{kr})\,, \tag{5.42}$$

with the constraints $\delta\phi'_{\mathbf{k}}=\delta\phi'_{-\mathbf{k}}$ and $\delta\phi''_{\mathbf{k}}=\delta\phi''_{-\mathbf{k}}$ and thus get

$$A=A_0+\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\sum_{\mathbf{k}}\begin{pmatrix}\delta\phi'_{\mathbf{k}}(\tau)\\ \delta\phi''_{\mathbf{k}}(\tau)\end{pmatrix}\cdot\begin{pmatrix}\epsilon_{\mathbf{k}} & -\mathrm{i}\hbar\frac{\partial}{\partial\tau}\\ \mathrm{i}\hbar\frac{\partial}{\partial\tau} & \epsilon_{\mathbf{k}}+2\mu\end{pmatrix}\begin{pmatrix}\delta\phi'_{\mathbf{k}}(\tau)\\ \delta\phi''_{\mathbf{k}}(\tau)\end{pmatrix} \tag{5.43}$$

with the free-particle dispersion relation $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$. It is further possible to perform a Fourier transformation in the imaginary time coordinate as well, namely

$$\delta\phi'_{\mathbf{k}}(\tau) = \sum_n \delta\phi'_{\mathbf{k},\omega_n} \cos(\omega_n\tau) \tag{5.44}$$

$$\delta\phi''_{\mathbf{k}}(\tau) = \sum_n \delta\phi''_{\mathbf{k},\omega_n} \cos(\omega_n\tau) \ , \tag{5.45}$$

with the Matsubara frequencies (4.11) and the constraints $\delta\phi'_{\mathbf{k},\omega_n} = \delta\phi'_{\mathbf{k},-\omega_n}$ and $\delta\phi''_{\mathbf{k},\omega_n} = \delta\phi''_{\mathbf{k},-\omega_n}$, which leads to the form

$$A = A_0 + \frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \sum_{\mathbf{k},n} \begin{pmatrix} \delta\phi'_{\mathbf{k},\omega_n} \\ \delta\phi''_{\mathbf{k},\omega_n} \end{pmatrix} \cdot \mathcal{G}^{-1}(\mathbf{k},\omega_\nu) \begin{pmatrix} \delta\phi'_{\mathbf{k},\omega_n} \\ \delta\phi''_{\mathbf{k},\omega_n} \end{pmatrix} \ , \tag{5.46}$$

and allows to identify the quasiparticle Green's function (a 2×2 matrix in this case)

$$\mathcal{G}^{-1}(\mathbf{k},\omega_n) = \begin{pmatrix} \epsilon_{\mathbf{k}} & \mathrm{i}\hbar\omega_n \\ \mathrm{i}\hbar\omega_n & \epsilon_{\mathbf{k}} + 2\mu \end{pmatrix} \ . \tag{5.47}$$

The excitation energies of the quasiparticles are given by the poles of the quasiparticle Green's function, which are found by solving the equation

$$\det\, \mathcal{G}^{-1}(\mathbf{k},\omega_n) = 0 \ , \tag{5.48}$$

and performing the analytic continuation

$$\mathrm{i}\hbar\omega_n \longrightarrow E_{\mathbf{k}} \ .$$

The solution

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}\left(2\mu + \epsilon_{\mathbf{k}}\right)} \tag{5.49}$$

is identical to the Bogoliubov spectrum (5.11), if the relation $n_0 = \mu/g$ is inserted.

5.6 Partition function and correlation functions

To find the correct expression for the grand canonical partition function as well as for the correlation functions, we have to perform the same steps as in section 4.2, namely to start with the discrete-time functional integral and sending the number of time steps M to infinity at the end. In analogy to eq. (4.14), the discrete-time version of eq. (5.43) is

$$A_{\mathrm{discrete}} = A_0 + \sum_{\mathbf{k}} \sum_{n,m=1}^{M} \begin{pmatrix} \delta\phi'_{\mathbf{k},n} \\ \delta\phi''_{\mathbf{k},n} \end{pmatrix} \cdot \hat{A}^{(\mathbf{k})}_{nm} \begin{pmatrix} \delta\phi''_{\mathbf{k},m} \\ \delta\phi'_{\mathbf{k},m} \end{pmatrix} \ , \tag{5.50}$$

where $\hat{A}^{(\mathbf{k})}_{nm}$ has the $M \times M$ structure

$$\hat{A}^{(\mathbf{k})} = \begin{bmatrix} \hat{B} & -\hat{b}^*_{\mathbf{k}} & 0 & \cdots & 0 & -\hat{b}_{\mathbf{k}} \\ -\hat{b}_{\mathbf{k}} & \hat{B} & -\hat{b}^*_{\mathbf{k}} & 0 & & \\ 0 & -\hat{b}_{\mathbf{k}} & \hat{B} & \ddots & & \vdots \\ & 0 & -\hat{b}_{\mathbf{k}} & \ddots & -\hat{b}^*_{\mathbf{k}} & 0 \\ \vdots & & 0 & \ddots & \hat{B} & -\hat{b}^*_{\mathbf{k}} \\ -\hat{b}^*_{\mathbf{k}} & & & \cdots & -\hat{b}_{\mathbf{k}} & \hat{B} \end{bmatrix} \tag{5.51}$$

in the imaginary time variables n and m, and each matrix entry is by itself a 2×2 matrix:

$$\hat{b}_{\mathbf{k}} = \frac{1}{2}\left(1 - \frac{\beta}{M}(\epsilon_{\mathbf{k}} + \mu)\right)\begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} 1 + \frac{\beta}{M}\mu & 0 \\ 0 & 1 - \frac{\beta}{M}\mu \end{pmatrix}. \tag{5.52}$$

The matrix can be diagonalised by using the same unitary transformation (4.20), which was applied for the ideal Bose gas. This yields

$$(U\hat{A}^{(\mathbf{k})}U^{+})_{kn} = \delta_{kn}\left[\begin{pmatrix} 1 + \frac{\beta}{M}\mu & 0 \\ 0 & 1 - \frac{\beta}{M}\mu \end{pmatrix} - \left(1 - \frac{\beta}{M}(\epsilon_{\mathbf{k}} + \mu)\right)\begin{pmatrix} \cos\left(\frac{2\pi}{M}n\right) & \sin\left(\frac{2\pi}{M}n\right) \\ -\sin\left(\frac{2\pi}{M}n\right) & \cos\left(\frac{2\pi}{M}n\right) \end{pmatrix}\right]. \tag{5.53}$$

Therefore, the determinant of the matrix is given as the product over the above 2×2 matrices:

$$\det\,\hat{A}^{(\mathbf{k})} = \prod_{n=1}^{M}\left[2\left(1 - \frac{\beta}{M}(\epsilon_{\mathbf{k}} + \mu)\right)\left(1 - \cos\left(\frac{2\pi}{M}n\right)\right) + \left(\frac{\beta}{M}\right)^2 \epsilon_{\mathbf{k}}\left(\epsilon_{\mathbf{k}} + 2\mu\right)\right]. \tag{5.54}$$

This is a product of the type (A.2) given in the Appendix and can be performed. The result is

$$\det\,\hat{A}^{(\mathbf{k})} = \left(1 - \frac{\beta}{M}\left(\epsilon_{\mathbf{k}} + \mu\right)\right)\Bigg[-2+ \left(1 + \frac{\beta}{M}\sqrt{\epsilon_{\mathbf{k}}\left(\epsilon_{\mathbf{k}} + 2\mu\right)} + \mathcal{O}\left(\frac{\beta}{M}\right)^2\right)^M + \left(1 - \frac{\beta}{M}\sqrt{\epsilon_{\mathbf{k}}\left(\epsilon_{\mathbf{k}} + 2\mu\right)} + \mathcal{O}\left(\frac{\beta}{M}\right)^2\right)^M\Bigg]. \tag{5.55}$$

Thus we obtain the grand canonical partition function of the Bogoliubov Hamiltonian (after omitting an uninteresting constant factor):

$$Z = e^{-A_0}\lim_{M\to\infty}\prod_{\mathbf{k}\neq 0}\left[\det\hat{A}^{(\mathbf{k})}\right]^{-\frac{1}{2}} = \exp\left(\frac{\beta V\mu^2}{2g}\right)\prod_{\mathbf{k}\neq 0} e^{\frac{\beta}{2}(\epsilon_{\mathbf{k}}+\mu)}\left[\cosh(\beta E_{\mathbf{k}}) - 1\right]^{-\frac{1}{2}}. \tag{5.56}$$

Thermodynamic quantities can be calculated as correlation functions, as was mentioned in section 3.2. The distribution function of the particles outside of the condensate is given as

$$\langle n_{\mathbf{k}} \rangle = \langle \delta\phi^*_{\mathbf{k}}(0)\delta\phi_{\mathbf{k}}(0) \rangle = \langle \delta\phi'_{\mathbf{k}}(0)^2 \rangle + \langle \delta\phi''_{\mathbf{k}}(0)^2 \rangle \; . \tag{5.57}$$

These expectation values are given by the diagonal elements of the matrix $[\hat{A}^{(\mathbf{k})}]^{-1}$. So we have to calculate

$$\langle n_{\mathbf{k}} \rangle = \lim_{M\to\infty} \frac{1}{2} \left(([\hat{A}^{(\mathbf{k})}]^{-1}_{11})_{nn} + ([\hat{A}^{(\mathbf{k})}]^{-1}_{22})_{nn} \right) \; ,$$

with the 11- and the 22-component of the matrix with respect to the 2×2 structure. After inversion of the matrix (5.53) and the back transformation like in section 4.3, we find the matrix elements

$$[\hat{A}^{(\mathbf{k})}]^{-1}_{11/22} = \frac{1}{2} \sum_{n=1}^{M} \frac{1}{M} \frac{\cos\left(\frac{2\pi}{M}n\right) - \frac{1 \mp \frac{\beta}{M}\mu}{1-\left(\frac{\beta}{M}\right)(\epsilon_{\mathbf{k}}+\mu)}}{\cos\left(\frac{2\pi}{M}n\right) - \frac{1-\left(\frac{\beta}{M}\right)(\epsilon_{\mathbf{k}}+\mu)+\frac{1}{2}\left(\frac{\beta}{M}\right)^2(\epsilon_{\mathbf{k}}^2+2\epsilon_{\mathbf{k}}\mu)}{1-\left(\frac{\beta}{M}\right)(\epsilon_{\mathbf{k}}+\mu)}} \; , \tag{5.58}$$

where the "minus" sign in the numerator holds for the 11 element and the "plus" sign for the 22 element. This sum is composed of sums of the type (A.5) and (A.6) in Appendix A.2. With the use of

$$\frac{1-\left(\frac{\beta}{M}\right)(\epsilon_{\mathbf{k}}+\mu)+\frac{1}{2}\left(\frac{\beta}{M}\right)^2(\epsilon_{\mathbf{k}}^2+2\epsilon_{\mathbf{k}}\mu)}{1-\left(\frac{\beta}{M}\right)(\epsilon_{\mathbf{k}}+\mu)} = 1 + \frac{1}{2}\left(\frac{\beta}{M}\right)E_{\mathbf{k}}^2 + \mathcal{O}\left(\frac{\beta}{M}\right)^2$$

we get

$$\langle n_{\mathbf{k}} \rangle = \lim_{M\to\infty} \frac{1}{2} \left[\frac{M}{\beta E_{\mathbf{k}}} \frac{\left(1-\frac{\beta}{M}E_{\mathbf{k}}\right)^M + \left(1+\frac{\beta}{M}E_{\mathbf{k}}\right)^M + 2}{\left(1-\frac{\beta}{M}E_{\mathbf{k}}\right)^M - \left(1+\frac{\beta}{M}E_{\mathbf{k}}\right)^M} \left(1 - \frac{\beta}{M}(\epsilon_{\mathbf{k}}-\mu)\right) \right.$$

$$\left. - \frac{M}{\beta E_{\mathbf{k}}} \frac{\left(1-\frac{\beta}{M}E_{\mathbf{k}}\right)^{M-1} + \left(1+\frac{\beta}{M}E_{\mathbf{k}}\right)^{M-1} + 2}{\left(1-\frac{\beta}{M}E_{\mathbf{k}}\right)^M - \left(1+\frac{\beta}{M}E_{\mathbf{k}}\right)^M} \right] + \mathcal{O}\left(\frac{\beta}{M}\right)^2 \; ,$$

which after performing the limit $M \to \infty$ yields the expression

$$\langle n_{\mathbf{k}} \rangle = -\frac{1}{2} + \frac{\epsilon_{\mathbf{k}}+\mu}{2E_{\mathbf{k}}} \coth\left(\frac{\beta}{2}E_{\mathbf{k}}\right) \; . \tag{5.59}$$

This expression can be shown to be identical to the previous result (5.25).

The static structure factor is given by the forth-order expectation value (4.38), which we used for the ideal gas before. We replace ϕ_0 by the order parameter Φ_0 and for non-zero momenta we replace $\phi_{\mathbf{k}} \to \delta\phi_{\mathbf{k}}$. After splitting the fluctuations into real and imaginary part and applying Wick's theorem for real variables, we get a similar result to (4.37). The difference to the ideals gas is, that the anomalous expectation values $\langle\phi^*_{\mathbf{k}}\phi^*_{-\mathbf{k}}\rangle$ and $\langle\phi_{\mathbf{k}}\phi_{-\mathbf{k}}\rangle$ also give a contribution here (for simplicity we have dropped the time variable). The contribution of the anomalous expectation values after splitting it into its real and imaginary part is

$$\left\langle\delta\phi^*_{\mathbf{q}}\delta\phi^*_{-\mathbf{q}}\right\rangle + \langle\delta\phi_{\mathbf{q}}\delta\phi_{-\mathbf{q}}\rangle = 2\left(\left\langle(\delta\phi'_{\mathbf{k}})^2\right\rangle - \left\langle(\delta\phi''_{\mathbf{k}})^2\right\rangle\right) \ ,$$

such that the static structure factor is given as

$$S(\mathbf{q}) = 1 + 2\frac{N_0}{N_{\text{tot}}}\langle n_{\mathbf{q}}\rangle + \frac{N_0}{N_{\text{tot}}}\left(\langle\delta\phi^*_{\mathbf{q}}\delta\phi^*_{-\mathbf{q}}\rangle + \langle\delta\phi_{\mathbf{q}}\delta\phi_{-\mathbf{q}}\rangle\right) + \sum_{\mathbf{k}\neq\{0,-\mathbf{q}\}}\langle n_{\mathbf{k}}\rangle\langle n_{\mathbf{k}+\mathbf{q}}\rangle =$$

$$1 + 4\frac{N_0}{N_{\text{tot}}}\left\langle(\delta\phi'_{\mathbf{k}})^2\right\rangle + \sum_{\mathbf{k}\neq\{0,-\mathbf{q}\}}\langle n_{\mathbf{q}}\rangle\langle n_{\mathbf{k}+\mathbf{q}}\rangle \ . \tag{5.60}$$

With the help of eq. (5.58) we find, after performing the limit $M \to \infty$ in the same way as above:

$$\left\langle(\delta\phi'_{\mathbf{q}})^2\right\rangle = \lim_{M\to\infty}\frac{1}{2}[\hat{A}^{(\mathbf{k})}]^{-1}_{11} = -\frac{1}{4} + \frac{1}{4}\frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\coth\left(\frac{\beta}{2}E_{\mathbf{k}}\right) \ . \tag{5.61}$$

If we neglect the last term in eq. (5.60) which is quadratic in the momentum distribution, this expression reduces to

$$S(\mathbf{q}) = \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\coth\left(\frac{\beta}{2}E_{\mathbf{k}}\right) \ , \tag{5.62}$$

which agrees with the former result (5.29), if we assume that $N_0/N_{\text{tot}} \approx 1$. In the following chapters the same procedure like here will be used to calculate physical quantities for hard-core Bose systems by means of expectation values, like densities and the static structure factor. We have seen that for an interacting Bose gas, these quantities can be found on the level of a saddle-point integration with Gaussian approximation. At least this method is powerful enough to find the same results as the standard Bogoliubov approximation.

6 Hard-core Bose gas in one dimension

6.1 General remarks

This chapter shall be devoted to the special case of a one-dimensional interacting Bose gas. The remarkable feature of this problem is its exact integrability. Lieb and Liniger showed, that this is even the case for a homogeneous Bose gas given by the one-dimensional equivalent of the general Hamiltonian (2.5) with an arbitrary interaction constant g [50]. However, in the first place we are interested in the hard-core interaction, which is related to the large g limit. In this case, the first full solution for a homogeneous system was given by Girardeau, and a system of this type is called a Tonks-Girardeau gas [51]. The limit of weak interaction is the Gross-Pitaevskii limit.

The main feature of the one-dimensional hard-core Bose gas is, that the particles cannot penetrate each other, i.e. they cannot interchange their position. An interesting consequence of this property is the equivalence to an ideal non-interacting one-dimensional Fermi gas. This can be understood when one considers that the difference between bosons and fermions is, that the wave function of bosons is symmetric under particle exchange, while it is antisymmetric for fermions. Because particle exchange is prohibited in the Tonks-Girardeau gas because of the hard-core interaction, and for fermions because of the Pauli principle, the symmetry of their wave function does not matter, therefore they are equivalent. However, it is important to mention, that this equivalence does not hold for all physical quantities in momentum space, namely those which are given by one-particle (more precisely: "odd-particle") correlation functions like the momentum-distribution [52, 53, 54, 55, 56]. The reason is that the different symmetry of the wave functions for bosons and fermions matter, if the Fourier transformation to k-space is performed. On the other hand, quantities given by two-particle ("even-particle") correlation functions like the density-density correlation function and the dynamic structure factor are the same for hard-core bosons and for ideal fermions.

The properties of a hard-core Bose gas in a one-dimensional optical lattice are not much different from those mentioned above for the homogeneous system. It is given by the one-dimensional equivalent of the hard-core Bose Hamiltonian (2.49) in terms of hard-core operators and is equivalent to the spin one-half Heisenberg model as mentioned in section 2.6. The exact mapping to fermions is done by a Jordan-Wigner transformation

[9, 39]:

$$\hat{a}_r^+ = \hat{c}_r^+ \prod_{r'=-\infty}^{\infty} e^{-\mathrm{i}\pi \hat{c}_{r'}^+ \hat{c}_{r'}} \ , \quad \hat{a}_r = \prod_{r'=-\infty}^{\infty} e^{-\mathrm{i}\pi \hat{c}_r^+ \hat{c}_r} \hat{c}_r \ , \tag{6.1}$$

where r denotes the lattice site by an integer number, so that the position of the lattice site in the direction of the lattice is ar, where a is the lattice constant. Further, $\hat{a}^+$ and $\hat{a}$ are the hard-core boson operators, $\hat{c}^+$ and $\hat{c}$ are fermionic operators. This approach has been used in a couple of works to calculate the momentum distribution of particles [34, 57, 58]. However, the calculation of the momentum distribution function shall not be discussed in this chapter, so this problem will not be addressed here.

The zero temperature phase diagram of a hard-core Bose gas in a one-dimensional optical lattice shows three phases: An empty phase (EP), an incommensurate phase (ICP) with a particle number per lattice site of $0 < n_{\mathrm{tot}} < 1$, and a Mott insulator (MI) with $n_{\mathrm{tot}} = 1$. A model with an infinite number of MI phases for arbitrary rational filling factors has been proposed in [59]. In a real one-dimensional optical lattice, the ICP phase is a BEC, because the Bose gas has a non-zero extension in all three spacial directions, as illustrated in fig. 2.1. However, if the extension in the two other directions could be suppressed completely, the BEC phase would break down completely, because it does not exist in one and two spacial dimensions due to the Mermin-Wagner theorem. Here we will especially be interested in the phase transition between the ICP and the MI phase [60]. Again, the quantity we chose for investigating this transition is the static structure factor which contains the information about the density fluctuations. It has also been considered in other works about one-dimensional Bose gases, in the weakly interacting regime as well as in the strongly interacting regime [30, 31, 61, 62].

In this chapter, we will use a functional integral approach to this problem. As has been demonstrated for the ideal Bose gas, a random walk expansion leads to a world-line picture. To make the mapping to a system of ideal fermions possible, it has to be assured that world-lines cannot intersect each other. So instead of constructing the functional integral by starting from the Hamiltonian, we choose a different way and construct it by starting out from the random-walk picture directly. For this purpose we adopt an approach to the statistics of directed polymers in two dimensions [63].

6.2 World-line model

When the random walk expansion for a system of ideal spinless fermions is performed, one obtains a sum which is analogous to the sum in eq. (4.45) with two important differences: Because of the nilpotent property of the Grassmann variables, the fermionic analog to eq. 4.44 reads

$$\int \bar{\psi}^m \psi^{m'} \, e^{-\bar{\psi}\psi} \, \mathrm{d}\psi \mathrm{d}\bar{\psi} = j! \, \delta_{m0} \delta_{m'0} \ . \tag{6.2}$$

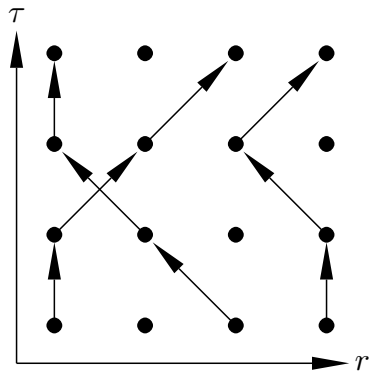

Figure 6.1: World-lines of spinless fermions can intersect each other, if the lattice has a square form.

This means, that all terms, where the particle number $m_{\mathrm{r},n} = m'_{\mathrm{r},n}$ is larger than 1 at lattice site r, do not contribute. This reflects the Pauli principle or in the case of hard-core bosons, the hard-core property. The second, more problematic difference to ideal bosons, is that the Grassmann variable analogue to eq. (4.43) gets an additional sign because of the anti-commutation property. In a one-dimensional system, this sign depends on the number of intersections between world-lines. These intersections must be excluded for a bosonic system, because all terms contributing to the grand canonical partition function from the random walk expansion should be positive. The problem is that if we start from a spinless fermionic Hamiltonian describing a homogeneous system, like

$$\hat{H} = \sum_{r,r'} \hat{\epsilon}_{rr'} \hat{c}_r^+ \hat{c}_{r'} \tag{6.3}$$

with fermionic operators and the matrix $\hat{\epsilon}_{rr'}$ given by the hopping matrix as defined in eq. 4.41, and perform the equivalent random walk expansion as in section 4.5, we get diagrams where intersections are still possible because of the square form of the lattice (see fig. 6.1).

To avoid this problem it is possible to construct a world-line model which consists of two sublattices as depicted in fig. 6.2 *(a)* and *(b)*. Each sublattice is by itself a square-lattice, illustrated by black and white dots respectively. Each site of both sublattices belongs to one point (r, τ) in space-time, where the imaginary time τ is again split into M discrete equidistant time steps. Because we work effectively with fermions, we impose anti-periodic boundary conditions in time. In the figure, the two sites of each sublattice belonging to the same point in space-time are surrounded by a dashed oval-shaped closed line. In the resulting chequered lattice structure bosons can propagate to the site vertically above them, which belongs to the same sublattice (black to black, white to white), or they can propagate diagonally to the next site above them, which belongs to the other lattice (black to white, white to black). In picture *(a)* we can see, that this structure excludes the possibility of intersecting world lines, so exact mapping

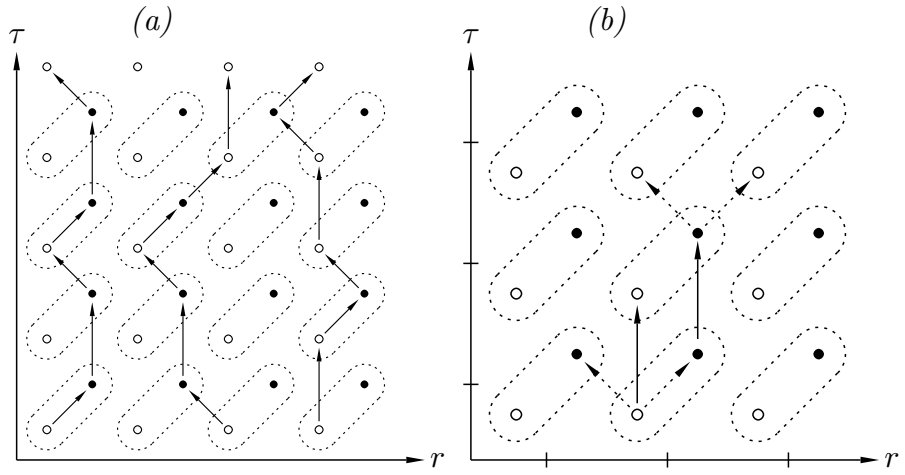

Figure 6.2: World-line model for hard-core bosons. Intersections of world-lines are prohibited by the sublattice structure, therefore an exact mapping to ideal fermions is possible.

to ideal fermions is possible. We assign unit weight to a step in the vertical direction, and a weight $J\beta/2M$ to a step along the diagonals of the lattice which represents a hopping event (the factor $1/2$ is necessary because of the two sublattices). The weight of an empty site is connected to the chemical potential and chosen to be $1 - \mu\beta/M$.

With these weights assigned to each element of a world-line diagram, it is possible to construct an inverse Green's function $\hat{G}^{-1}_{rr',nm}$. In contrary to the matrix $\hat{A}_{rr';nm}$ used in the functional integral (4.39) for an ideal Bose gas, the matrix $\hat{G}^{-1}$ has an additional 2×2 structure reflecting the two sublattices. All possible contributions to the Green's function are depicted in picture *(b)*:

- Propagation in the vertical direction from a black to a black and a white to a white site, respectively, with weight $\delta_{n,m+1}\delta_{r,r'}$,
- propagation from a white to a black site, to the left with weight $J\beta/2M\delta_{n,m}\delta_{r-1,r'}$ and to the right with weight $J\beta/2M\delta_{n,m}\delta_{r,r'}$,
- propagation from a black to a white site, to the left with weight $J\beta/2M\delta_{n,m+1}\delta_{r,r'}$ and to the right with weight $J\beta/2M\delta_{n,m+1}\delta_{r+1,r'}$,
- black and white sites with weight $-(1 - \mu\beta/M)\,\delta_{n,m}\delta_{r,r'}$.

Given these contributions, the matrix elements of the 2×2 structure of the inverse Green's function can be identified:

$$\hat{G}^{-1}_{rr';nm} = \begin{pmatrix} (-\delta_{n,m+1} + (1 - \frac{\beta}{M}\mu)\delta_{n,m})\delta_{r,r'} & -\frac{\beta}{M}\frac{J}{2}(\delta_{r,r'} + \delta_{r+1,r'})\delta_{n,m+1} \\ -\frac{\beta}{M}\frac{J}{2}(\delta_{r,r'} + \delta_{r-1,r'})\delta_{n,m} & (-\delta_{n,m+1} + (1 - \frac{\beta}{M}\mu)\delta_{n,m})\delta_{r,r'} \end{pmatrix} . \quad (6.4)$$

The grand canonical partition function is given by the functional integral

$$Z = \lim_{M\to\infty} \int \exp\left[-\sum_{r,r'} \sum_{n,m=1}^{M} \sum_{j,j'=1}^{2} \bar{\psi}_{r,n,j} \frac{[\hat{G}^{-1}_{rr';nm}]_{jj'}}{1-\frac{\beta}{M}\mu} \psi_{r',m,j'} \right] \prod_{r,n,j} \mathrm{d}\psi_{r,m,j}\, \mathrm{d}\bar{\psi}_{r,m,j} \quad (6.5)$$

with the sublattice index j, which can be performed and yields

$$Z = \lim_{M\to\infty} \left(1-\frac{\beta}{M}\mu\right)^{-2M\mathcal{N}} \det \hat{G}^{-1} \,, \quad (6.6)$$

where $\mathcal{N}$ is the number of lattice sites. The factor of $(1-\mu\beta/M)^{-1}$ in the exponent is necessary to cancel the main diagonal term to unity (note that the main diagonal elements of the matrix $\hat{A}^{(\mathbf{k})}$ given in eq. (4.15) are 1 as well).

6.3 Particle density and phase diagram

To calculate correlation functions, the Green's matrix has to be inverted. Fourier transformation of this matrix in the spacial coordinate is performed by the substitution

$$\delta_{r+1,r'} \to e^{\mathrm{i}k} \,, \quad \delta_{r-1,r'} \to e^{-\mathrm{i}k} \,.$$

Diagonalisation in the time structure is not possible with the unitary transformation given in (4.20) because the fermionic system requires anti-periodic boundary conditions $\hat{G}^{-1}_{nm} = -\hat{G}_{n,m+M}$. Instead, the correct transformation matrix is

$$\tilde{U}_{nm} = \frac{1}{\sqrt{M}}\, e^{\frac{2\pi\mathrm{i}}{M}\left(n-\frac{1}{2}\right)m} \,, \quad \tilde{U}^{+}_{nm} = \frac{1}{\sqrt{M}}\, e^{-\frac{2\pi\mathrm{i}}{M}\, n\left(m-\frac{1}{2}\right)} \,, \quad (6.7)$$

which leads to the diagonal form of the inverse Green's function:

$$(\tilde{U}\hat{G}^{-1}(k)\tilde{U}^{+})_{kn} = \delta_{kn} \begin{pmatrix} -e^{\frac{2\pi\mathrm{i}}{M}\left(n-\frac{1}{2}\right)} + 1 - \frac{\beta}{M}\mu & -\frac{\beta}{M}\frac{J}{2} e^{\frac{2\pi\mathrm{i}}{M}\left(n-\frac{1}{2}\right)}(1+e^{ik}) \\ -\frac{\beta}{M}\frac{J}{2}(1+e^{-ik}) & -e^{\frac{2\pi\mathrm{i}}{M}\left(n-\frac{1}{2}\right)} + 1 - \frac{\beta}{M}\mu \end{pmatrix} . \quad (6.8)$$

In analogy to eq. (4.19), the one-particle correlation function is given by the matrix elements of the Green's matrix $\hat{G}$. To describe particles, we need the diagonal matrix elements only. The 11-component and the 22-component are equal:

$$(\tilde{U}\hat{G}_{11/22}(k)\tilde{U}^{+})_{nm} = \frac{\delta_{nm}\left(-e^{\frac{2\pi\mathrm{i}}{M}\left(n-\frac{1}{2}\right)} + 1 - \frac{\beta}{M}\mu\right)}{\left(e^{\frac{2\pi\mathrm{i}}{M}\left(n-\frac{1}{2}\right)} - 1 + \frac{\beta}{M}\mu\right)^2 - e^{\frac{2\pi\mathrm{i}}{M}\left(n-\frac{1}{2}\right)}\left(\frac{\beta}{M}J\right)^2 \cos^2\frac{k}{2}} \,. \quad (6.9)$$

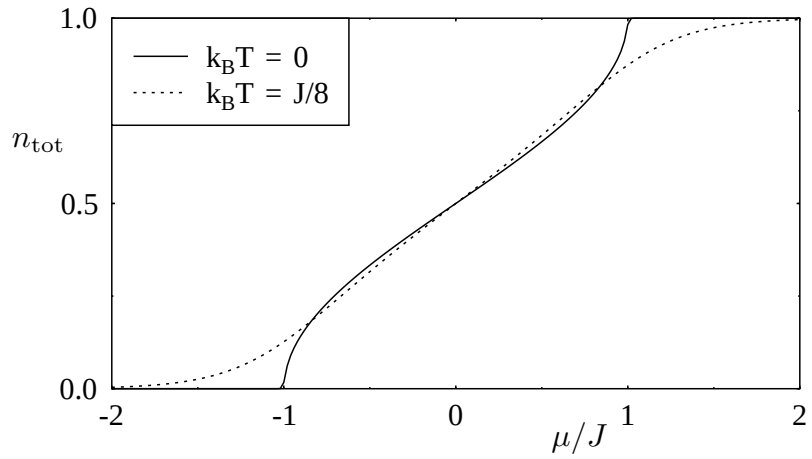

Figure 6.3: Total particle density of a hard-core Bose gas in a one-dimensional optical lattice calculated from eq. (6.15), for both zero temperature (solid line) and finite temperature (dashed line).

Since we are interested in the diagonal elements in the time structure, we get the one-particle correlation function of the fermions at equal times by taking the sum over indices of the time structure:

$$C(k) = \lim_{M\to\infty} \sum_{n,m=1}^{M} \frac{1}{M} \left(\tilde{U}\hat{G}_{11}(k)\tilde{U}^{+}\right)_{nm} \tag{6.10}$$

$$= \lim_{M\to\infty} \sum_{l=1}^{M} \frac{1}{M} \frac{\left[-e^{\frac{2\pi \mathrm{i}}{M}l} + e^{\frac{\pi \mathrm{i}}{M}}\left(1-\frac{\beta}{M}\mu\right)\right] e^{\frac{\pi i}{M}}}{\left(e^{\frac{2\pi \mathrm{i}}{M}l} - e^{\frac{\pi \mathrm{i}}{M}}\left(1-\frac{\beta}{M}\mu\right)\right)^2 - e^{\frac{2\pi \mathrm{i}}{M}l} e^{\frac{\pi \mathrm{i}}{M}} \left(\frac{\beta}{M}J\right)^2 \cos^2\frac{k}{2}} \,. \tag{6.11}$$

This sum is performed in Appendix A.2 d). After performing the limit $M \to \infty$, the result is

$$C(k) = \frac{1}{2}\left(\frac{1}{1+e^{-\beta\left(J\cos\frac{k}{2}-\mu\right)}} + \frac{1}{1+e^{-\beta\left(-J\cos\frac{k}{2}-\mu\right)}}\right) \,. \tag{6.12}$$

In the zero temperature limit we find

$$\lim_{\beta\to\infty} C(k) = \begin{cases} 1 & \text{if} \quad \mu < -\left|J\cos\frac{k}{2}\right| \\ \frac{1}{2} & \text{if} \quad -\left|J\cos\frac{k}{2}\right| < \mu < \left|J\cos\frac{k}{2}\right| \\ 0 & \text{if} \quad \mu > \left|J\cos\frac{k}{2}\right| \end{cases} \,. \tag{6.13}$$

As was mentioned before, the one-particle correlation function of the fermions in momentum space does not lead to the correct momentum distribution of the hard-core bosons, like it is possible for ideal bosons by means of eq. (4.24). However, the total

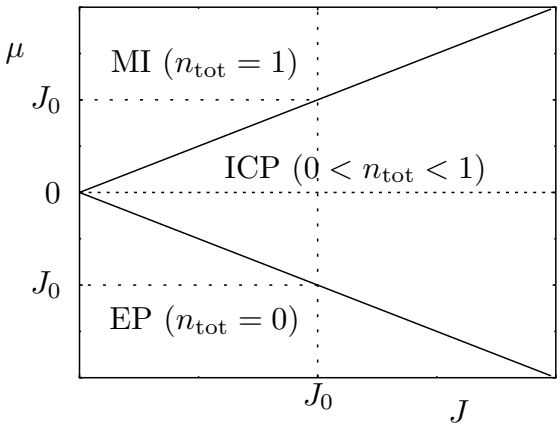

Figure 6.4: Phase diagram of the one-dimensional hard-core Bose gas at zero temperature with an empty phase (EP), an incommensurate phase (ICP), and a Mott insulator (MI).

particle density of the bosons is given by taking the fermionic one-particle correlation function in real space

$$C(r, r') = \int_0^{2\pi} C(k)\, e^{\mathrm{i}k(r-r')}\, \frac{\mathrm{d}k}{2\pi}\,, \tag{6.14}$$

at $r = r'$. This can be shown by applying the expression (3.20) of the total particle number to the partition function (6.5). We need an additional factor of 1/2 because of the two sublattices, which would otherwise count the particles twice:

$$N_{\mathrm{tot}} = \frac{1}{2\beta}\frac{\partial}{\partial\mu}\log Z = \lim_{M\to\infty}\frac{1}{2\beta}\frac{\partial}{\partial\mu}\left[-2M\mathcal{N}\log\left(1-\frac{\beta}{M}\mu\right) - \log\det\hat{G}\right]$$

$$= \mathcal{N} - \frac{1}{2\beta Z}\lim_{M\to\infty}\frac{\beta}{M}\sum_{r,n,j}\langle\bar{\psi}_{r,t,j}\psi_{r,t,j}\rangle$$

So, because of $\langle\bar{\psi}_{r,n,1}\psi_{r,n,1}\rangle = \langle\bar{\psi}_{r,n,2}\psi_{r,n,2}\rangle = C(r,r)$, we find the result

$$n_{\mathrm{tot}} = \frac{N_{\mathrm{tot}}}{\mathcal{N}} = 1 - C(r,r) \tag{6.15}$$

for the total particle density. Note that the time slice ε, which was necessary for the definition of the total particle density for conventional (non-hard-core) bosons, see eq. (3.21), is absent here, because of the construction of the Green's matrix. The zero temperature result is

$$\lim_{\beta\to\infty} n_{\mathrm{tot}} = \begin{cases} 0 & \text{if } \mu < -J \\ 1 - \frac{1}{\pi}\arccos\left(\frac{\mu}{J}\right) & \text{if } -J < \mu < J \\ 1 & \text{if } \mu < J \end{cases}\,. \tag{6.16}$$

Graphs for zero temperature and finite temperature are plotted in fig. 6.3. Both graphs are symmetric to the point $\mu/J = 0$, $n_{\text{tot}} = 1/2$. This reflects the particle hole symmetry of the system: Because of the Pauli principle a given configuration of the system is symmetric to the configuration, in which each occupied site is empty and vice versa. Further one can see that the system is empty ($n_{\text{tot}} = 0$) if $\mu/J < -1$, and it is a Mott-insulator ($n_{\text{tot}} = 1$) if $\mu/J > 1$. The phase transitions between the EP and the incommensurate phase with $0 < n_{\text{tot}} < 1$, and between the ICP and the MI, are abrupt with a diverging slope of the curve at the transition points. At non-zero temperatures the sharp phase transition is smeared out. The zero temperature phase diagram is depicted schematically in fig. 6.4.

6.4 Density correlations and static structure factor

As defined in eq. (3.26), the density-density correlation function $D(r - r')$ is the expectation value of the product of the local density operators at the points r and r'. Translated into an expectation value with respect to the Grassmann variables, we have to take into account, that the Grassmann field is associated to holes instead of particles, because according to eq. (6.15) the local density is given by

$$n_{\text{tot}} = 1 - \langle \bar{\psi}_{r,n,1} \psi_{r,n,1} \rangle \ .$$

We define the truncated density-density CF of the hard-core Bose gas with respect to holes as

$$D_{\text{trunc}}(r - r') = \left\langle \bar{\psi}_{r,n,1} \psi_{r,n,1} \bar{\psi}_{r',n,1} \psi_{r',n,1} \right\rangle - \underbrace{\left\langle \bar{\psi}_{r,n,1} \psi_{r,n,1} \right\rangle \left\langle \bar{\psi}_{r',n,1} \psi_{r',n,1} \right\rangle}_{= n_{\text{tot}}^2} \ . \tag{6.17}$$

In the following we will write $D(r - r')$ instead of $D_{\text{trunc}}(r - r')$ for simplicity. Using Wick's theorem for Grassmann variables given in eq. (B.5), we find

$$\left\langle \bar{\psi}_{r,n,1} \psi_{r,n,1} \bar{\psi}_{r',n,1} \psi_{r',n,1} \right\rangle = n_{\text{tot}}^2 - C(r, r') C(r', r) \ ,$$

leading to the result

$$D(r - r') = -C(r, r') C(r', r) \ . \tag{6.18}$$

The static structure factor is related to the density-density CF by means of a Fourier transformation which is shifted by unity, and a normalisation. We use the definition

$$S(q) = 1 + \frac{\sum_{r,r'} D(r - r') e^{\mathrm{i}q(r - r')}}{\sum_{r,r'} D(r - r')} \ . \tag{6.19}$$

The same definition has been used in ref. [60], and a similar one in ref. [31] except that there the normalisation is the total particle number. It is the analogue to the definition

of the static structure factor of an ideal Bose (4.38), where the term 1 appears when the time slice is canceled in the expectation value of the complex fields. Expressed in terms of the one-particle CF in momentum space $C(k)$ by applying the Fourier transformation in eq. (6.14), the above expression reads

$$S(q) = 1 + \frac{\int_0^{2\pi} C(k)C(k+q)}{\int_0^{2\pi} C(k)^2} \frac{\mathrm{d}k}{2\pi} \,. \tag{6.20}$$

We want to investigate the static structure factor at zero temperature in the ICP phase near the phase transitions to the EP and the MI. Beacuse of the particle-hole symmetry discussed in the previous section, both transitions should be symmetrical with respect to the physics of light scattering as well: Near the EP light is scattered by particles and near the MI it is scattered by holes. Let us first discuss the region $\mu > 0$, where light scattering is done by holes. Defining the *characteristic wave vector*

$$k^\star = 2 \arccos\left(\frac{|\mu|}{J}\right) \,, \tag{6.21}$$

we find from eq. (6.13) for the zero temperature one-particle CF

$$C(k) = \begin{cases} 0 & \text{if } k^\star < k < 2\pi - k^\star \\ \frac{1}{2} & \text{if } k < k^\star \text{ or } k > 2\pi - k^\star \end{cases} \,, \tag{6.22}$$

and thus

$$\begin{aligned} \int_0^{2\pi} C(k)C(k+q) \frac{\mathrm{d}k}{2\pi} &= \frac{1}{2} \int_0^{k^\star} C(k+q) \frac{\mathrm{d}k}{2\pi} + \frac{1}{2} \int_{2\pi-k^\star}^{2\pi} C(k+q) \frac{\mathrm{d}k}{2\pi} \\ &= \begin{cases} \frac{1}{4\pi}\left(k^\star - \frac{q}{2}\right) & \text{if } q < 2k^\star \\ 0 & \text{if } 2k^\star < q < 2\pi - 2k^\star \\ \frac{1}{4\pi}\left(k^\star - \frac{2\pi - q}{2}\right) & \text{if } q > 2\pi - 2k^\star \end{cases} \,. \end{aligned} \tag{6.23}$$

The normalisation in eq. (6.20) is given by the above expression for $q = 0$:

$$\int_0^{2\pi} C(k)^2 \frac{\mathrm{d}k}{2\pi} = \frac{k^\star}{4\pi} \,. \tag{6.24}$$

We find the result

$$S(q) = \begin{cases} \frac{q}{2k^\star} & \text{if } q < 2k^\star \\ 1 & \text{if } 2k^\star < q < 2\pi - 2k^\star \\ \frac{2\pi - q}{2k^\star} & \text{if } q > 2\pi - 2k^\star \end{cases} \,. \tag{6.25}$$

In order to keep the particle hole symmetry for the static structure factor, in the region $\mu < 0$ we do the substitution $C(k) \to 1 - C(k)$ in the expression (6.20), and find the

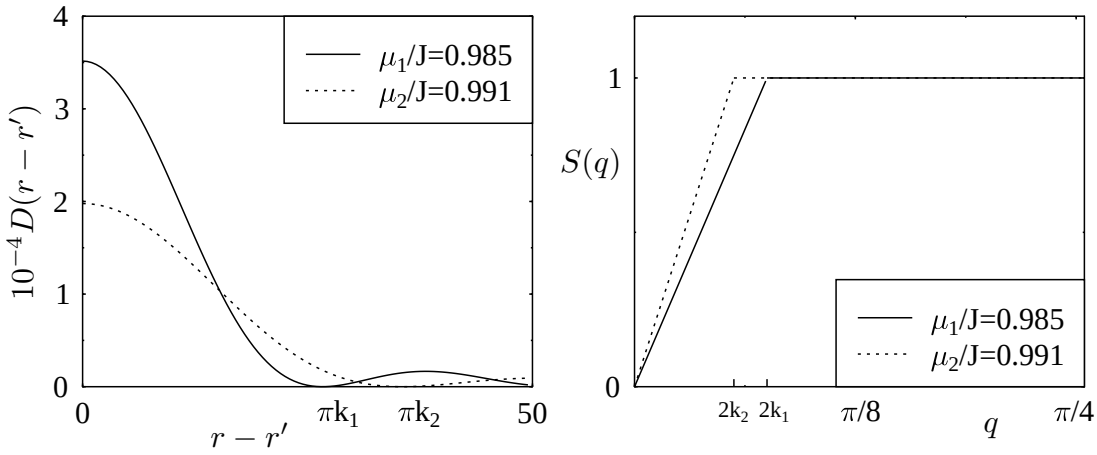

Figure 6.5: Truncated density-density correlation function $D(r-r')$ and static structure factor $S(q)$ in the vicinity of the ICP-MI phase transition. The transition point is at $\mu_c = J$. For the ICP-EP phase transition, the situation is symmetrical.

same result as in eq. (6.25). The expression for the density-density CF $D(r-r')$ near both phase transitions, we get from the eqs. (6.14), (6.18), and (6.22):

$$D(r-r') = \left(\frac{\sin(k^\star(r-r')}{2\pi(r-r'))}\right)^2 . \tag{6.26}$$

The characteristic wave vector can be written in terms of the total particle density (6.15):

$$k^\star = \begin{cases} 2\pi n_{\mathrm{tot}} & \text{if } n_{\mathrm{tot}} < 1/2 \\ 2\pi(1-n_{\mathrm{tot}}) & \text{if } n_{\mathrm{tot}} > 1/2 \end{cases} . \tag{6.27}$$

Near the phase transitions where $\delta := |\mu - \mu_c|/J \ll 1$, we have $\mu = (1-\delta)J$ at the ICP-MI phase transition, and $\mu = -(1-\delta)J$ at the ICP-EP transition. Here, we can approximate

$$k^\star \approx \sqrt{8\delta} . \tag{6.28}$$

For a homogeneous impenetrable Bose gas the role of $k^\star$ is played by the Fermi wave vector $k_{\mathrm{F}} = \pi n_{\mathrm{tot}}$ [31]. In our result (6.27), $k^\star$ depends linearly on the density as well in the region $n_{\mathrm{tot}} < 1/2$, but the discontinuous slope of the function $k^\star(n_{\mathrm{tot}})$ at the point $n_{\mathrm{tot}} = 1/2$ is a consequence of the optical lattice potential. The Feynman relation (2.37) allows us to identify the excitation spectrum

$$\epsilon(q) = \hbar c q + \mathcal{O}(q^2) , \quad c = \frac{\hbar k^\star}{m} . \tag{6.29}$$

which is linear for small values of q, where c is the sound velocity. The density-density CF and the static structure factor near the ICP-MI phase transition are plotted in fig. 6.5.

The density-density CF shows characteristic oscillations with length $\lambda = \pi/k^\star$. This length scale diverges at the ICP-EP and ICP-MI phase transition with $1/n_{\mathrm{tot}}$ and $1/(1-n_{\mathrm{tot}})$ respectively. Thus it can be used as a measure for the distance of the system to one of the two phase transitions. In the EP and the MI phase, the density-density CF vanishes because of the absence of particle number fluctuations, and the static structure factor saturates to $S(q) \equiv 1$.

6.5 External trap potential

In the previous sections a system in a translational invariant lattice was considered. In real experiments about one-dimensional Bose gases in optical lattices as explained in section 2.6, the particles are contained in an external trap potential. As usually, we assume a harmonic trap potential

$$V_r := V(ar) = \frac{m}{2}\omega_{\mathrm{ho}}^2 (ar)^2 \,, \tag{6.30}$$

where again a is the lattice constant, r an integer number denoting the lattice site, and ω_{ho} the harmonic oscillator frequency of the trap. In order to include the external potential into our model which is defined by the grand canonical partition function given by the functional integral (6.5) for , it is possible to define a space-dependent chemical potential

$$\mu_r = \mu - V_r \tag{6.31}$$

and perform the substitution $\mu \to \mu_r$ in the Green's matrix (6.4). The problem is that this matrix cannot be inverted simply by a Fourier transformation, so it has to be inverted numerically. This was done in ref. [60] to calculate the zero temperature results for the local density, the density correlations and the static structure factor and to compare them to the translational invariant case. The methods which were used in this work and the results which were found will be discussed in the following.

Like in ref. [63], the discrete time approximation was used, which means that the distance between two discrete time steps $\hbar\beta/M$ in the Green's function (6.4) was kept constant, while the zero temperature limit is performed by $M \to \infty$. Then the quantity $Mk_{\mathrm{B}}T$ can be used as the unit of energy and can be set to 1. This means that we make the replacements $\beta J/M \to J$ and $\beta\mu/M \to \mu$ such that J and μ are dimensionless[1]. This approximation can affect the result of physical quantities, but it is sufficient to describe the main qualitative physical effects like phase transitions and critical behaviour, as far as J and μ are small compared to 1. The inverse Green's function is Fourier transformed

[1] Another possibility would be to consider β/M as an additional free parameter

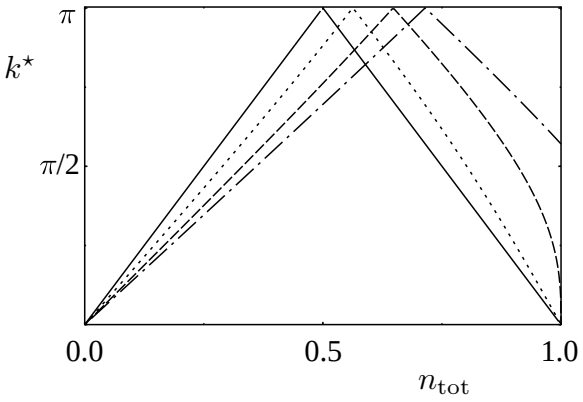

Figure 6.6: Characteristic wave vector in discrete time approximation as a function of the total particle density in the translational invariant case. Curves are plotted for different values of the tunneling rate: $J \to 0$ (solid), $J = 0.4$ (dotted), $J = 1.0$ (dashed), $J = 1.6$ (dashed-dotted; the MI phase is not reached here). The $J \to 0$ limit is equivalent to the $M \to \infty$ limit given in eq. (6.27).

with respect to the time structure by introducing a dimensionless "frequency" ω with $0 \leq \omega < 2\pi$:

$$\begin{aligned} \hat{G}^{-1}_{rr'}(\omega) &:= \sum_{m=1}^{\infty} \hat{G}^{-1}_{rr';nm}\, e^{\mathrm{i}\omega(n-m)} \\ &= \begin{pmatrix} (-e^{\mathrm{i}\omega} + (1-\mu_r)\delta_{n,m})\delta_{r,r'} & -\frac{J}{2}(\delta_{r,r'} + \delta_{r+1,r'})e^{\mathrm{i}\omega} \\ -\frac{J}{2}(\delta_{r,r'} + \delta_{r-1,r'}) & (-e^{\mathrm{i}\omega} + (1-\mu_r))\delta_{r,r'} \end{pmatrix} . \end{aligned} \tag{6.32}$$

This matrix was inverted numerically with respect to the 2×2 sublattice structure and the structure of the spacial indices r, r'. The 11- (or the identical 22-) component of the sublattice structure of this inverted matrix we denote by $G_{rr'}(\omega)$. From this the fermionic one-particle correlation function at equal times is obtained by integration with respect to ω:

$$C(r, r') = \int_0^{2\pi} G_{rr'}(\omega)\, \frac{\mathrm{d}\omega}{2\pi} . \tag{6.33}$$

Within this approach, the local density was calculated by means of the expression

$$n_r = 1 - (1 - \mu_r) C(r, r) . \tag{6.34}$$

In the translational invariant system we find the solution [63]

$$n_{\mathrm{tot}} = 1 - \frac{1}{2\pi}\left[\tilde{k} \mp (k^* - \pi)\right] , \tag{6.35}$$

where $\pm$ corresponds to the cases $\mu > 0$ and $\mu < 0$, respectively, $k^\star$ is given by eq. (6.21), and

$$\tilde{k} = \arccos\left(1 - \frac{(2-\mu)^2}{2\left(1 - \mu + \left(\frac{J}{2}\right)^2\right)}\right) . \tag{6.36}$$

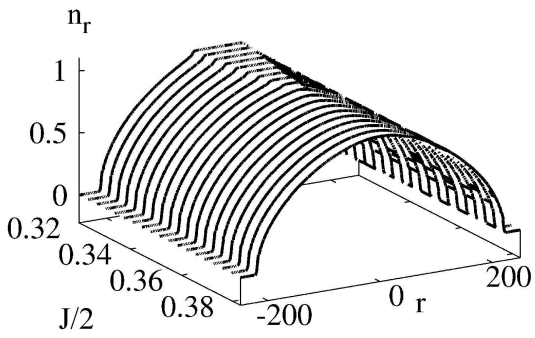

Figure 6.7: Local particle density for system in harmonic trap potential ($\mu = 0.7$, $ma^2\omega_{\rm ho}^2/2 = 3 \times 10^{-5}$) in discrete time approximation with varying tunneling rate J. A Mott plateau appears in the center of the trap (r=0) as J is decreased below a critical value $J_{\rm P} \approx 0.70$. (Fig. taken from ref. [60].)

While the phase diagram of the discrete time approximation is the same as the one plotted in fig. 6.4, the result for $k^\star$ as a function of the total particle density depends on J, as shown in the plots in fig. 6.6. The larger J, the stronger is the deviation from the $J \to 0$ limit. For $J > 1$ the MI phase is not reached any more. If we resubstitute $\mu \to \mu\beta/M$ and $J \to J\beta/M$ in eqs. (6.35) and (6.36), and perform the limit $M \to \infty$, we find $\tilde{k} \to \pi$ and obtain the result (6.27). The numerical solution for the trapped system is plotted in fig. 6.7, where the formation of a Mott plateau can be seen below a critical value $J_{\rm P}$. We find that $J_{\rm P}$ is close to the transition point of the translational invariant system $J_{\rm c}$. A similar behavior was found for the one-dimensional Bose-Hubbard model with a harmonic trapping potential [64]. The truncated density-density CF was calculated by

$$D(r - r') = (1 - \mu_r)(1 - \mu_{r'})C(r, r')C(r', r) - (1 - \mu_r)C(r, r)\delta_{rr'} \,, \tag{6.37}$$

and the static structure factor by

$$S(q) = 1 - \frac{\sum_r \left(D(r) + n_0\delta_{r0}\right) e^{-{\rm i}kr}}{\sum_r \left(D(r) + n_0\delta_{r0}\right)} \,. \tag{6.38}$$

Numerical results for a trapped system are shown in fig. 6.8. The results from the homogeneous system with the same parameters are plotted for reference. The parameters were chosen to be close to the ICP-MI phase transition.

In conclusion, we find that the properties of the density-density CF and the static structure factor of the trapped system are qualitatively the same as in the translational invariant case. $D(r)$ vanishes when $J_{\rm P}$ is reached, owing to the fact that there are no density fluctuations within the plateau. The characteristic length scales become larger as the Mott plateau is reached. Close to $J_{\rm P}$ the correlations of the density fluctuations are suppressed around the center of the trap leading to a local minimum of $D(r)$ at $r = 0$. This is accompanied by an increase of the slope of $S(q)$.

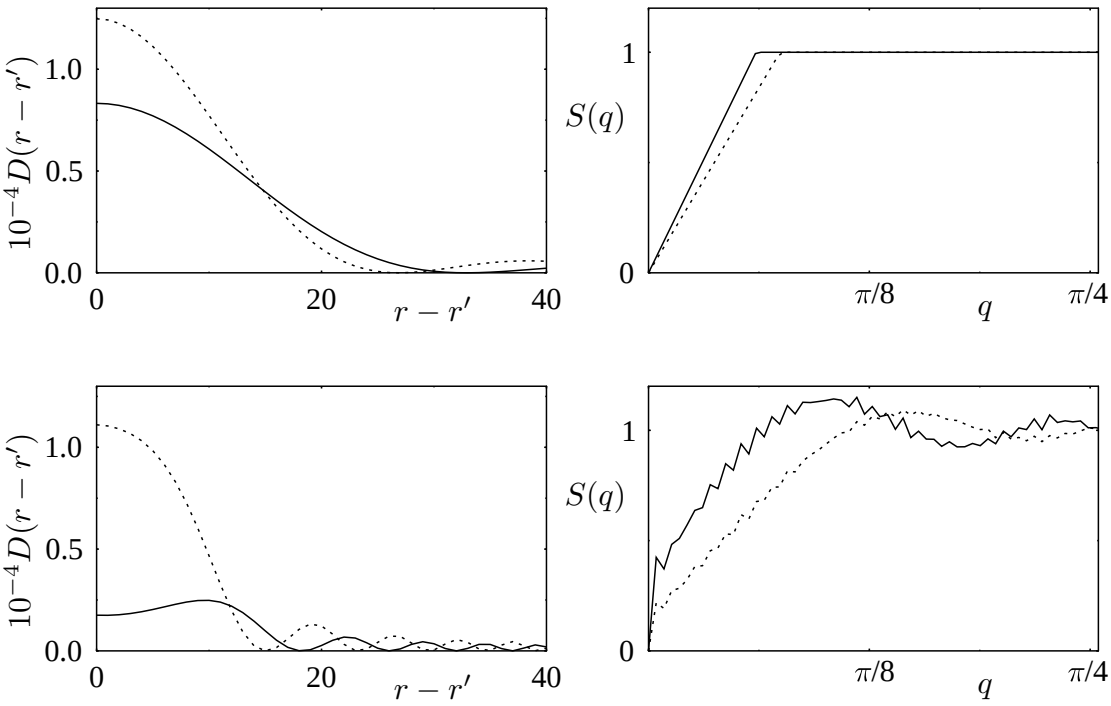

Figure 6.8: Density-density correlation function and static structure factor near the ICP-MI phase transition in discrete-time approximation ($\beta/M \equiv 1$) for different tunneling rates J. First row: Translational invariant system ($\mu = 0.7$). Second row: Harmonic trap potential ($\mu = 0.7$, $ma^2\omega_{\mathrm{ho}}^2/2 = 3 \times 10^{-5}$). Tunneling rates: $J_1 = 0.7012$ (solid lines) and $J_2 = 0.7008$ (dashed lines). The transition point of the translational invariant system is at $J_{\mathrm{c}} = 0.7000$. (Data taken from ref. [60]).

7 Hard-core Bose model in more than one dimension

7.1 Nilpotent algebra

In two and three dimensions, an exact mapping of the hard-core Bose model to ideal fermions is not possible. However, it is possible to construct a functional integral representation for hard-core bosons by means of Grassmann variables which can be viewed as a system of *interacting* fermions. In this chapter, we want to apply this approach to investigate the physics of a hard-core Bose gas in two- and three-dimensional lattices. Like in the previous chapter on one-dimensional lattice, the main interest lies on the zero temperature phase diagram and the static structure factor.

In this section we will construct the functional integral of the hard-core Bose model by introducing an algebra of nilpotent fields which are composed by a product of two Grassmann fields [44, 65, 66]. The validity of the hard-core property which excludes multiple occupation of lattice sites we explain within the world-line picture.

Like the complex field ϕ in the functional integral of the ideal Bose gas, the nilpotent field variables shall depend on the lattice site $\mathbf{r}$ and the discrete-time index n. We introduce two fields of pairs of conjugate Grassmann variables $\psi^1_{\mathbf{r},n}, \bar{\psi}^1_{\mathbf{r},n}$ and $\psi^2_{\mathbf{r},n}, \bar{\psi}^2_{\mathbf{r},n}$ and define the nilpotent field variables as a product of two Grassmann variables:

$$\bar{\eta}_{\mathbf{r},n} := \bar{\psi}^1_{\mathbf{r},n}\bar{\psi}^2_{\mathbf{r},n} \ , \quad \eta_{\mathbf{r},n} := \psi^2_{\mathbf{r},n}\psi^1_{\mathbf{r},n} \ . \tag{7.1}$$

Because of the anti-commutativity of the Grassmann variables, the variables of the field $\bar{\eta}$, η are commutative and nilpotent, reflecting the bosonic commutation property and the hard-core property of the particles, respectively:

$$\eta_{\mathbf{r},n}\eta_{\mathbf{r}',m} = \eta_{\mathbf{r}',m}\eta_{\mathbf{r},n} \ , \ \bar{\eta}_{\mathbf{r},n}\bar{\eta}_{\mathbf{r}',m} = \bar{\eta}_{\mathbf{r}',m}\bar{\eta}_{\mathbf{r},n} \ , \ \bar{\eta}_{\mathbf{r},n}\eta_{\mathbf{r}',m} = \eta_{\mathbf{r}',m}\bar{\eta}_{\mathbf{r},n} \ ,$$

$$(\eta_{\mathbf{r},n})^j = (\bar{\eta}_{\mathbf{r},n})^j = 0 \text{ for } j \geq 2 \ .$$

Integration of nilpotent field variables is defined as a Grassmann integral, see eqs. (3.8) and (3.9):

$$\int \bar{\eta}\eta \, \mathrm{d}\bar{\eta}\mathrm{d}\eta := \int \bar{\psi}^1\bar{\psi}^2\psi^2\psi^1 \, \mathrm{d}\psi^1\mathrm{d}\bar{\psi}^1\mathrm{d}\psi^2\mathrm{d}\bar{\psi}^2 = 1 \ ,$$

$$\int \bar{\eta} \, \mathrm{d}\bar{\eta}\mathrm{d}\eta = \int \eta \, \mathrm{d}\bar{\eta}\mathrm{d}\eta = 0 \ .$$

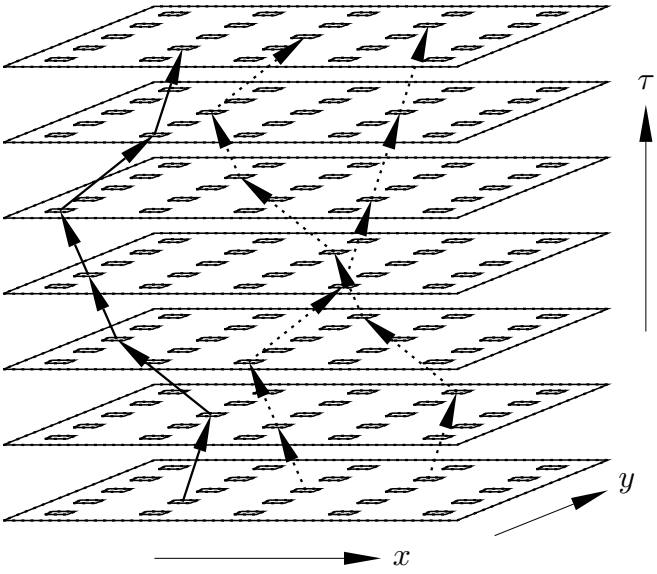

Figure 7.1: World-line diagram of a hard-core boson system in a two-dimensional lattice in the xy-plane. The lowest plane shall belong to the imaginary time $\tau = 0$ and the uppermost one to $\tau = \beta$. Because of the periodicity in imaginary time the full arrows form a world-line with periodicity 1 (winding number = 0) and the dashed arrows a world-line with periodicity 2 (winding number = 1).

With these definitions we can write down the grand canonical partition function of the hard-core Bose gas as

$$Z_{\mathrm{hc}} = \lim_{M\to\infty} \int \exp\left[-\sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m=1}^{M} \bar{\eta}_{\mathbf{r},n} \hat{A}^{\mathrm{hc}}_{\mathbf{r}\mathbf{r}';nm} \eta_{\mathbf{r}',m} \right] \prod_{\mathbf{r}} \prod_{n=1}^{M} \mathrm{d}\bar{\eta}_{\mathbf{r},n} \mathrm{d}\eta_{\mathbf{r},n} \,, \tag{7.2}$$

in analogy to the ideal system given by eq. (4.39). Here, we use the matrix

$$\hat{A}^{\mathrm{hc}}_{\mathbf{r}\mathbf{r}';nm} := -\delta_{nm}\delta_{\mathbf{r}\mathbf{r}'} - (\delta_{n,m+1} + \delta_{n1}\delta_{mM}) \left[\delta_{\mathbf{r}\mathbf{r}'} - \frac{\beta}{M} (\hat{J}_{\mathbf{r}\mathbf{r}'} - \mu\, \delta_{\mathbf{r}\mathbf{r}'}) \right] \,, \tag{7.3}$$

which differs from the matrix $\hat{A}_{\mathbf{r}\mathbf{r}';nm}$ given in eq. (4.42) only by the minus sign in front of the diagonal term $\delta_{nm}\delta_{\mathbf{r}\mathbf{r}'}$. Further we have used the hopping matrix $\hat{J}_{\mathbf{r}\mathbf{r}'}$ instead the shifted matrix $\hat{\epsilon}_{\mathbf{r}\mathbf{r}'}$ given in eq. (4.41) here, and included the diagonal term into the chemical potential by performing the shift $\mu \to \mu - J$, which doesn't have and physical consequence. Note that the functional integral (7.2) is of second order in the nilpotent field and thus of forth order in the Grassmann fields, which makes an exact solution impossible in general.

In order to demonstrate that this Grassmann integral really gives the grand canonical partition function of a hard-core Bose gas, one can perform a random walk expansion in the same way as it was done in section 4.5 for ideal bosons. It turns out that the only difference is, that in the hard-core case we have

$$\int \bar{\eta}^m \eta^{m'} e^{\bar{\eta}\eta} \mathrm{d}\bar{\eta}\mathrm{d}\eta = \begin{cases} 1 & \text{if } m = m' = 0 \text{ or } m = m' = 1 \\ 0 & \text{else} \end{cases}$$

instead of the complex-variable Gaussian integral (4.44). Therefore the result of the random walk expansion differs from the ideal gas result (4.45) only in the way that the number of particles $m_{\mathbf{r},n}$ at lattice site $\mathbf{r}$ to the time $n\beta/M$ is restricted to 0 or 1. All diagrams where two or more world-lines meet at the same point in space-time fall out. This is exactly the requirement of the hard-core condition. As an example for a world-line diagram of a system in a two-dimensional lattice see fig. 7.1. The picture illustrates that every world-line has a winding number [66], which counts the number of periods in imaginary time until it reaches its starting point again. The existence of odd winding numbers indicates that it is possible for particles to exchange their position. It was argued in the previous chapter that the impossibility of particle exchange is the main condition for an exact mapping of the system to a system of ideal fermions. We have shown that it is possible to construct a model which prohibits particle exchange in a one-dimenional system such that the nilpotent field can just be replaced by a Grassmann field, but in two- and three-dimensional systems this is impossible.

Another way to find the expression (7.2) is to start from the hard-core Bose Hamiltonian (2.49) directly and to construct a coherent state functional integral of the nilpotent variables for the hard-core boson's creation and annihilation operators. This is demonstrated in Appendix C. Here, we proceeded "the other way round" by postulating the functional integral expression first and verifying it by means of a random walk expansion. It can be viewed as a fermionic functional integral as given in (3.10), with the Grassmannian action

$$A_{\mathrm{hc}}(\bar{\psi},\psi) = \sum_{n=1}^{M} \Bigg\{ \sum_{\mathbf{r}} \bar{\psi}^1_{\mathbf{r},n+1}\bar{\psi}^2_{\mathbf{r},n+1}(-\psi^2_{\mathbf{r},n+1}\psi^1_{\mathbf{r},n+1} - \psi^2_{\mathbf{r},n}\psi^1_{\mathbf{r},n})$$

$$- \frac{\beta\mu}{M}\sum_{\mathbf{r}} \bar{\psi}^1_{\mathbf{r},n+1}\bar{\psi}^2_{\mathbf{r},n+1}\psi^2_{\mathbf{r},n}\psi^1_{\mathbf{r},n} + \frac{\beta}{M}\sum_{\mathbf{r},\mathbf{r}'} \hat{J}_{\mathbf{r}\mathbf{r}'}\bar{\psi}^1_{\mathbf{r},n+1}\bar{\psi}^2_{\mathbf{r},n+1}\psi^2_{\mathbf{r}',n}\psi^1_{\mathbf{r}',n} \Bigg\} . \tag{7.4}$$

The boundary conditions in imaginary time are anti-periodic in the discrete-time index n for the Grassmann variables, but they are periodic for the nilpotent variables because of their commutativity.

7.2 Hubbard-Stratonovich decoupling

The idea of a Hubbard-Stratonovich transformation is to decouple a quartic interaction term of a many-body system by writing it in terms of a Gaussian integral [67]. The original field variables are then only of second order and can be integrated out such that the system is represented only by the field variables of the Gaussian integral. In the following we will present the decoupling of the system given by the action (7.4) of the nilpotent field variables [65].

As in the previous chapters, physical quantities we get from correlation functions. For bosons, they are given as expectation values of a complex field as explained in section 3.2, and for fermions and one-dimensional hard-core bosons they are expectation values of a Grassmann field. Consequently, for the hard-core Bose system described here they are expectation values of pairs of Grassmann variables, i.e. of the nilpotent variables defined in eq. (7.1). For this purpose it is advisable to introduce a **generating functional** with a generating real field $\xi^{\sigma}_{\mathbf{r},n}$ by

$$Z^{\mathrm{gen}}_{\mathrm{hc}}(\xi) = \int \exp\left[A^{\mathrm{gen}}_{\mathrm{hc}}(\bar{\psi},\psi,\xi)\right] \prod_{\mathbf{r}} \prod_{n=1}^{M} \mathrm{d}\bar{\eta}_{\mathbf{r},n}\mathrm{d}\eta_{\mathbf{r},n} \ , \tag{7.5}$$

with the generating action

$$A^{\mathrm{gen}}_{\mathrm{hc}}(\bar{\psi},\psi,\xi) = A(\bar{\psi},\psi) - \sum_{\mathbf{r}} \sum_{n=1}^{M} \left(\bar{\eta}_{\mathbf{r},n}\xi^{1}_{\mathbf{r},n} + \eta_{\mathbf{r},n}\xi^{2}_{\mathbf{r},n}\right) \ . \tag{7.6}$$

The grand canonical partition function is then given as $Z_{\mathrm{hc}} = Z^{\mathrm{gen}}_{\mathrm{hc}}(\xi \equiv 0)$. The general static n-particle CF can be defined in analogy to the definition (3.19) for a complex field, and with the help of the generating functional, is can be written as a derivative with respect to the field ξ:

$$\begin{aligned} C_n(\mathbf{r}_1,\ldots,\mathbf{r}_n;\mathbf{r}'_n,\ldots,\mathbf{r}'_1) &= \langle \bar{\eta}_{\mathbf{r}_1,0}\cdots\bar{\eta}_{\mathbf{r}_n,0}\eta_{\mathbf{r}'_n,0}\cdots\eta_{\mathbf{r}'_1,0}\rangle \\ &= \frac{1}{Z_{\mathrm{hc}}} \frac{\partial^{2n} Z^{\mathrm{gen}}_{\mathrm{hc}}}{\partial\xi^{1}_{\mathbf{r}_1,0}\ldots\partial\xi^{1}_{\mathbf{r}_n,0}\partial\xi^{2}_{\mathbf{r}'_n,0}\ldots\partial\xi^{2}_{\mathbf{r}'_1,0}}\bigg|_{\xi\equiv 0} \ . \end{aligned} \tag{7.7}$$

We will apply the Hubbard-Stratonovich transformation to the functional integral (7.5) by introducing two new complex fields φ and χ, and the Grassmann field will be integrated out. The resulting expression will contain the field ξ from which the CFs will be derived of. Usually there are more than one way of performing a Hubbard-Stratonovich decoupling. For the hard-core Bose model we choose to decouple the whole off-diagonal term. We write

$$\begin{aligned} \hat{v}^{\mathrm{hc}}_{\mathbf{r}\mathbf{r}';nm} &= -A^{\mathrm{hc}}_{\mathbf{r}\mathbf{r}';nm} - (1-s)\delta_{nm}\delta_{\mathbf{r}\mathbf{r}'} \\ &= (\delta_{n,m+1} + \delta_{n1}\delta_{mM}) \left[\delta_{\mathbf{r}\mathbf{r}'} - \frac{\beta}{M}(\hat{J}_{\mathbf{r}\mathbf{r}'} - \mu\,\delta_{\mathbf{r}\mathbf{r}'})\right] + s\,\delta_{nm}\delta_{\mathbf{r}\mathbf{r}'} \ , \end{aligned} \tag{7.8}$$

and insert the identity

$$\text{const.} \times \exp\left\{ \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m=1}^{M} \bar{\eta}_{\mathbf{r},n} (\hat{v}^{\text{hc}}_{\mathbf{r}\mathbf{r}';nm} - s\,\delta_{nm}\delta_{\mathbf{r}\mathbf{r}'}) \eta_{\mathbf{r}',m} \right\}$$

$$= \int \exp\left\{ -\sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m} \varphi^*_{\mathbf{r},n} (\hat{v}^{\text{hc}}_{\mathbf{r}\mathbf{r}';nm})^{-1} \varphi_{\mathbf{r}',m} - \frac{1}{s} \sum_{\mathbf{r},n} \chi^*_{\mathbf{r},n} \chi_{\mathbf{r},n} \right.$$

$$\left. + \sum_{\mathbf{r},n} \left[\eta_{\mathbf{r},n} (\varphi^*_{\mathbf{r},n} + \mathrm{i}\chi^*_{\mathbf{r},n}) + \bar{\eta}_{\mathbf{r},n} (\varphi_{\mathbf{r},n} + \mathrm{i}\chi_{\mathbf{r},n}) \right] \right\} \prod_{\mathbf{r},n} \frac{\mathrm{d}\varphi^*_{\mathbf{r},n} \mathrm{d}\varphi_{\mathbf{r},n} \mathrm{d}\chi^*_{\mathbf{r},n} \mathrm{d}\chi_{\mathbf{r},n}}{(2\pi\mathrm{i})^2} \,, \tag{7.9}$$

which can be checked easily by applying the relation (B.2). The constant is given by a determinant and is of no physical importance, therefore it can be put to unity without changing any results. The parameter $s > 1$ takes care for the convergence of the Gaussian integral with respect to φ^*, φ. The eigenvalues of the matrix $\hat{v}^{\text{hc}}_{\mathbf{r}\mathbf{r}';nm}$ are

$$v^{\text{hc}}_{\mathbf{k},n} = e^{-\mathrm{i}\frac{2\pi}{M}n} \left(1 - \frac{\beta}{M} (\tilde{\epsilon}_{\mathbf{k}} - \mu) \right) + s \,, \quad \text{where} \quad \tilde{\epsilon}_{\mathbf{k}} := \frac{J}{2d} \sum_{\nu=1}^{d} \cos(a k_\nu) \,. \tag{7.10}$$

For the convergence of the integral, it is necessary that the real part of all eigenvalues is non-negative, which is the case for large values of M if we choose $s > 1$. Physical quantities should not depend on s. The Grassmann integral in eq. (7.5) can be performed by using the integral relations for the nilpotent field variables:

$$\int \exp\left\{ \sum_{\mathbf{r},n} \left[\bar{\eta}_{\mathbf{r},n} \eta_{\mathbf{r},n} + \bar{\eta}_{\mathbf{r},n} (\varphi_{\mathbf{r},n} + \mathrm{i}\chi_{\mathbf{r},n} + \xi^1_{\mathbf{r},n}) + \eta_{\mathbf{r},n} (\varphi^*_{\mathbf{r},n} + \mathrm{i}\chi^*_{\mathbf{r},n} + \xi^2_{\mathbf{r},n}) \right] \right\} \prod_{\mathbf{r},n} \mathrm{d}\bar{\eta}_{\mathbf{r},n} \mathrm{d}\eta_{\mathbf{r},n}$$

$$= \prod_{\mathrm{r},n} \left[1 + \left(\varphi_{\mathbf{r},n} + \mathrm{i}\chi_{\mathbf{r},n} + \xi^1_{\mathbf{r},n} \right) \left(\varphi^*_{\mathbf{r},n} + \mathrm{i}\chi^*_{\mathbf{r},n} + \xi^2_{\mathbf{r},n} \right) \right] \,.$$

Thus we obtain for the generating functional the expression

$$Z^{\text{gen}}_{\text{hc}}(\xi) = \int \exp\left[-\tilde{A}^{\text{gen}}_{\text{hc}} (\varphi^*, \varphi, \chi^*, \chi, \xi) \right] \prod_{\mathbf{r},n} \frac{\mathrm{d}\varphi^*_{\mathbf{r},n} \mathrm{d}\varphi_{\mathbf{r},n} \mathrm{d}\chi^*_{\mathbf{r},n} \mathrm{d}\chi_{\mathbf{r},n}}{(2\pi\mathrm{i})^2} \tag{7.11}$$

with the generating action of the new complex fields

$$\tilde{A}^{\text{gen}}_{\text{hc}} (\varphi^*, \varphi, \chi^*, \chi, \xi) = \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m} \varphi^*_{\mathbf{r},n} (\hat{v}^{\text{hc}}_{\mathbf{r}\mathbf{r}';nm})^{-1} \varphi_{\mathbf{r}',m} + \frac{1}{s} \sum_{\mathbf{r},n} \chi^*_{\mathbf{r},n} \chi_{\mathbf{r},n}$$

$$- \sum_{\mathbf{r},n} \log \left[1 + \left(\varphi_{\mathbf{r},n} + \mathrm{i}\chi_{\mathbf{r},n} + \xi^1_{\mathbf{r},n} \right) \left(\varphi^*_{\mathbf{r},n} + \mathrm{i}\chi^*_{\mathbf{r},n} + \xi^2_{\mathbf{r},n} \right) \right] \,. \tag{7.12}$$

This transformation has been exact so far. In the following we will apply a saddle point approximation to the generating action $\tilde{A}^{\text{gen}}_{\text{hc}}$.

7.3 Saddle point approximation

In section 5.5 it has been demonstrated that the Bogoliubov approximation of an interacting Bose gas can be derived within the functional integral approach by means of a saddle point approximation. We will apply the same idea to the hard-core Bose system given by the action $\tilde{A}_{\mathrm{hc}} = \tilde{A}^{\mathrm{gen}}_{\mathrm{hc}}(\xi \equiv 0)$ in eq. (7.12). For this purpose it is necessary to find the mean-field solution via the variational principle $\delta\tilde{A}_{\mathrm{hc}} = 0$ which leads to a discretised form of the Gross-Pitaevskii equation for the two complex fields

$$\frac{\partial\tilde{A}_{\mathrm{hc}}}{\partial\varphi^*_{\mathbf{r},n}} = \frac{\partial\tilde{A}_{\mathrm{hc}}}{\partial\varphi_{\mathbf{r},n}} = 0\,, \quad \frac{\partial\tilde{A}_{\mathrm{hc}}}{\partial\chi^*_{\mathbf{r},n}} = \frac{\partial\tilde{A}_{\mathrm{hc}}}{\partial\chi_{\mathbf{r},n}} = 0\,. \tag{7.13}$$

Here, we assume a mean-field solution that is constant in space and time, like it was done for the Bogoliubov gas, cf. eq. (5.34):

$$\varphi^*_0 \equiv \varphi^*_{\mathbf{r},n} \quad \varphi_0 \equiv \varphi_{\mathbf{r},n} \quad \chi^*_0 \equiv \chi^*_{\mathbf{r},n} \quad \chi_0 \equiv \chi_{\mathbf{r},n}\,. \tag{7.14}$$

The saddle point approximation is done by expanding the action $\tilde{A}_{\mathrm{hc}}$ up to second order in the field fluctuations around the mean-field solution. We split the fields into real and imaginary part ($\varphi = \varphi' + \mathrm{i}\varphi''$, $\chi = \chi' + \mathrm{i}\chi''$) and use the notation

$$\begin{pmatrix} \varphi'_{\mathbf{r},n} \\ \varphi''_{\mathbf{r},n} \\ \chi'_{\mathbf{r},n} \\ \chi''_{\mathbf{r},n} \end{pmatrix} = \begin{pmatrix} \phi^1_0 + \delta\phi^1_{\mathbf{r},n} \\ \phi^2_0 + \delta\phi^2_{\mathbf{r},n} \\ \phi^3_0 + \delta\phi^3_{\mathbf{r},n} \\ \phi^4_0 + \delta\phi^4_{\mathbf{r},n} \end{pmatrix}\,, \tag{7.15}$$

where ϕ^γ_0, $\gamma = 1,\ldots,4$ denotes the mean-field solution (7.14) and $\delta\phi^\gamma_{\mathbf{r},n}$ the Gaussian fluctuations around ϕ^γ_0. Thus the saddle-point approximation is given by the relation

$$\tilde{A}_{\mathrm{hc}} = \tilde{A}_0 + \sum_{\mathbf{r},\mathbf{r}'}\sum_{n,m}\sum_{\gamma,\gamma'} \delta\phi^\gamma_{\mathbf{r},n}\left(\hat{\mathcal{G}}^{\gamma\gamma'}_{\mathbf{r}\mathbf{r}';nm}\right)^{-1}\delta\phi^{\gamma'}_{\mathbf{r}',m}\,, \quad \text{where} \quad \tilde{A}_0 = \tilde{A}_{\mathrm{hc}}(\phi_0)\,. \tag{7.16}$$

Here, $\hat{\mathcal{G}}$ represents the Green's function of quasiparticle fluctuations. For convenience introduce the following abbreviation:

$$\tilde{\mu} := \frac{\beta}{M}(\mu + J)\,. \tag{7.17}$$

For the action $\tilde{A}_{\mathrm{hc}}$ we find by the use of $\sum_{\mathbf{r}',m}(\hat{v}^{\mathrm{hc}}_{\mathbf{r}\mathbf{r}';nm})^{-1} = (1+s-\tilde{\mu})^{-1}$ the mean-field result

$$\frac{\tilde{A}^{\mathrm{hc}}_0}{\mathcal{N}M} = \frac{\varphi^*_0\varphi_0}{1+s+\tilde{\mu}} + \frac{1}{s}\chi^*_0\chi_0 - \log\left[1 + (\varphi_0 + \mathrm{i}\chi_0)\,(\varphi^*_0 + \mathrm{i}\chi^*_0)\right]\,, \tag{7.18}$$

where $\mathcal{N}$ denotes the number of lattice sites. With eq. (7.13) this leads to the equations

$$0 = \frac{\varphi_0}{1+s+\tilde{\mu}} - \frac{\varphi_0 + \mathrm{i}\chi_0}{1+(\varphi_0+\mathrm{i}\chi_0)(\varphi_0^*+\mathrm{i}\chi_0^*)} , \tag{7.19}$$

$$0 = \frac{\varphi_0^*}{1+s+\tilde{\mu}} - \frac{\varphi_0^* + \mathrm{i}\chi_0^*}{1+(\varphi_0+\mathrm{i}\chi_0)(\varphi_0^*+\mathrm{i}\chi_0^*)} , \tag{7.20}$$

$$0 = \frac{\chi_0}{s} - \frac{\mathrm{i}(\varphi_0 + \mathrm{i}\chi_0)}{1+(\varphi_0+\mathrm{i}\chi_0)(\varphi_0^*+\mathrm{i}\chi_0^*)} , \tag{7.21}$$

$$0 = \frac{\chi_0^*}{s} - \frac{\mathrm{i}(\varphi_0^* + \mathrm{i}\chi_0^*)}{1+(\varphi_0+\mathrm{i}\chi_0)(\varphi_0^*+\mathrm{i}\chi_0^*)} . \tag{7.22}$$

These equations are invariant with respect to the $U(1)$ transformation $\varphi \to e^{\mathrm{i}\alpha}\varphi$, $\chi \to e^{\mathrm{i}\alpha}\chi$. We find two solutions: A *trivial solution*

$$\phi_0^\gamma = 0 , \quad \gamma = 1, \ldots, 4 , \tag{7.23}$$

and a *non-trivial solution* with broken $U(1)$ symmetry

$$\phi_0^1 = \frac{1+s+\tilde{\mu}}{1+\tilde{\mu}}\sqrt{\tilde{\mu}} , \quad \phi_0^2 = 0 , \quad \phi_0^3 = \frac{s}{1+\tilde{\mu}}\sqrt{-\tilde{\mu}} , \quad \phi_0^4 = 0 . \tag{7.24}$$

The solutions ϕ_0^γ can be imaginary (depending on the sign of μ) because of the fact that the eqs. (7.19) and (7.20) on the one hand, and (7.21) and (7.22) on the other hand, are not complex conjugate to each other, so φ,φ^* and χ,χ^* are not, either. It should be noted that the non-trivial saddle point vanishes as well, if the limit $M \to \infty$ is performed.

- For the trivial solution we find $\tilde{A}_0^{\mathrm{hc}} = 0$ and, after using the expansion $\log(1+x) = x + \mathcal{O}(x^2)$, the Green's matrix

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} (\hat{v}^{\mathrm{hc}})^{-1} - 1 & -\mathrm{i}(\hat{v}^{\mathrm{hc}})^{-1} & -\mathrm{i} & 0 \\ \mathrm{i}(\hat{v}^{\mathrm{hc}})^{-1} & (\hat{v}^{\mathrm{hc}})^{-1} - 1 & 0 & -\mathrm{i} \\ -\mathrm{i} & 0 & \frac{1}{s}+1 & 0 \\ 0 & -\mathrm{i} & 0 & \frac{1}{s}+1 \end{pmatrix} , \tag{7.25}$$

  where the entries of the 4×4 matrix represent the structure of the index γ, and the structure of the indices $\mathbf{r}$ and n are contained in the matrix $(\hat{v}^{\mathrm{hc}})^{-1}$. All constants represent diagonal terms and have to be multiplied by $\delta_{\mathbf{r}\mathbf{r}'}\delta_{nm}$ in principle.

- For the non-trivial solution we find

$$\frac{\tilde{A}_0^{\mathrm{hc}}}{\mathcal{N}M} = \frac{\tilde{\mu}}{1+\tilde{\mu}} - \log[1+\tilde{\mu}] = \frac{1}{2}\tilde{\mu}^2 + \mathcal{O}(\tilde{\mu}^3) . \tag{7.26}$$

  Expanding the logarithmic term

$$\log\left[1 + \left(\sqrt{\tilde{\mu}} + \delta\phi^1 + \mathrm{i}\delta\phi^3\right)^2 - \left(\mathrm{i}\delta\phi^2 - \delta\phi^4\right)^2\right]$$

up to second order in the fluctuations, we find the Green's function to be

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} (\hat{v}^{\mathrm{hc}})^{-1} - 1 & -\mathrm{i}(\hat{v}^{\mathrm{hc}})^{-1} & -\mathrm{i} & 0 \\ \mathrm{i}(\hat{v}^{\mathrm{hc}})^{-1} & (\hat{v}^{\mathrm{hc}})^{-1} - 1 & 0 & -\mathrm{i} \\ -\mathrm{i} & 0 & \frac{1}{s} + 1 & 0 \\ 0 & -\mathrm{i} & 0 & \frac{1}{s} + 1 \end{pmatrix} + \tilde{\mu} \begin{pmatrix} 3 & 0 & 3\mathrm{i} & 0 \\ 0 & 1 & 0 & \mathrm{i} \\ 3\mathrm{i} & 0 & -3 & 0 \\ 0 & \mathrm{i} & 0 & -1 \end{pmatrix} + \mathcal{O}\left(\tilde{\mu}^2\right) . \tag{7.27}$$

The higher order terms in $\tilde{\mu}$ can be neglected because $\tilde{\mu}$ is of the order $1/M$, so they vanish in the limit $M \to \infty$.

The matrix $\hat{\mathcal{G}}$ can be diagonalised in the coordinates of space and time like demonstrated in the previous chapters, and the 4×4 structure can be written in the more convenient form

$$(\hat{\mathcal{G}}_{\mathbf{k},n})^{-1} = \begin{pmatrix} (\tilde{v}^{\mathrm{hc}}_{\mathbf{k},n})^{-1} - \hat{B} & -\mathrm{i}\hat{B} \\ -\mathrm{i}\hat{B} & \frac{1}{s} + \hat{B} \end{pmatrix} \tag{7.28}$$

with the 2×2 matrix

$$(\tilde{v}^{\mathrm{hc}}_{\mathbf{k},n})^{-1} = \frac{1}{\tilde{b}^2_{\mathbf{k}} + s^2 + 2\tilde{b}_{\mathbf{k}} s \cos\left(\frac{2\pi}{M} n\right)} \begin{pmatrix} \tilde{b}_{\mathbf{k}} \cos\left(\frac{2\pi}{M} n\right) + s & \tilde{b}_{\mathbf{k}} \sin\left(\frac{2\pi}{M} n\right) \\ -\tilde{b}_{\mathbf{k}} \sin\left(\frac{2\pi}{M} n\right) & \tilde{b}_{\mathbf{k}} \cos\left(\frac{2\pi}{M} n\right) + s \end{pmatrix} \tag{7.29}$$

with

$$\tilde{b}_{\mathbf{k}} = 1 - \frac{\beta}{M} \left(\tilde{\epsilon}_{\mathbf{k}} - \mu\right) \tag{7.30}$$

where $\tilde{\epsilon}_{\mathbf{k}}$ is given in eq. (7.10), and

$$\hat{B} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{or} \quad \hat{B} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \tilde{\mu} \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix} + \mathcal{O}\left(\frac{1}{M^2}\right) \tag{7.31}$$

for the trivial and the non-trivial saddle point, respectively.

7.4 Results for the hard-core Bose model

In the remaining part of this chapter the main calculations and results for the hard-core Bose model shall be presented. We will consider a three-dimensional system so that the mean-field solution with broken $U(1)$ symmetry is considered to be associated to a BEC phase. It is stable at $\mu > -J$. For $\mu < -J$ the non-trivial mean-field solution is stable and is associated with the non-condensed phase. A solution which describes

a Mott-insulator is not found. It should be noted that all results which were found on the level of Gaussian fluctuations are independent of the free parameter s which was introduced in eq. (7.8) for the convergence of the decoupling.

It was shown that the quasiparticle spectrum within Bogoliubov theory is given by the poles of the Green's function of Gaussian fluctuations, cf. eq. (5.48). Similarly, we find the excitation spectrum of the hard-core Bose model by the equation

$$\det \hat{\mathcal{G}}^{-1} = 0 \,,$$

identifying the Matsubrara frequencies with eq. (4.11), and performing the analytic continuation $\mathrm{i}\hbar\omega_n \to E_{\mathbf{k}}$. Keeping only the lowest order in $1/M$, we find the solutions

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + |\mu + J| \tag{7.32}$$

in the non-condensed phase $\mu < -J$ and

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} \left(2(\mu + J) + \epsilon_{\mathbf{k}}\right)} \tag{7.33}$$

in the condensed phase $\mu > -J$. Here, $\epsilon_{\mathbf{k}}$ is again the lattice dispersion (4.7) which goes like $\propto k^2$ for small wave vectors. The spectrum in the non-condensed phase shows a gap $|\mu + J|$, which is a measure for the distance of the system to the phase transition to the BEC phase. Inside the BEC phase we find a result which is identical to the Bogoliubov result (5.11). The linearity of the spectrum for small wave vectors reflects the Goldstone mode due to the broken $U(1)$ symmetry.

In section 3.2 it was argued that the total particle density and the condensate density are derived from the one-particle CF. The static structure factor will be derived from the two-particle CF, like it was done for the one-dimensional system in chapter 6. Applying the definition of the CFs for our model given in eq. (7.7), we find expressions in terms of expectation values of the complex fields $\varphi_{\mathbf{r},0}$ and $\chi_{\mathbf{r},0}$. In the following we will drop the imaginary-time index "0" because we only need equal-time CFs. The CFs of interest here are:

- One-particle CF at one site:

$$C_1(\mathbf{r}, \mathbf{r}) = \left\langle [1 + (\varphi_{\mathbf{r}} + \mathrm{i}\chi_{\mathbf{r}})(\varphi^*_{\mathbf{r}} + \mathrm{i}\chi^*_{\mathbf{r}})]^{-1} \right\rangle \,. \tag{7.34}$$

  This CF gives the total particle density per site and component:

$$n_{\mathrm{tot}} = 1 - C_1(\mathbf{r}, \mathbf{r}) \,. \tag{7.35}$$

- Single particle CF on different sites, i.e. $\mathbf{r} \neq \mathbf{r}'$:

$$C_1(\mathbf{r}, \mathbf{r}') = \left\langle \frac{(\varphi_{\mathbf{r}} + \mathrm{i}\chi_{\mathbf{r}})(\varphi^*_{\mathbf{r}'} + \mathrm{i}\chi^*_{\mathbf{r}'})}{[1 + (\varphi_{\mathbf{r}} + \mathrm{i}\chi_{\mathbf{r}})(\varphi^*_{\mathbf{r}} + \mathrm{i}\chi^*_{\mathbf{r}})] \left[1 + (\varphi_{\mathbf{r}'} + \mathrm{i}\chi_{\mathbf{r}'})(\varphi^*_{\mathbf{r}'} + \mathrm{i}\chi^*_{\mathbf{r}'})\right]} \right\rangle \,. \tag{7.36}$$

This correlation function we will use to define the condensate density:

$$n_0 := \lim_{\mathbf{r}-\mathbf{r}'\to\infty} C_1(\mathbf{r},\mathbf{r}') \; . \tag{7.37}$$

- Density-density CF for $\mathbf{r} \neq \mathbf{r}'$:

$$D(\mathbf{r}-\mathbf{r}') = 2n_{\mathrm{tot}} - 1 + C_2(\mathbf{r},\mathbf{r}';\mathbf{r}',\mathbf{r}) \; , \tag{7.38}$$

with

$$C_2(\mathbf{r},\mathbf{r}';\mathbf{r}',\mathbf{r}) = \left\langle [1+(\varphi_{\mathbf{r}}+\mathrm{i}\chi_{\mathbf{r}})(\varphi^*_{\mathbf{r}}+\mathrm{i}\chi^*_{\mathbf{r}})]^{-1}\,[1+(\varphi_{\mathbf{r}'}+\mathrm{i}\chi_{\mathbf{r}'})(\varphi^*_{\mathbf{r}'}+\mathrm{i}\chi^*_{\mathbf{r}'})]^{-1} \right\rangle \; . \tag{7.39}$$

To calculate these expectation values within the saddle point approximation we expand the functions inside the angled brackets up to second order in the field fluctuations. They can then be expressed in terms of the expectation values

$$F_1(\mathbf{r}-\mathbf{r}') := \langle(\varphi_{\mathbf{r}}+\mathrm{i}\chi_{\mathbf{r}})(\varphi_{\mathbf{r}'}+\mathrm{i}\chi_{\mathbf{r}'})\rangle = \langle(\varphi^*_{\mathbf{r}}+\mathrm{i}\chi^*_{\mathbf{r}})(\varphi^*_{\mathbf{r}'}+\mathrm{i}\chi^*_{\mathbf{r}'})\rangle \; , \tag{7.40}$$

$$F_2(\mathbf{r}-\mathbf{r}') := \langle(\varphi_{\mathbf{r}}+\mathrm{i}\chi_{\mathbf{r}})(\varphi^*_{\mathbf{r}'}+\mathrm{i}\chi^*_{\mathbf{r}'})\rangle \; . \tag{7.41}$$

The expansion of the CFs as well as the evaluation of the functions F_1 and F_2 is given in Appendix D.

In the limit $M \to \infty$, the results for this model are somewhat disappointing. For the total density of excited particles we find in the non-condensed phase ($\mu < -J$) the expression

$$n_{\mathrm{tot}} = \int \frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-(\mu+J))}-1}\,\frac{\mathrm{d}^d k}{(2\pi)^d} \; . \tag{7.42}$$

In the BEC phase ($\mu > -J$) we find

$$n_{\mathrm{tot}} - n_0 = \int \left[\frac{\epsilon_{\mathbf{k}}+(\mu+J)}{2E_{\mathbf{k}}}\,\coth\left(\frac{\beta}{2}\,E_{\mathbf{k}}\right) - \frac{1}{2}\right]\,\frac{\mathrm{d}^d k}{(2\pi)^d} \; . \tag{7.43}$$

A comparison with eqs. (4.24) and (5.59) shows that the solution is equivalent to the ideal gas in the non-condensed phase, whereas we find the condensate depletion of the Bogoliubov gas in the condensed phase. The only difference here is, that we have chosen the phase boundary to be at the point $\mu = -J$ instead of $\mu = 0$, but this choice is arbitrary because the chemical potential can be shifted by a constant without changing the physics. The total density of the particles out of the condensate is plotted against the chemical potential in fig. 7.2. It is peaked at the phase transition at $\mu = -J$. At zero temperature the non-condensed phase is empty.

It turns out that predictions about the condensate density cannot be made in the limit $M \to \infty$. The one-particle CF vanishes for large distances, and the density-density CF is

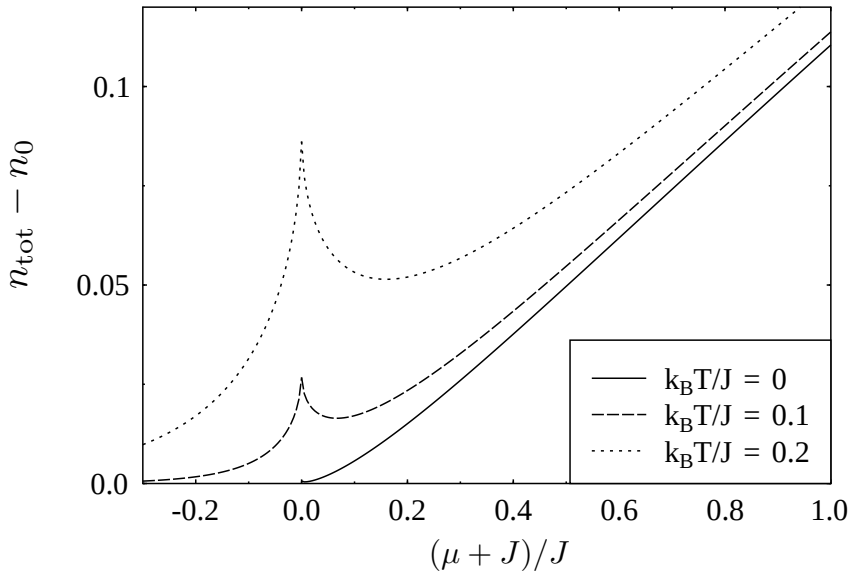

Figure 7.2: Total density of non-condensed particles plotted against the normalised chemical potential for different temperatures T. The phase transition is at the point $(\mu + J)/J = 0$. The density of non-condensed particles is peaked there. The condensate density n_0 is unknown.

constant. However, the static structure factor, which is its Fourier transform normalised by $\tilde{\mu}$, stays finite in the BEC phase because $\tilde{\mu}$ cancels out. The term of first order in $\tilde{\mu}$ survives in the condensed phase and leads to

$$\begin{aligned} S(\mathbf{q}) &= 2\left(F_1^{\rm nt}(\mathbf{q}) + F_2^{\rm nt}(\mathbf{q})\right) + \mathcal{O}(\tilde{\mu}) \\ &= \frac{\epsilon_{\mathbf{q}}}{E_{\mathbf{q}}} \coth\left(\frac{\beta}{2} E_{\mathbf{q}}\right) , \end{aligned} \tag{7.44}$$

which is proportional to the static structure factor which was obtained from Bogoliubov theory, given in eq. (5.62).

To determine the type of the decay of the density-density correlations for large distances (i.e. exponentially or algebraically) at zero temperature in d dimensions in the BEC phase, we Fourier transform the static structure factor for small wave vectors, because they are relevant for large distances $\mathbf{r}$:

$$D(\mathbf{r}) \sim \int S(\mathbf{q}) e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \mathrm{d}^d q \sim \int \frac{\mathbf{q}^2}{\sqrt{2(\mu+J)\mathbf{q}^2 + \mathbf{q}^4}} e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \mathrm{d}^d q \sim \int \frac{|\mathbf{q}|}{\sqrt{2(\mu+J)}} e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \mathrm{d}^d q \, . \tag{7.45}$$

This expression shows an algebraic decay. In $d = 1$ the decay is proportional to $1/r^2$ (in agreement with the result (6.26) of the one-dimensional system), in $d = 2$ it decays like $1/r^3$, and in $d = 3$ like $1/r^4$ (see Appendix D.1).

In the empty phase, all CFs vanish completely at zero temperature, because the expressions F_1^{tr} and F_2^{tr} given in the Appendix in eqs. (D.1) and (D.2) vanish. Thus, the static structure factor is constantly unity.

7.5 The N-component model

The hard-core Bose model has been extended to a N-component system of bosons. In this model, each particle can be assigned to one of N types of bosons. The hard-core interaction only shows up for bosons which belong to the same component. We allow that particles may change their identity during the hopping process, i.e. they can switch the component that they are belonging to like it might be possible e.g. for hyperfine states. This is a difference to the system given by the Hamiltonian (2.38) where particles are assumed to stay in the same state always, which is accounted for by the δ-function in the kinetic term. In our model, all components are treated equally and can be considered as N degenerate states per site of the optical lattice, assuming that there is a hard-core interaction only in the same state. Thus, the bosons can avoid hard-core interaction by choosing an unoccupied state, leading to an effective interaction between the bosons that becomes weaker with an increasing number of states N.

This model has been chosen because a $1/N$ expansion can be performed, and all the results which were presented previously for the hard-core Bose model can be used again. In the limit $N \to \infty$, the mean-field solution is exact and the results we get from the Gaussian approximation lead to corrections to the mean-field result of the order $1/N$. To make qualitative predictions for zero temperature results, we used the same discrete-time approximation that was used for the treatment of the trapped one-dimensional system discussed in section 6.5. We kept the imaginary time step $\hbar\beta/M$ constant and used it as the unit of energy, and performed the limit $M \to \infty$ to reach the zero temperature result. We did the replacement $\beta J/M \to J$ and used the parameter $\zeta = \exp(\beta\mu/M)$ instead of the chemical potential μ. We replaced $1 + \beta\mu/M \to \zeta$, which is a good approximation if $\beta\mu/M$ is small compared to 1. Otherwise, quantitative deviations from the $\hbar\beta/M \to 0$ limit are expected. Within the discrete-time approximation we find non-vanishing mean-field results which vanish in the limit $\hbar\beta/M \to 0$, which was shown in the previous section.

The model is constructed by assigning an additional index $\alpha = 1, \ldots, N$ to the nilpotent field η, $\bar{\eta}$, which denotes the component. In analogy to eq. (7.2) the model is defined via the grand canonical partition function:

$$Z_N = \lim_{M\to\infty} \int \exp\left[-\sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m} \sum_{\alpha,\alpha'} \bar{\eta}^{\alpha}_{\mathbf{r},n} (\hat{A}_N)^{\alpha\alpha'}_{\mathbf{r}\mathbf{r}';nm} \eta^{\alpha'}_{\mathbf{r}',m} \right] \prod_{\mathbf{r}} \prod_{n=1}^{M} \prod_{\alpha=1}^{N} \mathrm{d}\bar{\eta}^{\alpha}_{\mathbf{r},n} \mathrm{d}\eta^{\alpha}_{\mathbf{r},n} \tag{7.46}$$

with the matrix

$$(\hat{A}_N)^{\alpha\alpha'}_{\mathbf{r}\mathbf{r}';nm} := -\delta_{nm}\delta_{\mathbf{r}\mathbf{r}'}\delta_{\alpha\alpha'} - \frac{\zeta}{N}(\delta_{n,m+1} + \delta_{n1}\delta_{mM})\left[\delta_{\mathbf{r}\mathbf{r}'} - \hat{J}_{\mathbf{r}\mathbf{r}'}\right] . \tag{7.47}$$

After resubstituting $J \to \beta J/M$ and $\zeta \to \exp(\beta\mu/M)$, neglecting all terms of higher than first order in β/M, in the case $N = 1$ the matrix $\hat{A}_N$ reduces to $\hat{A}^{\mathrm{hc}}$ like given in eq. (7.3). For the Hubbard-Stratonovich decoupling we define

$$\bar{\rho}_{\mathbf{r},n} = \sum_{\alpha} \bar{\eta}^{\alpha}_{\mathbf{r},n} , \quad \rho_{\mathbf{r}',m} = \sum_{\alpha'} \eta^{\alpha}_{\mathbf{r}',m} ,$$

and in analogy to eq. (7.9) insert the identity

$$\begin{aligned} &\text{const.} \times \exp\left\{ \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m=1}^{M} \bar{\rho}_{\mathbf{r},n}(\hat{v}^{\mathrm{hc}}_{\mathbf{r}\mathbf{r}';nm} - s\,\delta_{nm}\delta_{\mathbf{r}\mathbf{r}'})\rho_{\mathbf{r}',m} \right\} \\ &= \int \exp\left\{ - N \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m} \varphi^*_{\mathbf{r},n}(\hat{v}^{\mathrm{hc}}_{\mathbf{r}\mathbf{r}';nm})^{-1}\varphi_{\mathbf{r}',m} - \frac{N}{s}\sum_{\mathbf{r},n} \chi^*_{\mathbf{r},n}\chi_{\mathbf{r},n} \right. \\ &\left. + \sum_{\mathbf{r},n} \left[\rho_{\mathbf{r},n}(\varphi^*_{\mathbf{r},n} + \mathrm{i}\chi^*_{\mathbf{r},n}) + \bar{\rho}_{\mathbf{r},n}(\varphi_{\mathbf{r},n} + \mathrm{i}\chi_{\mathbf{r},n})\right] \right\} \prod_{\mathbf{r},n} \frac{\mathrm{d}\varphi^*_{\mathbf{r},n}\mathrm{d}\varphi_{\mathbf{r},n}\mathrm{d}\chi^*_{\mathbf{r},n}\mathrm{d}\chi_{\mathbf{r},n}}{(2\pi\mathrm{i})^2} . \end{aligned} \tag{7.48}$$

The matrix $\hat{v}^{\mathrm{hc}}$ is the same as the one given in eq. (7.8), and we perform the same transformation as for the single-component system. For the generating functional we find the result

$$Z^{\mathrm{gen}}_N(\xi) = \int \exp\left[-N\tilde{A}^{\mathrm{gen}}_{\mathrm{hc}}(\varphi^*,\varphi,\chi^*,\chi,\xi)\right] \prod_{\mathbf{r},n} \frac{\mathrm{d}\varphi^*_{\mathbf{r},n}\mathrm{d}\varphi_{\mathbf{r},n}\mathrm{d}\chi^*_{\mathbf{r},n}\mathrm{d}\chi_{\mathbf{r},n}}{(2\pi\mathrm{i})^2} , \tag{7.49}$$

which differs from the single-component generating functional (7.11) only in the way that the number of components N appears in front of the generating action. This allows the $1/N$ expansion that was mentioned above. In the limit $N \to \infty$ only the mean-field result survives and the Gaussian fluctuations provide corrections of the order $1/N$.

Results were published in ref. [68] and are depicted in figs. 7.3, 7.4, and 7.5 for the number of components being $N = 5$. In the large-N limit we find for the total particle density per site and component the result

$$n_{\mathrm{tot}} = \begin{cases} 0 & \text{if} \quad \zeta < 1 \\ 1 - \zeta^{-1} & \text{if} \quad \zeta > 1 \end{cases} ,$$

and for the condensate density per site and component, got by means of eq. (7.37) we find

$$n_0 = \begin{cases} 0 & \text{if} \quad \zeta < 1 \\ \zeta^{-1} - \zeta^{-2} & \text{if} \quad \zeta > 1 \end{cases} .$$

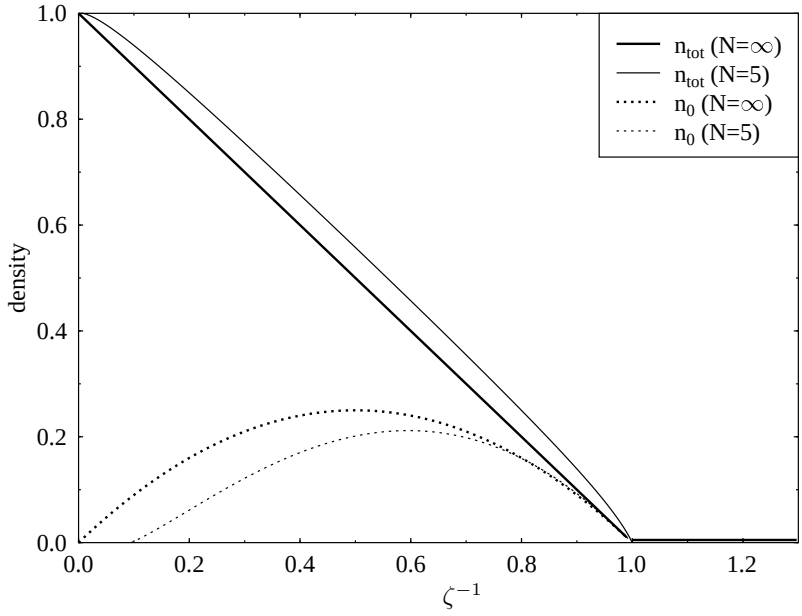

Figure 7.3: Total particle density and condensate density for $J = 0.1$ in three dimensions.

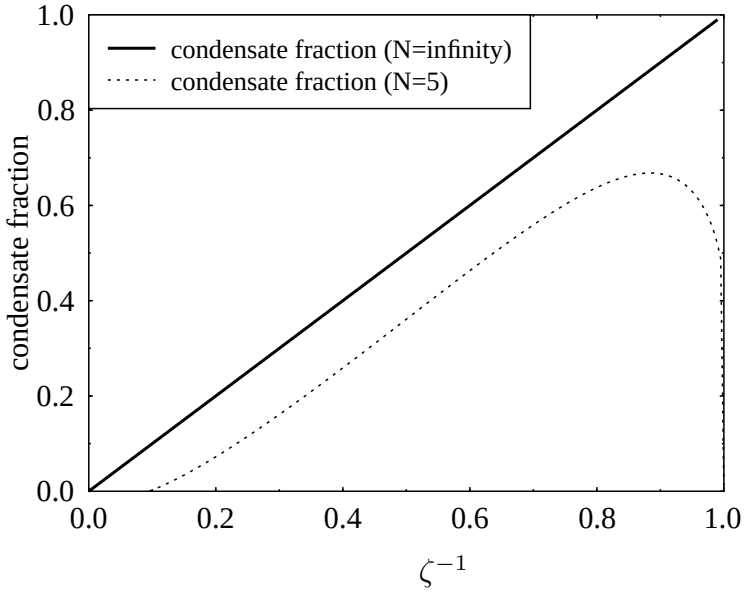

Figure 7.4: Condensate fraction n_0/n_{tot} for $J = 0.1$ in three dimensions.

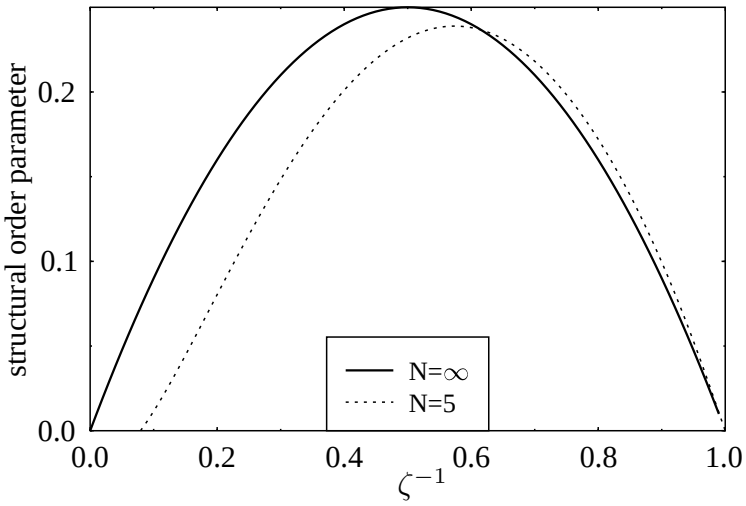

Figure 7.5: Structural order parameter $C_1(\mathbf{r}\alpha, \mathbf{r}\alpha')$ for $J = 0.1$ in three dimensions.

It can be seen in fig. 7.3, that the $1/N$-corrections lead to a depletion of the condensate density caused by strong interaction. This effect leads eventually to the destruction of the condensate and to the formation of a Mott-insulator for sufficiently large fugacity ζ. Quantitative predictions about the transition point to the Mott-insulator cannot be made within this approximation, but at least we find the tendency towards a MI phase. However, the condensate survives in the limit $N \to \infty$, since the interaction is always weak in this case. On the other hand, in the very dilute regime (i.e. for $\zeta \approx 1$; this is the regime that survives in the limit $\hbar\beta/M \to 0$), the condensate density increases with decreasing N. This reflects the well-known fact that increasing interaction supports BEC formation in a dilute Bose gas [69, 70]. The quantity which is plotted in fig. 7.5 is the CF of the type $C_1(\mathbf{r}\alpha, \mathbf{r}\alpha')$, where α and α' denote components which are not of the same type. This is the appropriate quantity describing the correlation of the internal structure of the components of a given site. We call it the structural order parameter. Its $N \to \infty$ limit is equal to that of the condensate density, but the $1/N$ correction is slightly different: The dilute regime where the interaction supports this parameter is broader, and its destruction happens at higher values of ζ.

Again, it should be noted that if we substitute back $\zeta \to \exp(\beta\mu/M)$ and $J \to \beta J/M$ in these results, and perform the limit $\hbar\beta M \to 0$ subsequently, we find all the results that were given in the previous section. This also means that the large-N limit vanishes like $1/M$ such that we loose all qualitative information about it. Therefore it might be adequate to look at the results derived from the discrete-time approximation like they are presented here.

The same N-component model, like it was used here for a system with N types of bosons, was also applied to analyse the statistics of a system of complex directed macromolecules (polymers) [71]. Here, the N components are represented by constituting molecules of which the macromolecules are formed. Those constituting molecules could e.g. be amino acids which form proteins, or molecular sequences along a DNA helix. We assumed that the macromolecules are directed, i.e. they have a preferred direction. This direction is identified by the imaginary-time axis in a world-line diagram like shown in fig. (7.1). The dimension of the space perpendicular to the axis of the direction is identified by the spacial dimension of the bosonic model. That means, a three-dimensional system of directed macromolecules is described by a two-dimensional system of hard-core bosons. The hard-core property of the N-component model means that the interaction of different molecule types is neglected. This can be understood as a chemical property of the molecules. The density of constituting molecules we describe by the one-particle CF at one site and for the same component via eq. (7.35), like for the two-dimensional boson system. The large scale behaviour of the one-particle CF (7.36) is associated with the probability of the breaking of a macromolecule, which depends of the distance of the remaining ends; if this distance is large, it can by described by the quantity which is analogue to the condensate density of the two-dimensional boson system. The probability that a constituting molecule is replaced by one of another type is associated to the structural order parameter.

The hard-core Bose model has also been applied to the statistics of flux lines in type-II superconductors [72]. Similar to the system of macromolecules, the imaginary-time axis of the bosonic system is identified by the spacial direction in which the macromolecules are aligned, which is parallel to the macroscopic magnetic field.

8 Paired-fermion model

8.1 Bosonic molecules of spin-$1/2$ fermions

The aim of this chapter is to show that a system of hard-core bosons can be represented by molecules consisting of pairs of spin-1/2 fermions, as an alternative to the hard-core Bose model which was discussed in the previous chapter. In order to distinguish it from the latter this model will be referred to as "paired-fermion model".

A general model which was introduced to study the dissociation of bosonic molecules into pairs of fermionic atoms in an optical lattice was proposed in ref. [73]. It is given by the Hamiltonian

$$\hat{H} - \mu \hat{N}_{\mathrm{tot}} = -\frac{\bar{t}}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \sum_{\sigma=\uparrow,\downarrow} \hat{c}^{+}_{\mathbf{r},\sigma} \hat{c}_{\mathbf{r},\sigma} - \frac{J}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \hat{c}^{+}_{\mathbf{r}\uparrow} \hat{c}_{\mathbf{r}'\uparrow} \hat{c}^{+}_{\mathbf{r}\downarrow} \hat{c}_{\mathbf{r}'\downarrow} - \mu \sum_{\mathbf{r}} \sum_{\sigma=\uparrow\downarrow} \hat{c}^{+}_{\mathbf{r}\sigma} \hat{c}_{\mathbf{r}\sigma} \,. \quad (8.1)$$

The index $\sigma = \uparrow, \downarrow$ denotes the spin. The first term describes tunneling of individual fermions with rate $\bar{t}$ and the second term tunneling of local fermion pairs. Similar Hamiltonians were proposed in a couple of works for homogeneous systems, in order to study the BEC-BCS crossover [74, 75, 76]. They are similar to the BCS-Hamilonian (2.39) with two additional terms, one describing the kinetic energy of bosonic molecules and one describing the interaction between molecules and individual fermions. In contrary to the lattice-Hamiltonian (8.1) they do not exhibit a Mott insulating phase.

Because the main interest here shall be the model of hard-core bosons, we consider the case $\bar{t} = 0$ in the following, i.e. we exclude the existence of dissociated fermionic atoms. Further we will write the index $\sigma = 1, 2$ as superscript instead of the spin indices $\uparrow, \downarrow$. We write the grand canonical partition function of the system in terms of a fermionic functional integral of a field of conjugate Grassmann variables as defined in eq. (3.10) with the action

$$A_{\mathrm{ferm}}(\bar{\psi}, \psi) = \sum_{n=1}^{M} \Bigg\{ \sum_{\mathbf{r},\sigma} \bar{\psi}^{\sigma}_{\mathbf{r},n+1} (\psi^{\sigma}_{\mathbf{r},n+1} - \psi^{\sigma}_{\mathbf{r},n}) - \frac{\beta\mu}{M} \sum_{\mathbf{r},\sigma} \bar{\psi}^{\sigma}_{\mathbf{r},n+1} \psi^{\sigma}_{\mathbf{r},n}$$

$$+ \frac{\beta}{M} \sum_{\mathbf{r},\mathbf{r}'} \hat{J}_{\mathbf{r}\mathbf{r}'} \bar{\psi}^{1}_{\mathbf{r},n+1} \psi^{1}_{\mathbf{r}',n} \bar{\psi}^{2}_{\mathbf{r},n+1} \psi^{2}_{\mathbf{r}',n} \Bigg\} \,, \quad (8.2)$$

and anti-periodic boundary conditions in time. A comparison of this action with the action (7.4) for the hard-core Bose model shows that the last term, which describes

tunneling of bosons, is identical after two exchanges of Grassmann variables. However, the first two terms are different because in A_{ferm} they are of the second order in the Grassmann variables, while they are of forth order in A_{hc}.

Despite their difference, the hard-core Bose model and the paired-fermion model are expected to describe the same physics. Because the effects of unpaired fermionic atoms are neglected in the action in (8.2), the term containing the chemical potential μ is associated only to the number of *paired* fermions (i.e. to the bosonic molecules) and we could in principle make the substitution

$$-\frac{\beta\mu}{M}\sum_{\mathbf{r},n,\sigma}\left(\bar{\psi}^1_{\mathbf{r},n+1}\psi^1_{\mathbf{r},n}+\bar{\psi}^2_{\mathbf{r},n+1}\psi^2_{\mathbf{r},n}\right)\to-\frac{\beta\mu}{M}\sum_{\mathbf{r},n}\bar{\psi}^1_{\mathbf{r},n+1}\psi^1_{\mathbf{r},n}\bar{\psi}^2_{\mathbf{r},n+1}\psi^2_{\mathbf{r},n}\ .$$

This is identical to the μ-term in (7.4). Note that in A_{hc} the total particle number is given by the number of bosons and in A_{ferm} it is given by the number of fermionic atoms which the 2-atomic bosonic molecules consist of. So if we assume that there are no unpaired fermions, we can write (we always assume the limit $M\to\infty$, but we will not write it everywhere for simplicity):

$$\begin{aligned}N_{\text{hc}}&=\sum_{\mathbf{r}}\langle\bar{\eta}_{\mathbf{r},n+1}\eta_{\mathbf{r},n}\rangle=\sum_{\mathbf{r}}\langle\bar{\psi}^1_{\mathbf{r},n+1}\bar{\psi}^2_{\mathbf{r},n+1}\psi^2_{\mathbf{r},n}\psi^1_{\mathbf{r},n}\rangle\\&=\frac{1}{2}\sum_{\mathbf{r},\sigma}\langle\bar{\psi}^\sigma_{\mathbf{r},n+1}\psi^\sigma_{\mathbf{r},n}\rangle=\frac{N_{\text{ferm}}}{2}\ .\end{aligned}$$

In the following we will always write N_{tot} instead of N_{hc}. Under the same assumption it is also possible to perform the equivalent substitution in the first term representing the "discrete-time derivative",without changing the physics:

$$-\sum_{\sigma=1,2}\bar{\psi}^\sigma_{\mathbf{r},n+1}(\psi^\sigma_{\mathbf{r},n+1}-\psi^\sigma_{\mathbf{r},n})\to\bar{\psi}^1_{\mathbf{r},n+1}\psi^1_{\mathbf{r},n+1}\bar{\psi}^2_{\mathbf{r},n+1}\psi^2_{\mathbf{r},n+1}+\bar{\psi}^1_{\mathbf{r},n+1}\psi^1_{\mathbf{r},n}\bar{\psi}^2_{\mathbf{r},n+1}\psi^2_{\mathbf{r},n}\ .$$

For this reason, we can regard the two actions A_{hc} and A_{ferm} as representing the same model of hard-core bosons. In the following they will be referred to as hard-core Bose model and paired-fermion model, respectively.

In the world-line picture, the paired-fermion model given by A_{ferm} is represented by pairs of fermions with opposite "spin" 1 and 2 whose world-lines always stay together while they tunnel through the lattice. Tunneling of unpaired fermions does not exist. The world-lines of paired fermions can then be seen as the world-lines of bosonic molecules like in fig. 7.1.

We will treat the paired-fermion model in mean-field theory. Therefore it is necessary to get rid of the Grassmann integral. We will show that it is possible to decouple the forth order Grassmann term by means of a Hubbard-Stratonovich transformation. However,

we will see that the decoupling that we choose for this model leads to a different mean-field theory, than the one we found for the previously discussed hard-core Bose model. This difference is not so much caused by the difference in the models but rather by the different types of decoupling.

8.2 Hubbard-Stratonovich decoupling

We perform a Hubbard-Stratonovich transformation on the system of paired fermions [73] given by eq. (8.2). Because we will not discuss so many physical quantities for this model, we will not define a generating functional analogous to eq. (7.5) here, but will apply the decoupling directly to the grand canonical partition function which is defined by the action A_{ferm} in eq. (8.2). Only the term which describes hopping of fermion pairs is quartic, so we will decouple it. In contrary to the case of the hard-core Bose model, it is not necessary here to decouple the entire off-diagonal term, because the term describing the discrete-time derivative and the term containing the chemical potential are already of second order. For the matrix with fermionic boundary conditions we write

$$\hat{v}^{\text{ferm}}_{\mathbf{r}\mathbf{r}';nm} = (\delta_{n,m+1} - \delta_{n1}\delta_{mM})\,\frac{\beta}{M}\,\hat{J}_{\mathbf{r}\mathbf{r}'} + s\,\delta_{nm}\ , \tag{8.3}$$

and insert the identity

$$\text{const.} \times \exp\left\{ -\frac{\beta}{M} \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m=1}^{M} \hat{J}_{\mathbf{r}\mathbf{r}'} \bar{\psi}^1_{\mathbf{r},n+1} \psi^1_{\mathbf{r}',n} \bar{\psi}^2_{\mathbf{r},n+1} \psi^2_{\mathbf{r}',n} \right\}$$

$$= \int \exp\left\{ -\frac{\beta}{M} \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m} \varphi^*_{\mathbf{r},n} (\hat{v}^{\text{ferm}}_{\mathbf{r}\mathbf{r}';nm})^{-1} \varphi_{\mathbf{r}',m} - \frac{1}{s} \sum_{\mathbf{r},n} \chi^*_{\mathbf{r},n}\chi_{\mathbf{r},n} \right.$$

$$\left. + \sum_{\mathbf{r},n} \left[\psi^2_{\mathbf{r},n}\psi^1_{\mathbf{r},n}(\mathrm{i}\varphi^*_{\mathbf{r},n} + \chi^*_{\mathbf{r},n}) + \bar{\psi}^1_{\mathbf{r},n+1}\bar{\psi}^2_{\mathbf{r},n+1}(\mathrm{i}\varphi_{\mathbf{r},n} + \chi_{\mathbf{r},n}) \right] \right\} \prod_{\mathbf{r},n} \frac{\mathrm{d}\varphi^*_{\mathbf{r},n}\mathrm{d}\varphi_{\mathbf{r},n}\mathrm{d}\chi^*_{\mathbf{r},n}\mathrm{d}\chi_{\mathbf{r},n}}{(2\pi\mathrm{i})^2}\ . \tag{8.4}$$

Again, the parameter s cares for the convergence of the integral of the complex field φ. For $\hat{v}^{\text{ferm}}_{\mathbf{r}\mathbf{r}';nm}$ we have the eigenvalues

$$v^{\text{ferm}}_{\mathbf{k},n} = e^{-\mathrm{i}\frac{2\pi}{M}\left(n-\frac{1}{2}\right)} \frac{\beta}{M} \tilde{\epsilon}_{\mathbf{k}} + s\ , \tag{8.5}$$

therefore one has to choose s large enough such that all eigenvalues are non-negative, but besides this condition the choice of s is free. We integrate out the Grassmann field in the functional integral representation of the partition function:

$$\int \exp\left\{\sum_{n=1}^{M}\left[-\sum_{\mathbf{r},\sigma}\bar{\psi}^{\sigma}_{\mathbf{r},n+1}(\psi^{\sigma}_{\mathbf{r},n+1}-\psi^{\sigma}_{\mathbf{r},n})+\frac{\beta\mu}{M}\sum_{\mathbf{r},\sigma}\bar{\psi}^{\sigma}_{\mathbf{r},n+1}\psi^{\sigma}_{\mathbf{r},n}\right.\right.$$

$$\left.\left.+\,\psi^{2}_{\mathbf{r},n}\psi^{1}_{\mathbf{r},n}(\mathrm{i}\varphi^{*}_{\mathbf{r},n}+\chi^{*}_{\mathbf{r},n})+\bar{\psi}^{1}_{\mathbf{r},n+1}\bar{\psi}^{2}_{\mathbf{r},n+1}(\mathrm{i}\varphi_{\mathbf{r},n}+\chi_{\mathbf{r},n})\right]\right\}\prod_{\mathbf{r},n}\mathrm{d}\bar{\eta}_{\mathbf{r},n}\mathrm{d}\eta_{\mathbf{r},n}=\prod_{\mathbf{r}}\det\hat{\mathbb{G}}^{-1}_{\mathbf{r}}\ , \tag{8.6}$$

where we have introduced the matrix

$$\begin{aligned}\hat{\mathbb{G}}^{-1}_{\mathbf{r}} &= \delta_{nm}\begin{pmatrix}\mathrm{i}\varphi_{\mathbf{r},n}+\chi_{\mathbf{r},n} & 1\\ 1 & -(\mathrm{i}\varphi^{*}_{\mathbf{r},n}+\chi^{*}_{\mathbf{r},n})\end{pmatrix}\\ &\quad -(\delta_{n,m+1}-\delta_{n1}\delta_{mM})\begin{pmatrix}0 & 1+\frac{\beta\mu}{M}\\ 1-\frac{\beta\mu}{M} & 0\end{pmatrix}\ .\end{aligned} \tag{8.7}$$

For the grand canonical partition function we obtain the expression

$$Z_{\mathrm{ferm}}=\int\exp\left[-\tilde{A}_{\mathrm{ferm}}(\varphi^{*},\varphi,\chi^{*},\chi)\right]\prod_{\mathbf{r},n}\frac{\mathrm{d}\varphi^{*}_{\mathbf{r},n}\mathrm{d}\varphi_{\mathbf{r},n}\mathrm{d}\chi^{*}_{\mathbf{r},n}\mathrm{d}\chi_{\mathbf{r},n}}{(2\pi\mathrm{i})^{2}} \tag{8.8}$$

with the action

$$\tilde{A}_{\mathrm{ferm}}(\varphi^{*},\varphi,\chi^{*},\chi)=\sum_{\mathbf{r},\mathbf{r}'}\sum_{n,m}\varphi^{*}_{\mathbf{r},n}(\hat{v}^{\mathrm{ferm}}_{\mathbf{r}\mathbf{r}';nm})^{-1}\varphi_{\mathbf{r}',m}+\frac{1}{s}\sum_{\mathbf{r},n}\chi^{*}_{\mathbf{r},n}\chi_{\mathbf{r},n}-\sum_{\mathbf{r}}\log\det\hat{\mathbb{G}}^{-1}_{\mathbf{r}}\ . \tag{8.9}$$

A comparison of the two actions in eqs. (7.12) and (8.9) shows that the logarithmic term of the former is decoupled in the time structure (i.e. in the index n) whereas it is contained inside the logarithmic term of the latter.

8.3 Saddle point expansion

The mean-field solution of the paired-fermion model is more complicated than the one of the hard-core Bose model. Under the assumption (7.14) that the mean-field solution is spatially constant, we can Fourier transform the matrix $\hat{\mathbb{G}}^{-1}_{\mathbf{r}}\equiv\hat{\mathbb{G}}^{-1}$ in eq. (8.7) with respect to the discrete-time index:

$$\mathbb{G}^{-1}_{n}=\begin{pmatrix}\mathrm{i}\varphi_{0}+\chi_{0} & 1-e^{-\frac{\mathrm{i}2\pi}{M}\left(n-\frac{1}{2}\right)}\left(1+\frac{\beta\mu}{M}\right)\\ 1-e^{-\frac{\mathrm{i}2\pi}{M}\left(n-\frac{1}{2}\right)}\left(1-\frac{\beta\mu}{M}\right) & -(\mathrm{i}\varphi^{*}_{0}+\chi^{*}_{0})\end{pmatrix}\ . \tag{8.10}$$

By the use of the identity $\sum_{\mathbf{r}',m}(\hat{v}^{\text{ferm}}_{\mathbf{r}\mathbf{r}';nm})^{-1} = (s - \beta J/M)^{-1}$ we have:

$$\frac{\tilde{A}_0^{\text{ferm}}}{\mathcal{N}M} = \frac{\varphi_0^*\varphi_0}{s+\frac{\beta J}{M}} + \frac{1}{s}\chi_0^*\chi_0$$

$$-\frac{1}{M}\sum_{n=1}^{M}\log\left[-(\mathrm{i}\varphi_0+\chi_0)(\mathrm{i}\varphi_0^*+\chi_0^*) - 1 - e^{-2\frac{\mathrm{i}2\pi}{M}(n-\frac{1}{2})}\left(1-\left(\frac{\beta\mu}{M}\right)^2\right) + 2\,e^{-\frac{\mathrm{i}2\pi}{M}(n-\frac{1}{2})}\right]. \tag{8.11}$$

From the saddle point conditions

$$\frac{\partial\tilde{A}_{\text{ferm}}}{\partial\varphi^*_{\mathbf{r},n}} = \frac{\partial\tilde{A}_{\text{ferm}}}{\partial\varphi_{\mathbf{r},n}} = 0\,, \quad \frac{\partial\tilde{A}_{\text{ferm}}}{\partial\chi^*_{\mathbf{r},n}} = \frac{\partial\tilde{A}_{\text{ferm}}}{\partial\chi_{\mathbf{r},n}} = 0 \tag{8.12}$$

we find the mean-field equations

$$\frac{\chi_0}{s} = -\mathrm{i}G\,, \quad \frac{\varphi_0}{s+\frac{\beta J}{M}} = G\,, \tag{8.13}$$

where

$$G := \frac{1}{M}\sum_{n=1}^{M}\frac{\mathrm{i}(\mathrm{i}\varphi_0+\chi_0)}{1+(\mathrm{i}\varphi_0+\chi_0)(\mathrm{i}\varphi_0^*+\chi_0^*) - 2\,e^{-\frac{\mathrm{i}2\pi}{M}(n-\frac{1}{2})} + \left(1-\left(\frac{\beta\mu}{M}\right)^2\right)e^{-2\frac{\mathrm{i}2\pi}{M}(n-\frac{1}{2})}}\,. \tag{8.14}$$

This sum is performed in Appendix A.2 e) and after taking the $M\to\infty$ limit, the result is

$$G = \frac{J\varphi_0/s}{\sqrt{\mu^2+\left(\frac{J|\varphi_0|}{s}\right)^2}}\tanh\left[\frac{\beta}{2}\sqrt{\mu^2+\left(\frac{J|\varphi_0|}{s}\right)^2}\right]. \tag{8.15}$$

Here, we have used the relation

$$\mathrm{i}\varphi_0+\chi_0 = \mathrm{i}\frac{\beta J\varphi_0}{sM} + \mathcal{O}\left(\frac{1}{M}\right)^2\,, \tag{8.16}$$

which follows from eq. (8.13). Again, we find a trivial solution with $\varphi_0 = \varphi_0^* = \chi_0 = \chi_0^* = 0$ and a non-trivial solution with broken $U(1)$ symmetry. For the mean-field action we find (after integrating G with respect to $\mathrm{i}\varphi_0+\chi_0$):

$$\tilde{A}_0^{\text{ferm}} = \mathcal{N}\left[\frac{\beta J}{s^2}|\varphi_0|^2 - \frac{\beta\mu}{2} - \log\cosh\left(\frac{1}{\beta}\sqrt{\mu^2+\left(\frac{J|\varphi_0|}{s}\right)^2}\right)\right]. \tag{8.17}$$

The level of the Gaussian fluctuations will not be discussed in this thesis because those calculations were not done by me any more. In principle this can be done by expanding $\tilde{A}_{\text{ferm}}$ up to second order around the mean-field solution in the field fluctuations.

8.4 Results for the paired-fermion model

It turns out that even on the mean-field level, the paired-fermion model shows some interesting physical results. This is in contrary to the hard-core Bose model, where the mean-field results vanish in the $M \to \infty$ limit and some interesting physical results have only been found on the level of the Gaussian fluctuations.

The condensate density we get via the definition (2.6) and the mean-field assumption that the CF factorises for large distances:

$$n_0 = \lim_{\mathbf{r}-\mathbf{r}'\to\infty} \langle \bar{\psi}^1_{\mathbf{r},n+1} \bar{\psi}^2_{\mathbf{r},n+1} \psi^2_{\mathbf{r}',n} \psi^1_{\mathbf{r}',n} \rangle = \langle \bar{\psi}^1_{\mathbf{r},n+1} \bar{\psi}^2_{\mathbf{r},n+1} \rangle \langle \psi^2_{\mathbf{r}',n} \psi^1_{\mathbf{r}',n} \rangle \; . \tag{8.18}$$

Further, the CFs which are of second order in the Grassmann field, are given by the diagonal elements of the matrix $\hat{\mathbb{G}}$ whose inverse is given in eq. (8.7), and these diagonal elements are equal to $G/2$ from eq. (8.14):

$$\langle \bar{\psi}^1_{\mathbf{r},n+1} \bar{\psi}^2_{\mathbf{r},n+1} \rangle = \langle \psi^2_{\mathbf{r}',n} \psi^1_{\mathbf{r}',n} \rangle = \frac{G}{2} \implies n_0 \equiv \frac{G^2}{4} \; . \tag{8.19}$$

Thus, from the eqs. (8.15) and (8.19), together with the $M \to \infty$ limit of eq. (8.13), one finds a self-consistent equation for the condensate density:

$$J = \sqrt{\mu^2 + 4J^2\, n_0}\, \coth\left[\frac{\beta}{2}\sqrt{\mu^2 + 4J^2\, n_0}\right] \; . \tag{8.20}$$

The total particle density we get from the mean-field action (8.17):

$$n_{\mathrm{tot}} = -\frac{1}{\beta\mathcal{N}} \frac{\partial \tilde{A}_0^{\mathrm{ferm}}}{\partial \mu} = \frac{1}{2} + \frac{1}{2} \frac{\mu}{\sqrt{\mu^2 + 4J^2\, n_0}} \tanh\left[\frac{\beta}{2}\sqrt{\mu^2 + 4J^2\, n_0}\right] \tag{8.21}$$

$$= \begin{cases} \dfrac{1}{2}\left(1 + \dfrac{\mu}{J}\right) & \text{in the condensed phase } (n_0 > 0) \\[2ex] \dfrac{1}{2}\left[1 + \tanh\left(\dfrac{\beta\mu}{2}\right)\right] & \text{in the non-condensed phase } (n_0 = 0). \end{cases} \tag{8.22}$$

It might be interesting to mention that all these mean-field results do not depend on the parameter s which was introduced in the Hubbard-Stratonovich transformation for the convergence of the Gaussian integral.

The phase boundary between the BEC and the non-condensed phase we get from eq. (8.20) by finding the solution for $n_0 = 0$. The resulting phase diagram is depicted in fig. 8.1. We see in picture *(a)* that for $T > 0$ the phase diagram is separated into two parts, a BEC phase and a non-condensed phase. But at $T = 0$ there are three phases: A BEC, an empty phase ($n_{\mathrm{tot}} = 0$) for $\mu < -J$, and a Mott-insulator ($n_{\mathrm{tot}} = 1$) for

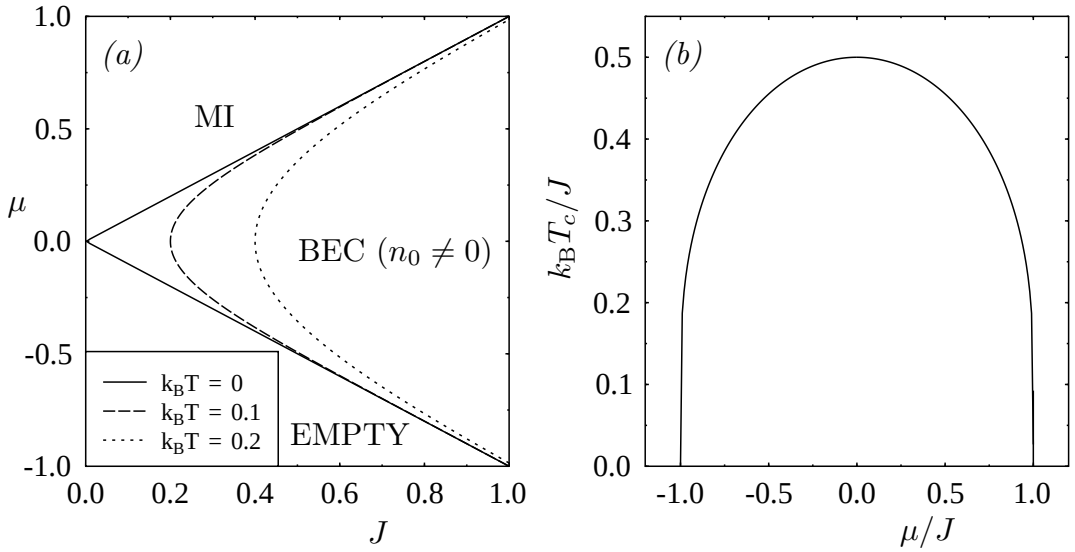

Figure 8.1: *(a)* Phase diagram with phase boundaries between the BEC and the non-condensed phase for different temperatures. For $k_BT \neq 0$ there is only one phase boundary between a BEC and a non-condensed phase. The energy unit is arbitrary because of a simple scaling behaviour. *(b)* Critical temperature of BEC formation.

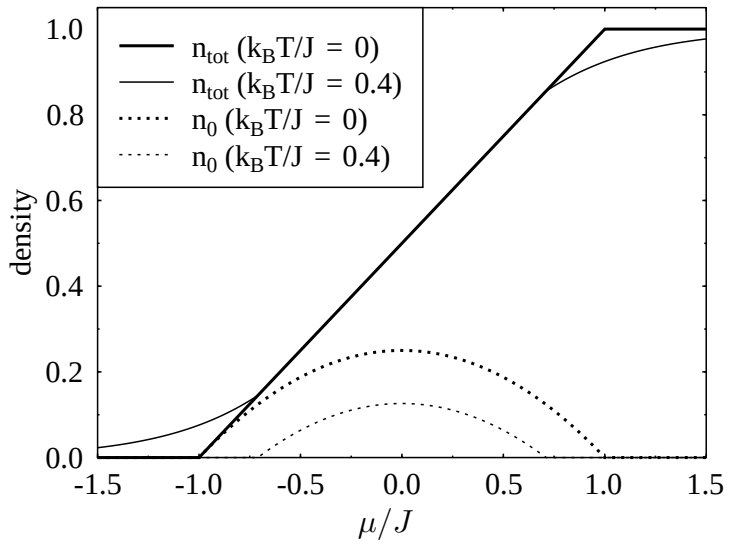

Figure 8.2: Total particle density and condensate density for zero temperature (thick lines, given by eqs. (8.23) and (8.24)) and for non-zero temperature (thin lines) plotted against chemical potential.

$\mu > J$. Recall that for the hard-core Bose model the only phase boundary is the one given by the equation $\mu = -J$ and is independent of temperature. A density profile of n_{tot} and n_0 is plotted in fig. 8.2. At zero temperature the sharp transitions between the empty phase and the BEC, and the BEC and the MI, can be seen on the plot of the total particle density. The zero temperature result is

$$n_0 = \begin{cases} \frac{1}{4}\left(1 - \frac{\mu^2}{J^2}\right) & \text{if } -J < \mu < J \\ 0 & \text{else ,} \end{cases} \tag{8.23}$$

$$n_{\text{tot}} = \begin{cases} 0 & \text{if } \mu \leq -J \\ \frac{1}{2}\left(1 - \frac{\mu}{J}\right) & \text{if } -J < \mu < J \\ 1 & \text{if } J \leq \mu \,. \end{cases} \tag{8.24}$$

If the temperature increases, the sharp transitions are smeared out. It might be interesting to mention that in the zero temperature limit near the phase transition to the empty phase where $\mu = -J + \Delta\mu$ with $\Delta\mu \ll J$, i.e. in the dilute regime, it is possible to approximate

$$n_0 = \frac{\Delta\mu}{2J} + \mathcal{O}(\Delta\mu^2) = n_{\text{tot}} + \mathcal{O}(\Delta\mu^2) \,. \tag{8.25}$$

After neglecting the term of order $\Delta\mu^2$, this agrees with the Gross-Pitaevskii result (5.6), if the identification $g \equiv 2J$ is made.

Calculations for the quasiparticle spectrum by finding the poles of the Green's matrix $\hat{\mathcal{G}}$ of the Gaussian fluctuations have been made for the zero temperature phase diagram [77]. The zero temperature result in the empty phase and in the MI phase is

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + |\mu| - J \,, \tag{8.26}$$

with the gap $\Delta = |\mu| - J$, and in the BEC phase it is

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} \left[J \left(1 - \left(\frac{\mu}{J}\right)^2 \right) + \left(\frac{\mu}{J}\right)^2 \epsilon_{\mathbf{k}} \right]} \,. \tag{8.27}$$

These spectra agree with the results for the hard-core Bose model given in the eqs. (7.32) and (7.33) near the phase boundary between the empty phase and the BEC, i.e. if $\mu = -J(1 - \delta)$, with $\delta \ll 1$. In analogy with the result (7.44), the static structure factor is given as

$$S(\mathbf{q}) = \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \coth\left(\frac{\beta}{2} E_{\mathbf{k}}\right) \tag{8.28}$$

in the BEC phase.

In conclusion, we can say that the paired-fermion model reveals more interesting physics than the hard-core Bose model. At zero temperature it shows three phases, an empty phase, a MI, and a BEC, even on the mean-field level. In the hard-core Bose

model, the MI phase is not found. The empty phase and the MI vanish at non-zero temperatures. As mentioned at the beginning of this chapter, the differences between both models is assumed to arise from the different Hubbard-Stratonovich decouplings in the first place, which has a significant influence on the type mean-field theory.

9 Slave boson model

9.1 Hamiltonian and functional integral

In this chapter it shall be shown that a slave-boson approach can be applied to describe a system of hard-core bosons. The slave boson representation was originally developed for fermion systems, e.g. the Hubbard model [78, 79]. It allows to account for many aspects of strong correlations even on the mean-field level. The slave-boson approach to hard-core bosons that will be presented here, has been developed in the refs. [69, 80, 81, 82]. It is an alternative to the fermionic models which were discussed in the previous chapter.

Again, the starting point is the Hamiltonian

$$\hat{H}_{\rm hc} = -\frac{J}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \hat{a}^+_{\mathbf{r}} \hat{a}_{\mathbf{r}'} + \sum_{\mathbf{r}} V_{\mathbf{r}}\, \hat{a}^+_{\mathbf{r}} \hat{a}_{\mathbf{r}} \ , \tag{9.1}$$

where $\hat{a}^+_{\mathbf{r}}$, $\hat{a}_{\mathbf{r}}$ are the creation- and annihilation operators of hard-core bosons with the property $\hat{a}^2_{\mathbf{r}} = (\hat{a}^+_{\mathbf{r}})^2 = 0$. The Fock space of the system is given by the direct product (2.50). The operators act locally on the two-dimensional subspace of a given lattice site $\mathbf{r}$:

$$\hat{a}^+_{\mathbf{r}} |0\rangle_{\mathbf{r}} = |1\rangle_{\mathbf{r}} \quad ; \quad \hat{a}_{\mathbf{r}} |1\rangle_{\mathbf{r}} = |0\rangle_{\mathbf{r}} \ . \tag{9.2}$$

We extend the basis of the Fock space by decomposing the original occupation number states $|n_{\mathbf{r}}\rangle_{\mathbf{r}}$ as $|n^e_{\mathbf{r}}, n^b_{\mathbf{r}}\rangle_{\mathbf{r}}$, where $n^e_{\mathbf{r}}$ is the number of empty sites, and $n^b_{\mathbf{r}}$ is the number of occupies sites. Furthermore we introduce bosonic creation- and annihilation operators of unoccupied ($\hat{e}^+_{\mathbf{r}}$, $\hat{e}_{\mathbf{r}}$) and occupied ($\hat{b}^+_{\mathbf{r}}$, $\hat{b}_{\mathbf{r}}$) sites which act on the extended Fock space ("slaves"), such that

$$\hat{e}^+_{\mathbf{r}} |0,0\rangle_{\mathbf{r}} = |1,0\rangle_{\mathbf{r}} \ , \quad \hat{b}^+_{\mathbf{r}} |0,0\rangle_{\mathbf{r}} = |0,1\rangle_{\mathbf{r}} \ .$$

In the hard-core Bose system the condition $n^e_{\mathbf{r}} + n^b_{\mathbf{r}} = 1$ has to be fulfilled, to assure that a lattice site $\mathbf{r}$ is either empty or occupied by a boson. Thus only the two states $|1,0\rangle_{\mathbf{r}}$ (empty site) and $|0,1\rangle_{\mathbf{r}}$ (occupied site) are physical. To ensure this condition, we impose the constraint

$$\hat{b}^+_{\mathbf{r}} \hat{b}_{\mathbf{r}} + \hat{e}^+_{\mathbf{r}} \hat{e}_{\mathbf{r}} = 1. \tag{9.3}$$

To transfer the Hamiltonian to the extended Fock space, we replace the hard-core Bose operators by

$$\hat{a}^+_{\mathbf{r}} \rightarrow \hat{b}^+_{\mathbf{r}} \hat{e}_{\mathbf{r}} \quad ; \quad \hat{a}_{\mathbf{r}} \rightarrow \hat{e}^+_{\mathbf{r}} \hat{b}_{\mathbf{r}} \ . \tag{9.4}$$

Then the Hamiltonian is replaced by

$$\hat{H}_{\mathrm{hc}} \to \hat{H}_{\mathrm{sb}} = -\frac{J}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \hat{b}^+_{\mathbf{r}} \hat{e}_{\mathbf{r}} \hat{e}^+_{\mathbf{r}'} \hat{b}_{\mathbf{r}'} + \sum_{\mathbf{r}} V_{\mathbf{r}}\, \hat{b}^+_{\mathbf{r}} \hat{b}_{\mathbf{r}} \; . \tag{9.5}$$

A hopping process can be understood as a swapping of an occupied site and an empty site: Annihilation of a particle and creation of a hole at site $\mathbf{r}'$, creation of a particle and annihilation of a hole at site $\mathbf{r}$. The occupation number operator of site $\mathbf{r}$ is $\hat{b}^+_{\mathbf{r}} \hat{b}_{\mathbf{r}}$.

A similar theory for the Bose-Hubbard model has been established in refs. [83, 84]. In this case, an infinite number of operators $(\hat{b}^{\alpha}_{\mathbf{r}})^+$, $\hat{b}^{\alpha}_{\mathbf{r}}$ for each occupation number α has to be introduced at each lattice site, because multiple occupation is possible. In this respect, the slave-boson approach for hard-core bosons is much simpler. The grand canonical partition function of the system given by the bosonic Hamiltonian (9.5), can be expressed as a functional integral with two complex fields $b_{\mathbf{r}}(\tau)$ and $e_{\mathbf{r}}(\tau)$. The constraint $|b_{\mathbf{r}}(\tau)|^2 + |e_{\mathbf{r}}(\tau)|^2 = 1$ is enforced by a δ-function in the integration measure. Again we discretise the imaginary time τ into M equidistant steps and denote each time step by an index n:

$$Z_{\mathrm{sb}} = \int \mathrm{e}^{-A[b,b^*,e,e^*]}\, \mathcal{D}[b,b^*,e,e^*] \; , \tag{9.6}$$

with the integration measure

$$\mathcal{D}[b,b^*,e,e^*] = \lim_{M\to\infty} \prod_{\mathbf{r},n} \left(|b_{\mathbf{r},n}|^2 + |e_{\mathbf{r},n}|^2 - 1 \right) \mathrm{d}b_{\mathbf{r},n} \mathrm{d}b^*_{\mathbf{r},n} \mathrm{d}e_{\mathbf{r},n} \mathrm{d}e^*_{\mathbf{r},n} \tag{9.7}$$

and the action

$$\begin{aligned} A[b,b^*,e,e^*] = \lim_{M\to\infty} \sum_{n=1}^{M} \Bigg\{ \sum_{\mathbf{r}} \Bigg[b^*_{\mathbf{r},n+1} \left(b_{\mathbf{r},n+1} - \left(1 + \frac{\beta}{M} \mu_{\mathbf{r}} \right) b_{\mathbf{r},n} \right) \\ - e^*_{\mathbf{r},n+1} \left(e_{\mathbf{r},n+1} - e_{\mathbf{r},n} \right) \Bigg] - \frac{J}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} b^*_{\mathbf{r},n+1} e_{\mathbf{r},n} e^*_{\mathbf{r}',n+1} b_{\mathbf{r}',n} \Bigg\} \; , \end{aligned} \tag{9.8}$$

where the space-dependent chemical potential is $\mu_{\mathbf{r}} = \mu - V_{\mathbf{r}}$. Using a continuous time variable τ the action can be written as

$$\begin{aligned} A[b,b^*,e,e^*] = \frac{1}{\hbar} \int_0^{\hbar\beta} \mathrm{d}\tau \Bigg\{ \sum_{\mathbf{r}} b^*_{\mathbf{r}}(\tau) \left(\hbar \frac{\partial}{\partial \tau} - \mu_{\mathbf{r}} \right) b_{\mathbf{r}}(\tau) + \sum_{\mathbf{r}} e^*_{\mathbf{r}}(\tau)\, \hbar \frac{\partial}{\partial \tau} e_{\mathbf{r}}(\tau) \\ - \frac{J}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} b^*_{\mathbf{r}}(\tau) e_{\mathbf{r}}(\tau) e^*_{\mathbf{r}'}(\tau) b_{\mathbf{r}'}(\tau) \Bigg\} \; . \end{aligned} \tag{9.9}$$

9.2 Two-fluid theory in classical approximation

The hopping term of the action is of forth order in the field variables. Therefore it is not possible to perform the integration directly. However, it is possible to decouple the hopping term by introducing two new fields, a complex field Φ and a real field φ, and perform a Hubbard-Stratonovich transformation. The fields b and e can be integrated out then, and a mean-field approximation can be applied to the fields Φ and φ.

The idea of the Hubbard-Stratonovich decoupling is similar to the one used in the chapters 7 and 8 to decouple the forth order terms of the Grassmann fields. For simplicity we will proceed with the continuous-time notation of the action like given in eq. (9.9). We insert the identity

$$\begin{aligned}\text{const.} \times e^{-A[b,b^*,e,e^*]} = \int \exp\Bigg\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \Bigg[\sum_{\mathbf{r},\mathbf{r}'} \Phi^*_{\mathbf{r}}(\tau) \left[\frac{s-\hat{J}}{s^2}\right]^{-1}_{\mathbf{r}\mathbf{r}'} \Phi_{\mathbf{r}}(\tau) + s\sum_{\mathbf{r}} \varphi_{\mathbf{r}}(\tau)^2 \\ + \sum_{\mathbf{r}} (e_{\mathbf{r}}(\tau), b_{\mathbf{r}}(\tau)) \begin{pmatrix} 2s\varphi_{\mathbf{r}}(\tau) + s + \hbar\frac{\partial}{\partial\tau} & s\Phi_{\mathbf{r}}(\tau) \\ s\Phi^*_{\mathbf{r}}(\tau) & -\mu_{\mathbf{r}} + \hbar\frac{\partial}{\partial\tau} \end{pmatrix} \begin{pmatrix} e^*_{\mathbf{r}}(\tau) \\ b^*_{\mathbf{r}}(\tau) \end{pmatrix} \Bigg] \Bigg\} \mathcal{D}[\Phi^*, \Phi, \varphi] \,,\end{aligned} \tag{9.10}$$

with the integration measure

$$\mathcal{D}[\Phi^*, \Phi, \varphi] = \prod_{\mathbf{r},\tau} \frac{\mathrm{d}\Phi^*_{\mathbf{r}}(\tau)\mathrm{d}\Phi_{\mathbf{r}}(\tau)\mathrm{d}\varphi_{\mathbf{r}}(\tau)}{(2\pi)^{3/2}} \,. \tag{9.11}$$

Here, $\hat{J}$ is the hopping matrix (4.40). The constant factor is of no physical relevance. Like for the two fermionic models which were discussed before, the parameter s takes care for the convergence of the Gaussian integral. It has the unit of an energy and should not be too small compared to J. Although the exact identity does not depend on s, we will see subsequently that the mean-field equation we will derive, does. This is a difference to the previously discussed models, where the results which were derived on the mean-field level and on the level of Gaussian fluctuations, did not depend on the free parameter s.

After substituting the identity (9.10) into the functional integral (9.9), the integral with respect to the fields b and e are only of second order. However, it is not known how to integrate out the constraint because of the time-derivative in the quadratic form. Therefore it is advisable to use the so-called classical approximation here. This means that for the fields in Matsubara representation

$$\Phi_{\mathbf{r}}(\tau) = \sum_n \Phi_{\mathbf{r},\omega_n} e^{\mathrm{i}\omega_n\tau} \,; \quad \Phi^*_{\mathbf{r}}(\tau) = \sum_n \Phi^*_{\mathbf{r},\omega_n} e^{-\mathrm{i}\omega_n\tau} \,; \quad \varphi_{\mathbf{r}}(\tau) = \sum_n \varphi_{\mathbf{r},\omega_n} \cos(\omega_n\tau) \,,$$

with the bosonic Matsubara frequencies (4.11), only the terms with Matsubara frequency $\omega_0 = 0$ is taken into account, if one assumes that

$$\Phi_{\mathbf{r},\omega_n} \approx \Phi^*_{\mathbf{r},\omega_n} \approx \varphi_{\mathbf{r},\omega_n} \approx 0 \,, \quad \text{if } n \neq 0. \tag{9.12}$$

Because the Matsubara frequencies are separated from each other by a gap of the magnitude $2\pi k_\mathrm{B}T/\hbar$, this is the case if the temperature is not too low, such that quantum fluctuations (which are neglected in the classical approximation) are small compared to thermal fluctuations. It has been used e.g. in ref. [85] to calculate corrections to the critical temperature T_c of BEC formation in a homogeneous weakly interacting Bose gas in variational perturbation theory. A consequence of the classical approximation is, that all energies scale with the thermal energy $k_\mathrm{B}T$.

Because the derivative with respect to imaginary time only acts on the parts with non-vanishing Matsubara frequency, it vanishes in the classical approximation, and the fields can be approximated by

$$\Phi_\mathbf{r}(\tau) \approx \Phi_{\mathbf{r},\omega_0} \; ; \quad \Phi^*_\mathbf{r}(\tau) \approx \Phi^*_{\mathbf{r},\omega_0} \; ; \quad \varphi_\mathbf{r}(\tau) \approx \varphi_{\mathbf{r},\omega_0} \; ,$$

where in the following we will drop the index ω_0 such that the fields only depend on space. Thus the grand canonical partition function in classical approximation is given by the expression

$$\begin{aligned} Z_\mathrm{sb} \;=\; \int \exp\Bigg\{ -\beta \Bigg[\sum_{\mathbf{r},\mathbf{r}'} \Phi^*_\mathbf{r} \left[\frac{s-\hat{J}}{s^2} \right]^{-1}_{\mathbf{r}\mathbf{r}'} \Phi_{\mathbf{r}'} + s \sum_\mathbf{r} \varphi^2_\mathbf{r} \\ + \sum_\mathbf{r} (e_\mathbf{r}, b_\mathbf{r}) \begin{pmatrix} 2s\varphi_\mathbf{r} + s & s\Phi_\mathbf{r} \\ s\Phi^*_\mathbf{r} & -\mu_\mathbf{r} \end{pmatrix} \begin{pmatrix} e^*_\mathbf{r} \\ b^*_\mathbf{r} \end{pmatrix} \Bigg] \Bigg\} \mathcal{D}[\Phi^*, \Phi, \varphi]\, \mathcal{D}[b, b^*, e, e^*] \; . \end{aligned} \tag{9.13}$$

Integration over the fields Φ and φ leads back to the expression

$$Z_\mathrm{sb} = \int \exp\left[-\frac{\beta J}{2d} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} b^*_\mathbf{r} e_\mathbf{r} e^*_{\mathbf{r}'} b_{\mathbf{r}'} + \beta \sum_\mathbf{r} \mu_\mathbf{r} b^*_\mathbf{r} b_\mathbf{r} \right] \mathcal{D}[b, b^*, e, e^*] \; , \tag{9.14}$$

which is the classical approximation of the partition function (9.6). On the other hand, the fields b and e together with the constraint in the integration measure, can be integrated out exactly. This is shown in Appendix E.1. The result for the partition function is

$$Z_\mathrm{sb} = \int e^{-\tilde{A}(\Phi^*,\Phi)} \prod_\mathbf{r} \mathrm{d}\Phi_\mathbf{r} \mathrm{d}\Phi^*_\mathbf{r} \tag{9.15}$$

with the new action

$$\tilde{A}(\Phi^*, \Phi) = \beta \sum_{\mathbf{r},\mathbf{r}'} \Phi^*_\mathbf{r} \left[\frac{s-\hat{J}}{s^2} \right]^{-1}_{\mathbf{r}\mathbf{r}'} \Phi_{\mathbf{r}'} - \sum_\mathbf{r} \log \left[Z'_\mathbf{r}\, e^{\frac{\beta\mu_\mathbf{r}}{4}} \right] \; , \tag{9.16}$$

and the function

$$Z'_\mathbf{r} = \int_{-\infty}^{\infty} \mathrm{d}\varphi_\mathbf{r} \, \frac{\sinh\left[\beta \sqrt{\left(\varphi_\mathbf{r} s + \frac{\mu_\mathbf{r}}{2}\right)^2 + s^2 |\Phi_\mathbf{r}|^2} \right]}{\beta \sqrt{\left(\varphi_\mathbf{r} s + \frac{\mu_\mathbf{r}}{2}\right)^2 + s^2 |\Phi_\mathbf{r}|^2}} e^{-\beta s \varphi^2_\mathbf{r}} \; . \tag{9.17}$$

Note that the action $\tilde{A}(\Phi^*, \Phi)$ does not depend on the real field $\varphi_{\mathbf{r}}$ explicitly, because it appears inside the function Z' only as an integration variable.

The form (9.15) of the grand canonical partition function can be understood as a two-fluid theory. It is shown in Appendix E.2 that the condensate density is related to the field Φ and is given by the relation

$$n_0 \approx \frac{s^2}{(s+J)^2} \lim_{\mathbf{r}-\mathbf{r}'\to\infty} \langle \Phi_{\mathbf{r}} \Phi^*_{\mathbf{r}'} \rangle \ , \tag{9.18}$$

and that the total particle density at site $\mathbf{r}$ is related to the field $\varphi_{\mathbf{r}}$ by means of the expectation value

$$n_{\mathbf{r}} = \langle \varphi_{\mathbf{r}} \rangle + \frac{1}{2} \ . \tag{9.19}$$

9.3 Mean-field theory

A mean-field solution is found by minimising the action via the variational principle $\delta \tilde{A} = 0$, which leads to a saddle point approximation, the way like it was done for the previously discussed models. Because the field φ can be integrated out (e.g. numerically) inside the function $Z'_{\mathbf{r}}$ given in eq. (9.17), minimisation has to be done with respect to the complex field Φ only:

$$\frac{\partial \tilde{A}}{\partial \Phi_{\mathbf{r}}} = \frac{\partial \tilde{A}}{\partial \Phi^*_{\mathbf{r}}} = 0 \ . \tag{9.20}$$

This yields the mean-field equation, which is a discretised equivalent to the stationary Gross-Pitaevskii (GP) eq. (2.16):

$$\sum_{\mathbf{r}'} \left[\frac{s - \hat{J}}{s^2} \right]^{-1}_{\mathbf{r}\mathbf{r}'} \Phi_{\mathbf{r}'} - \frac{1}{\beta} \left[\frac{\partial}{\partial(|\Phi_{\mathbf{r}}|^2)} \log Z'_{\mathbf{r}} \right] \Phi_{\mathbf{r}} = 0 \ . \tag{9.21}$$

In the case of a spatially constant field without external trapping potential, i.e. if we assume that $\Phi_{\mathbf{r}} \equiv \Phi_0$ and $\mu_{\mathbf{r}} \equiv \mu$, the mean-field equation is

$$\frac{s^2}{s+J} - \frac{1}{\beta} \frac{\partial}{\partial(|\Phi_0|^2)} \log Z' = 0 \ . \tag{9.22}$$

If the field $\Phi_{\mathbf{r}}$ is varying only very slowly between neighbouring lattice sites, we can approximate

$$\sum_{\mathbf{r}'} \left[\frac{s - \hat{J}}{s^2} \right]^{-1}_{\mathbf{r}\mathbf{r}'} \Phi_{\mathbf{r}'} \approx \frac{s^2}{s+J} \Phi_{\mathbf{r}} + \frac{s^2}{(s+J)^2} \sum_{\mathbf{r}'} \left(J \, \delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'} \right) \Phi_{\mathbf{r}'} \ . \tag{9.23}$$

It turns out that the mean-field result depends significantly on the freely arbitrary parameter s. This is a difference to the calculations which were shown before for the

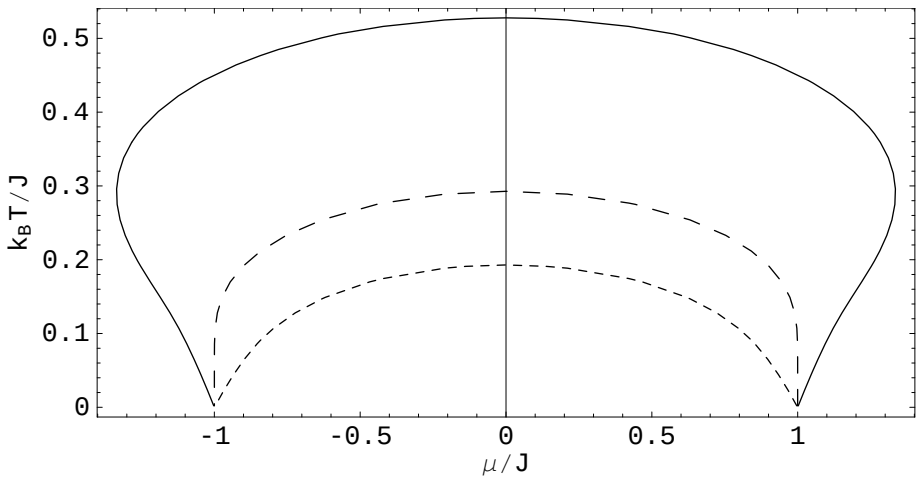

Figure 9.1: Phase boundary between the BEC and the non-condensed phase for $s/J = 3$ (solid line), $s/J = 1$ (long dashes), $s/J = 0.2$ (short dashes). Compare these graphs with the right graph of fig. 8.1, where the critical temperature of the mean-field result for the paired-fermion model is plotted.

hard-core Bose model and the paired-fermion model, and where the mean-field results did not depend on s. The dependence of the mean-field theory on s reflects the ambiguity of the Hubbard-Stratonovich decoupling. Although the decoupling is exact, the resulting mean-field theory can depend on the applied form of the decoupling, which was chosen out of many possibilities. In in fig. 9.1 the phase boundary between the BEC and the non-condensed phase is plotted for different values of s. The phase boundary solves eq. (9.22) for $\Phi_0 = 0$, and has been calculated numerically.

One can see that the BEC phase forms a "bubble" in the phase diagram, if $s/J > 1$. This behaviour is unexpected because the BEC phase should become narrower, if temperature is increased. This means that for too large values of s/J the mean-field theory seems to be incorrect, therefore it is reasonable to keep it smaller than 1.

It is possible to find an exact solution for zero temperature, which does *not* depend on s. This calculation is shown in Appendix E.3. Two phase boundaries are found: A boundary between the BEC and an empty phase with $\mu_c = -J$ and a phase boundary between the BEC and the Mott-insulator with $\mu_c = J$. It is identical to the zero temperature mean-field result in eqs. (8.23) and (8.24) that was found for the paired-fermion model, and agrees with it qualitatively at finite temperatures (see fig. 9.2). When temperature increases, results strongly depend on s.

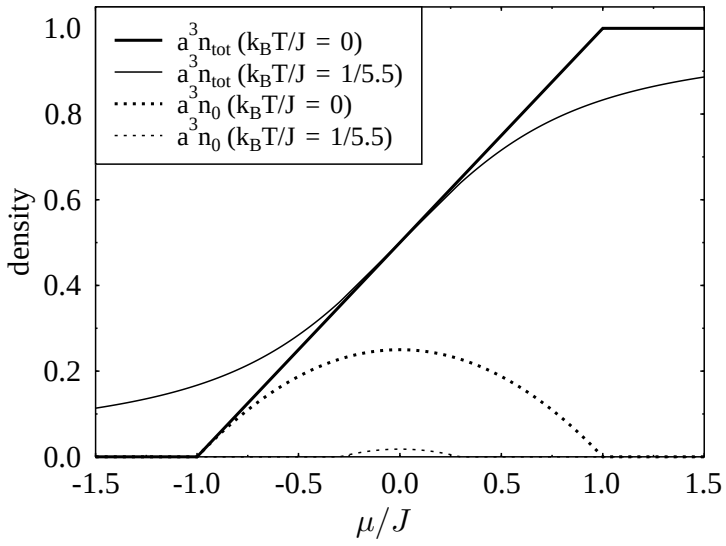

Figure 9.2: Total particle density and condensate density for zero temperature (thick lines) and for non-zero temperature (thin lines, $s/J = 1/5.5$) against chemical potential. Compare this graph with the result for the paired-fermion model plotted in fig. 8.2.

9.4 Quasiparticle spectrum

We get the quasiparticle spectrum from the Gaussian fluctuations, the same way as it was done for the hard-core Bose model and the paired-fermion model. We write

$$\Phi_{\mathbf{r}} = \Phi_0 + \delta\Phi_{\mathbf{r}} \,, \quad \Phi^*_{\mathbf{r}} = \Phi^*_0 + \delta\Phi^*_{\mathbf{r}} \,,$$

and assume that the fluctuations $\delta\Phi$, $\delta\Phi^*$ about the mean-field solution Φ_0 are small. Substituting this expression into the action (9.16), and expanding it up to second order in the fluctuations, one finds

$$\tilde{A} = \beta \frac{s^2}{s+J} |\Phi_0|^2 - \log Z' \left(|\Phi_0|^2\right) - \frac{\beta}{2} \sum_{\mathbf{r},\mathbf{r}'} (\delta\Phi_{\mathbf{r}}, \delta\Phi^*_{\mathbf{r}}) \, \hat{\mathcal{G}}^{-1}_{\mathbf{r}\mathbf{r}'} \begin{pmatrix} \delta\Phi^*_{\mathbf{r}'} \\ \delta\Phi_{\mathbf{r}'} \end{pmatrix} \,, \tag{9.24}$$

with the matrix

$$\hat{\mathcal{G}}^{-1}_{\mathbf{r}\mathbf{r}'} = \begin{pmatrix} \frac{J\,\delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'}}{s+J} + (\tilde{a}_2 + |\Phi_0|^2 \tilde{a}_4)\delta_{\mathbf{r}\mathbf{r}'} & (\Phi^*_0)^2 \, \tilde{a}_4 \delta_{\mathbf{r}\mathbf{r}'} \\ \Phi_0^2 \, \tilde{a}_4 \delta_{\mathbf{r}\mathbf{r}'} & \frac{J\,\delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'}}{s+J} + (\tilde{a}_2 + |\Phi_0|^2 \tilde{a}_4)\delta_{\mathbf{r}\mathbf{r}'} \end{pmatrix} \,. \tag{9.25}$$

Here, we have introduced the abbreviations

$$\tilde{a}_2 := -\frac{1}{\beta}\frac{\partial}{\partial(|\Phi|^2)}\log Z'\Big|_{\Phi=\Phi_0} + \frac{s^2}{s+J}\,, \tag{9.26}$$

$$\tilde{a}_4 := -\frac{1}{\beta}\frac{\partial^2}{\partial(|\Phi|^2)^2}\log Z'\Big|_{\Phi=\Phi_0}\,, \tag{9.27}$$

and used the approximation in eq. (9.23). The matrix $\mathcal{G}$ has no time-structure because of the classical approximation. To find the Green's function of quasiparticles, we *artificially* introduce the imaginary time by writing

$$\hat{\mathcal{G}}^{-1}_{\mathbf{r}\mathbf{r}'} = \begin{pmatrix} \frac{J\,\delta_{\mathbf{r}\mathbf{r}'}+\hat{J}_{\mathbf{r}\mathbf{r}'}+\hbar\frac{\partial}{\partial\tau}}{s+J} + \tilde{a}_2 + |\Phi_0|^2\tilde{a}_4\delta_{\mathbf{r}\mathbf{r}'} & (\Phi_0^*)^2\,\tilde{a}_4\delta_{\mathbf{r}\mathbf{r}'} \\ \Phi_0^2\,\tilde{a}_4\delta_{\mathbf{r}\mathbf{r}'} & \frac{J\,\delta_{\mathbf{r}\mathbf{r}'}+\hat{J}_{\mathbf{r}\mathbf{r}'}-\hbar\frac{\partial}{\partial\tau}}{s+J} + \tilde{a}_2 + |\Phi_0|^2\tilde{a}_4\delta_{\mathbf{r}\mathbf{r}'} \end{pmatrix}, \tag{9.28}$$

which has the same structure as the matrix which is given in (5.36) where the interacting Bose gas was treated in Bogoliubov theory. After a Fourier transformation it leads to the Green's function

$$\hat{\mathcal{G}}^{-1}(\mathbf{k},\omega_n) = \frac{s^2}{(s+J)^2}\begin{pmatrix} \epsilon_{\mathbf{k}} + \frac{(s+J)^2}{s^2}\tilde{a}_2 & \mathrm{i}\hbar\omega_n \\ \mathrm{i}\hbar\omega_n & \epsilon_{\mathbf{k}} + \frac{(s+J)^2}{s^2}\left(\tilde{a}_2 + 2\tilde{a}_4|\Phi_0|^2\right) \end{pmatrix}, \tag{9.29}$$

which is the equivalent to the matrix (5.47), and $\epsilon_{\mathbf{k}}$ is the lattice dispersion (4.7). The quasiparticle spectrum is given by the poles of $\hat{\mathcal{G}}$, and can be found by performing the analytic continuation $\mathrm{i}\hbar\omega_n \to E_{\mathbf{k}}$ and solving the equation $\det\hat{\mathcal{G}}^{-1} = 0$. We find solutions for both the BEC phase and the non-condensed phase:

Condensed phase

In the BEC phase, where $|\Phi_0|^2 > 0$, the coefficient $\tilde{a}_2$ vanishes, because Φ_0 solves the mean-field equation (9.22), which is equivalent to $\tilde{a}_2 = 0$. The solution is

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}\left(2\,\frac{(s+J)^2}{s^2}\,\tilde{a}_4\,|\Phi_0|^2 + \epsilon_{\mathbf{k}}\right)}\,. \tag{9.30}$$

It is gapless and agrees with the Bogoliubov spectrum (5.11), when the identifications $n_0 = s^2|\Phi_0|^2/(s+J)^2$ and $g = (s+J)^4\tilde{a}_4/s^4$ are made, where g is the interaction constant given in eq. (2.4). The coefficient $\tilde{a}_4$ depends on both temperature and chemical potential. Its zero temperature result is given in the Appendix E.3 in eq. (E.11). In the dilute gas (i.e. near the phase transition to the empty phase) where $n_0 \ll 1$, we find at zero temperature for the interaction constant the result $g \approx 2J$.

Non-condensed phase

In the non-condensed phase, where $|\Phi_0|^2 = 0$ and $\tilde{a}_2 \neq 0$, the quasiparticle spectrum is gapped, in agreement to the findings of the hard-core Bose and paired-fermion models:

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Delta \,, \tag{9.31}$$

with the gap $\Delta = (s+J)^2\tilde{a}_2/s^2$. At zero temperature and near the phase transitions, we find the result $\Delta = |\mu - \mu_c| + \mathcal{O}((\mu-\mu_c)^2)$ which is identical to the zero temperature result (8.26) for the composed-fermion model.

9.5 Renormalised Gross-Pitaevskii equation

In this section we will derive a mean-field equation which is appropriate to describe the condensate order parameter in a strongly interacting Bose gas, and which is similar to the stationary Gross-Pitaevskii eq. (2.16). In the absence of a trapping potential, a solution of the stationary GP equation is given by

$$n_0 = |\Phi_0|^2 = \frac{\mu}{g} \,. \tag{9.32}$$

This describes a linearly increasing condensate density n_0 with respect to the chemical potential. Although it takes the repulsion into account by a factor $1/g$ which is decreasing with increasing coupling constant g, the saturation of n_0 cannot be seen in this solution. From the physical point of view, in a realistic description for large densities, the particle density must saturate because there is a finite scattering volume around each particle. Furthermore, for increasing particle density, the condensate density should reach a maximum and for even larger densities, decrease again until its total destruction, because of the increasing interparticle interaction. This is the behaviour that we found for the slave-boson model in mean-field approximation (see fig. 9.2). A similar behaviour has also been found by variational perturbation theory [70], and diffusion Monte Carlo calculations [86]. In other words, the strong effect of the repulsion in a dense condensate is not really described by the conventional GP equation. In order to describe condensates at higher densities, the second order term in the low-density expansion of the energy density has been taken into account which leads to a modified GP theory [10, 86, 87, 88].

Although in many experimentally realised situations the BEC is in the weakly interacting regime where it is well described by GP theory, it might be possible to reach the strongly interacting regime. The main problem at high particle densities is the instability of the Bose gas by the formation of molecules due to three-particle interactions [89]. Here, we will assume that molecule formation does not occur. This might be unrealistic for some systems, but in others it is not, e.g. for Bose gases in optical lattices.

The mean-field equation for a hard-core Bose gas in an optical lattice within the slave-boson approach is given by

$$\frac{s^2}{(s+J)^2}\sum_{\mathbf{r}'}\left(J\,\delta_{\mathbf{r}\mathbf{r}'}+\hat{J}_{\mathbf{r}\mathbf{r}'}\right)\,\Phi_{\mathbf{r}'}+\frac{s^2}{s+J}\,\Phi_{\mathbf{r}}-\frac{1}{\beta}\left[\frac{\partial}{\partial(|\Phi_{\mathbf{r}}|^2)}\log Z'_{\mathbf{r}}\right]\Phi_{\mathbf{r}}=0\;. \tag{9.33}$$

This we get by applying the approximation (9.23) in eq. (9.21). However, it also possible to describe a system of strongly interacting bosons without lattice potential within this approximation. Therefore we perform a continuum approximation of the hopping term: If the lattice constant a is so small that the order parameter $\Phi_{\mathbf{r}}$ varies only slowly over neighbouring lattice sites, we can treat the 3-dimensional lattice approximately as a continuum:

$$\sum_{\mathbf{r}'}\left(J\,\delta_{\mathbf{r}\mathbf{r}'}+\hat{J}_{\mathbf{r}\mathbf{r}'}\right)\,\Phi_{\mathbf{r}'}=-\frac{Ja^2}{6}\sum_{j=1}^{3}\frac{\Phi_{\mathbf{r}+a\mathbf{e}_j}-2\Phi_{\mathbf{r}}+\Phi_{\mathbf{r}-a\mathbf{e}_j}}{a^2}\approx-\frac{Ja^2}{6}\nabla^2\Phi_{\mathbf{r}}\;. \tag{9.34}$$

When working on the continuum, we renormalise the order parameter by writing

$$\Phi(\mathbf{r}):=a^{-3/2}\Phi_{\mathbf{r}}\;, \tag{9.35}$$

such that the action (9.16) can be written as

$$\begin{aligned}\tilde{A}(\Phi^*,\Phi)\;\;=\;\;&\frac{\beta s^2}{(s+J)^2}\int\Bigg\{-\frac{Ja^2}{6}\Phi^*(\mathbf{r})\nabla^2\Phi(\mathbf{r})+(s+J)|\Phi(\mathbf{r})|^2\\&-\frac{(s+J)^2}{\beta s^2}\log\left[Z'(\mathbf{r})\,e^{\frac{\beta\mu(\mathbf{r})}{4}}\right]\Bigg\}\mathrm{d}^3r\end{aligned} \tag{9.36}$$

and the order parameter is normalised to the number of condensed particles by

$$N_0=\frac{s^2}{(s+J)^2}\int|\Phi(\mathbf{r})|^2\mathrm{d}^3r\;. \tag{9.37}$$

The replacement (9.35) has also to be made inside the function Z', of course. The corresponding mean-field equation for the continuum is

$$\left[-\frac{Ja^2}{6}\nabla^2+(s+J)-\frac{(s+J)^2}{\beta s^2}\,\frac{\partial}{\partial(a^3|\Phi(\mathbf{r})|^2)}\log Z'(\mathbf{r})\right]\Phi(\mathbf{r})=0\;. \tag{9.38}$$

This equation is the analogue of the stationary GP eq. in the case of our slave-boson approach. The parameters can be identified with those of the conventional GP eq.: The mass m of the particles is given by the hopping constant J and the original lattice constant a via

$$\frac{\hbar^2}{2m}\equiv\frac{Ja^2}{6}\;. \tag{9.39}$$

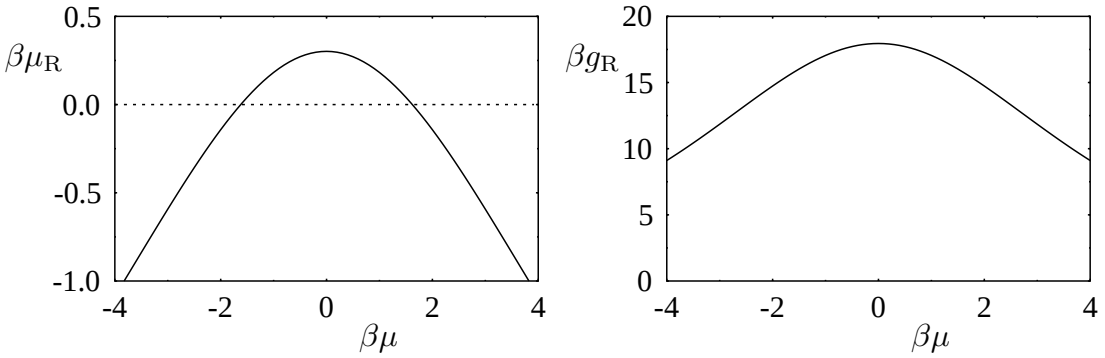

Figure 9.3: Coefficients μ_R and g_R of the renormalised GP theory plotted against the chemical potential μ. All parameters are normalised by the inverse temperature β. The tunneling rate was chosen to be $\beta J = 5.5$ and the free parameter was chosen as $s = k_B T$.

In the continuum a looses its identity as lattice constant, but describes a characteristic length scale that can be interpreted as the spacial extension of a boson. Thus, it should be of the same order of magnitude as the s-wave scattering length a_s.

If the order parameter Φ is small, we can expand the potential part of the action up to forth order:

$$\begin{aligned}&(s+J)a^3|\Phi(\mathbf{r})|^2 - \frac{(s+J)^2}{\beta s^2}\log\left[Z'(\mathbf{r})\,e^{\frac{\beta\mu(\mathbf{r})}{4}}\right]\\ &= a_0 - \mu_R|\Phi(\mathbf{r})|^2 + \frac{g_R}{2}\frac{s^2}{(s+J)^2}|\Phi(\mathbf{r})|^4 + \mathcal{O}(|\Phi|^6)\,,\end{aligned} \tag{9.40}$$

where we have introduced the coefficients

$$a_0 = -\frac{(s+J)^2}{\beta s^2}\log Z'(\mathbf{r})\big|_{\Phi=0} \tag{9.41}$$

$$\mu_R = -(s+J) + \frac{(s+J)^2}{\beta s^2}\frac{\partial}{\partial(a^3|\Phi(\mathbf{r})|^2)}\log Z'(\mathbf{r})\Big|_{\Phi=0} \tag{9.42}$$

$$g_R = -\frac{a^3(s+J)^4}{\beta s^4}\frac{\partial^2}{\partial(a^3|\Phi(\mathbf{r})|^2)^2}\log Z'(\mathbf{r})\Big|_{\Phi=0}\,. \tag{9.43}$$

They depend on μ, J, β, and $|\Phi(\mathbf{r})|^2$. Further, we introduce the rescaled order parameter

$$\Phi_R(\mathbf{r}) = \frac{s}{s+J}\,\Phi(\mathbf{r})\,. \tag{9.44}$$

With these coefficients, the full mean-field equation (9.38) can be approximated by the equation

$$\left[-\frac{Ja^2}{6}\nabla^2 - \mu_R + g_R|\Phi_R(\mathbf{r})|^2\right]\Phi_R(\mathbf{r}) = 0\,, \tag{9.45}$$

This equation has the same form as the conventional stationary GP equation, where μ_R and g_R play the role of a renormalised chemical potential and a renormalised interaction constant, respectively. Therefore we refer to this equation can be called a "renormalised GP equation". The μ-dependence of the coefficients μ_R and g_R is plotted in Fig. 9.3 for a special choice of the parameter s and the tunneling rate J. The zero temperature limits of the coefficients are calculated in Appendix E.3, see eq. (E.12). Near the phase transition to the empty phase, i.e. in the dilute regime, where $\mu = -J + \Delta\mu$, $\Delta\mu \ll J$, we find $\mu_R = \Delta\mu + \mathcal{O}(\Delta\mu^2)$. Thus, in the limiting case of a dilute BEC and zero temperature, the renormalised GP equation goes over to the conventional GP equation with the interaction parameter $g = g_R = 2a^3J$. In the case of a trapping potential, where the chemical potential $\mu(\mathbf{r})$ is space-dependent, μ_R and g_R are space-dependent as well. While g_R is always positive, μ_R can change sign. A BEC exists if $\mu_R > 0$, otherwise the order parameter vanishes. The phase transition between the BEC and the non-condensate phase is given by the relation $\mu_R = 0$, which is equivalent to eq. (9.22) in a translational-invariant system. Inside the BEC phase, μ_R increases linearly with increasing μ, reaches a maximum and decreases again until the condensate is destroyed totally due to strong interaction effects. We use this approach to calculate the condensate density profile of a trapped BEC.

9.6 Application to a trapped Bose-Einstein condensate

We consider a strongly interacting BEC in a spherical harmonic trap with trapping potential

$$V_{\mathrm{tr}}(\mathbf{r}) = \frac{m}{2}\omega_{\mathrm{ho}}^2\mathbf{r}^2 \,. \tag{9.46}$$

In typical experiments, the oscillator length $d_{\mathrm{ho}} = \sqrt{\hbar/m\omega_{\mathrm{ho}}}$ is of the order of a few μm [10], where ω_{ho} is the trap frequency measured in Hz. Considering, for instance, $\sim 10^5 \ldots 10^6$ ^{85}Rb atoms near a Feshbach resonance [3], we can study a Bose gas in a dense regime with a scattering length $a_s \sim a \sim 200$nm. In our calculations in ref. [90] we chose the parameters

$$\beta J = 5.5 \,, \quad \frac{k_{\mathrm{B}}T}{\hbar\omega_{\mathrm{ho}}} = 36.93 \,, \quad \frac{a}{d_{\mathrm{ho}}} = 0.1215 \,. \tag{9.47}$$

The parameter s was chosen to be equal to the thermal energy: $s = k_{\mathrm{B}}T$. For a non-interacting trapped Bose gas the critical temperature is given by eq. (2.18), which for the assumed particle number is close to the above chosen value of $k_{\mathrm{B}}T/\hbar\omega_{\mathrm{ho}}$. In this density and temperature regime the conventional GP equation is not applicable any more.

For conveniene we define dimensionless parameters by scaling all energies with the hopping rate J:

$$\mu \to \mu' := \frac{1}{\alpha J}\,\mu \,, \quad \beta \to \beta' := \alpha J \beta \,, \quad \text{where} \quad \alpha := \frac{s}{J} = \frac{1}{5.5} \,. \tag{9.48}$$

With the parameters given above, we have $\beta' = 1$. In the case of a trap that is rotating about the z-axis with an angular velocity Ω, one must include the additional angular momentum term $-\Omega \hat{L}_z \Phi(\mathbf{r})$ to the left hand side of the differential equation (9.38), where $\hat{L}_z$ is the z-component of the angular momentum operator (2.21). Thus, together with the identification of the mass (9.39), for our calculation we have to solve the mean-field equation

$$\left[-\frac{Ja^2}{6}\nabla^2 + (1+\alpha)J - k_\mathrm{B}T(1+1/\alpha)^2 \frac{\partial}{\partial(a^3|\Phi(\mathbf{r})|^2)} \log Z'(\mathbf{r}) - \Omega \hat{L}_z \right] \Phi(\mathbf{r}) = 0 \quad (9.49)$$

with the function Z' becoming

$$Z'(\mathbf{r}) = \int_{-\infty}^{\infty} e^{-\beta'\varphi^2} \frac{\sinh\left[\beta'\sqrt{(\varphi+\mu'/2)^2 + a^3|\Phi(\mathbf{r})|^2}\right]}{\beta'\sqrt{(\varphi+\mu'/2)^2 + a^3|\Phi(\mathbf{r})|^2}} \,\mathrm{d}\varphi \,.$$

In the renormalised GP approximation, eq. (9.49) is replaced by

$$\left[-\frac{Ja^2}{6}\nabla^2 - \mu_\mathrm{R} + g_\mathrm{R}|\Phi_\mathrm{R}(\mathbf{r})|^2 - \Omega \hat{L}_z \right] \Phi_\mathrm{R}(\mathbf{r}) = 0 \,, \quad (9.50)$$

where μ_R and g_R are plotted in fig. 9.3 with the same parameters which are chosen here.

Assuming a dense condensate, where the repulsive interaction between bosons dominates their kinetic energy, we neglect the differential term in eqs. (9.49) and (9.50). This is called the Thomas-Fermi (TF) approximation [10]. We calculated the density profiles of a vortex-free condensate with spherical symmetry and of a condensate with a single vortex with vortex core through the trap center parallel to the z-axis.

a) Vortex-free condensate

Because of the spherical symmetry the order parameter only depends on the radial coordinate r, but not on the angular coordinates. Therefore the contribution of the angular momentum operator $\hat{L}_z$ vanished, and the condensate shape is not affected by the angular velocity Ω. Thus we solve the TF equation

$$(1+1/\alpha) - \frac{1}{\beta'}(1+1/\alpha)^2 \frac{\partial}{\partial(a^3|\Phi(r)|^2)} \log Z(r) = 0 \,, \quad (9.51)$$

and compare it to the solution of the renormalised GP equation

$$n_0(r) = |\Phi_\mathrm{R}(r)|^2 = \frac{\mu_\mathrm{R}(r)}{g_\mathrm{R}(r)} \,. \quad (9.52)$$

Solutions for typical values of the parameters are plotted in Fig. 9.4. The results we get from the RGP approximation show only small deviations from the numerical solutions

of eq. (9.51). We find a condensate depletion at the trap center for $\beta\mu = 1$. This is due to the fact that the condensate is partly suppressed by strong interaction effects [70, 82, 86]. For $\beta\mu = 2$ the condensate is completely destroyed at the trap center. We note that the total particle density, which is given as

$$n_{\mathrm{tot}}(\mathbf{r}) = a^{-3}\left(\langle\varphi(\mathbf{r})\rangle + \frac{1}{2}\right) ,$$

is much larger than the condensate density n_0 and takes values of about $0.5\,a^{-3}$ at the trap center. Thus the interaction between the non-condensed and the condensed part of the Bose gas plays a significant role. This implies that the conventional GP equation, which neglects the non-condensed part, is not reliable in this parameter regime.

b) Rotating condensate with a single vortex

We assume a straight single vortex along the z-axis. This can be described by using cylindrical coordinates $(r_\perp, \varphi, z)$ and the ansatz $\Phi(\mathbf{r}) = \tilde{\Phi}(r_\perp, z)e^{i\varphi}$, where $r_\perp$ is the distance from the z-axis and φ the polar angle. In this case, the angular momentum operator is given as $\hat{L}_z = -\mathrm{i}\hbar\frac{\partial}{\partial\varphi}$. This gives rise to an additional term in the TF equation:

$$(1+1/\alpha) + \left(\frac{1}{6\alpha}\left(\frac{a}{r_\perp}\right)^2 - \frac{\hbar\Omega}{\alpha J}\right) - \frac{1}{\beta'}(1+1/\alpha)^2\frac{\partial}{\partial(a^3|\Phi(r)|^2)}\log Z(\mathbf{r}) = 0 . \tag{9.53}$$

The corresponding solution of the renormalised GP equation is

$$n_0(\mathbf{r}) = |\Phi_{\mathrm{R}}(\mathbf{r})|^2 = \frac{\mu_{\mathrm{R}}(\mathbf{r}) + \left(\frac{J}{6}\left(\frac{a}{r_\perp}\right)^2 - \hbar\Omega\right)}{g_{\mathrm{R}}(\mathbf{r})} . \tag{9.54}$$

A condensate that is rotating with given angular velocity Ω forms a stable vortex, if its total energy is lower than that of a vortex free condensate. This is equivalent to the condition

$$\tilde{A}^{\mathrm{vort}}(\Omega) - \tilde{A}^0 < 0 , \tag{9.55}$$

where $\tilde{A}(\Omega)$ is the mean-field action of a BEC with a single vortex in a trap rotating with angular velocity Ω, and $\tilde{A}^0$ is the mean-field action of a vortex-free BEC with spherical symmetry. In the TF approximation, they are given as

$$\tilde{A}^0 = \int\left\{\frac{|\Phi(\mathbf{r})|^2}{1+1/\alpha} - \frac{1}{\beta'}\log Z'(\mathbf{r})\right\}\mathrm{d}^3r , \tag{9.56}$$

$$\tilde{A}^{\mathrm{vort}}(\Omega) = \int\left\{\frac{|\Phi(\mathbf{r})|^2}{1+1/\alpha} + \frac{|\Phi(\mathbf{r})|^2}{(1+1/\alpha)^2}\left(\frac{1}{6\alpha}\left(\frac{a}{r_\perp}\right)^2 - \frac{\hbar\Omega}{\alpha J}\right) - \frac{1}{\beta'}\log Z'(\mathbf{r})\right\}\mathrm{d}^3r . \tag{9.57}$$

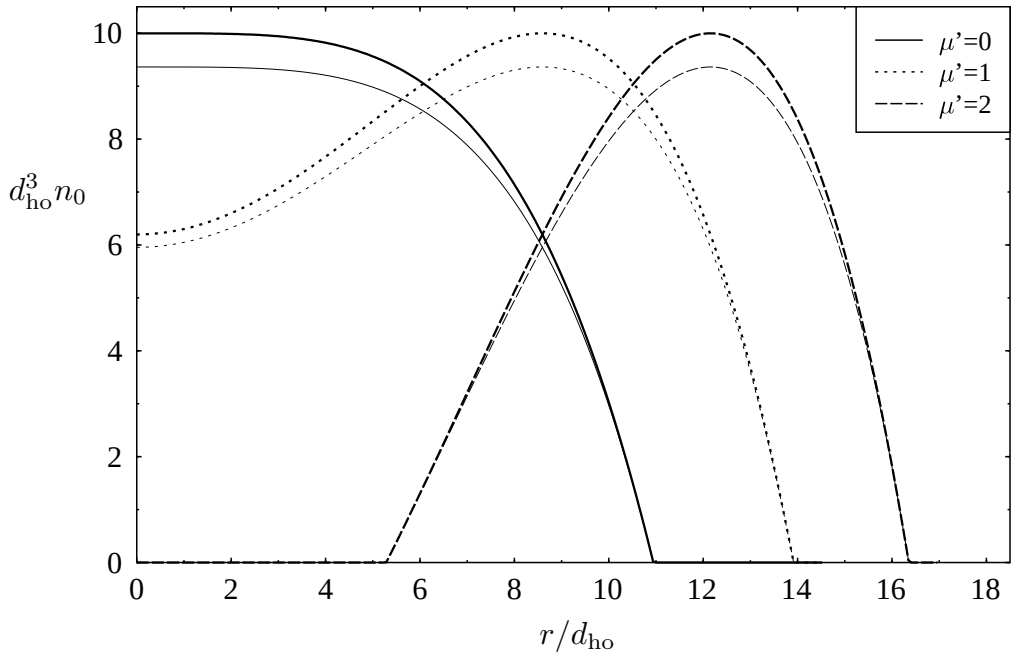

Figure 9.4: Condensate density n_0 of a vortex-free condensate in a spherical trap with the numerical parameters given in eq. (9.47) and different values of the chemical potential μ calculated in TF approximation from the full slave-boson mean-field eq. (9.51) (thick lines), and within RGP approximation (9.52) (thin lines). The spacial coordinate is scaled with the oscillator length $d_{\rm ho}$.

This can be checked numerically. The critical angular velocity $\Omega_{\rm c}$ above which the vortex is stable is plotted against the number of condensed bosons N_0 in Fig. 9.5, where N_0 can be calculated with eq. (9.37). The decreasing critical angular velocity for higher values of N_0 indicates that a high interaction energy favours the formation of a vortex. This agrees qualitatively with results derived from the GP eq. by perturbation theory [24] as well as numerically [22].

Typical solutions for shapes of condensate density profiles of BECs with a stable single vortex are shown in fig. 9.6. The graphs show the density profile perpendicular to the vortex core, where $r_\perp = 0$ represents the center of the trap. In contrast to the case without a vortex, the condensate is always completely destroyed at the trap center, a feature that also shows up in the conventional GP approximation. Again, the renormalised GP approximation is in good agreement with the numerical results from the full mean-field equation.

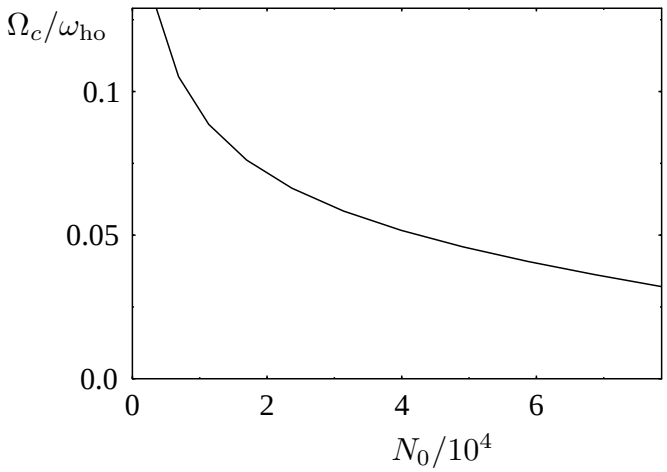

Figure 9.5: Critical angular velocity plotted against the total number of particles in the condensate.

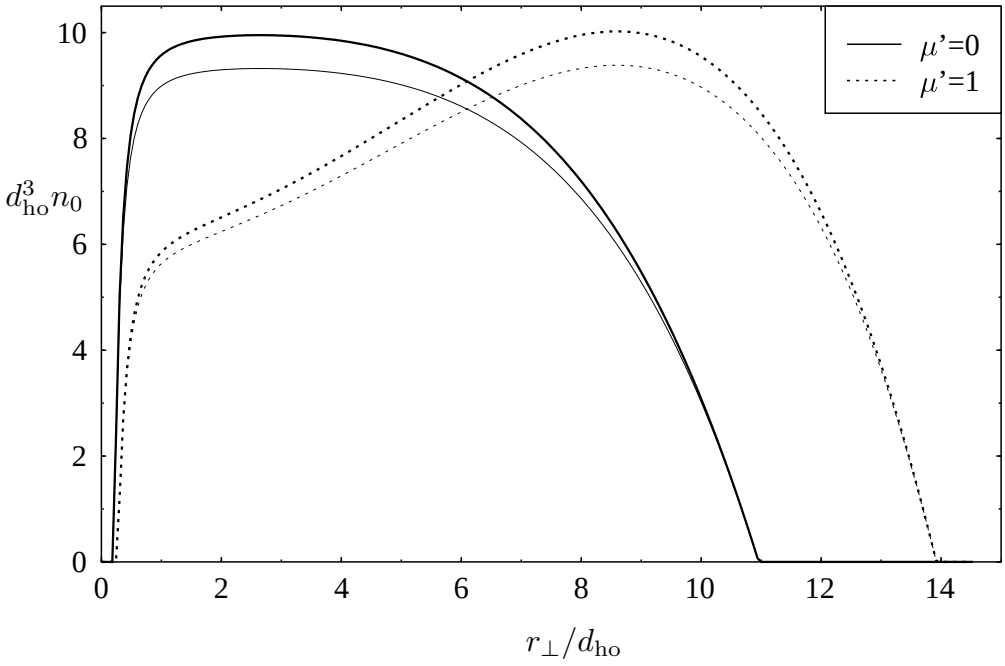

Figure 9.6: Condensate density of a condensate with a single vortex, with same parameters and normalisation as in Fig. 9.4, calculated from the full mean-field eq. (9.53) (thick lines) and within RGP approximation (9.54) (thin lines). The rotating frequencies of the trap were chosen to be close to the critical angular frequency $\Omega_{\rm c}$.

10 Discussion

10.1 Comparison of the results

The main results that we found for the one-dimensional model, the hard-core Bose model, the paired-fermion model, and the slave boson model, will be summarised and discussed in this section. Their common features and differences shall be pointed out.

a) Phase diagram

At zero temperature, the exact solution of the one-dimensional model exhibits three phases in the translational invariant case, as shown in fig. 6.4 in the J-μ plane: An empty phase which contains no particles in equilibrium (physically speaking, this means that the particles are driven apart from each other), an incommensurate phase with a particle number per lattice site n_{tot} between 0 and 1, and a Mott-insulator with $n_{\mathrm{tot}} = 1$. The same zero temperature phase diagram has been found for the paired-fermion model (see picture *(a)* in fig. 8.1) and the slave boson model on the mean-field level, as well. The only difference is that for the three-dimensional models, the incommensurate phase is also a BEC, which is not the case for the one-dimensional model due to the fact that there is no BEC in one dimension. At non-zero temperatures, the empty phase and the MI are affected by thermal fluctuations, and they have no clear phase boundary and more. However, the three-dimensional systems still have a single phase boundary between a BEC with a non-zero order parameter, and a non-condensed phase where the order parameter vanishes. The shape of this phase boundary depends on temperature, see right picture of fig. 8.1 for the paired-fermion model.

The hard-core Bose model does not show a MI phase. At zero temperature, it only shows the phase boundary between a BEC and the empty phase. At non-zero temperatures the empty phase vanishes and there is a phase boundary between a non-condensed phase and a BEC. However, the phase boundary which was derived from mean-field theory does not depend on the temperature. The reason for the non-existence of the MI phase can be understood when one considers the N-component extension of the hard-core Bose model as given in eq. (7.49): The mean-field result is exact in the large-N limit, and the hard-core interaction is very weak because of the large number of degenerate levels per lattice site. Thus the MI phase cannot be reached. For all the other models, which show an MI phase, we find a particle-hole symmetry: They are invariant under the substitution $\mu \to -\mu$ and $n_{\mathrm{tot}} \to 1 - n_{\mathrm{tot}}$.

b) Total density and condensate density

For the one-dimensional system a BEC does not exist, so the condensate density is zero. The total particle density for $T = 0$ and $T > 0$ is shown in fig. 6.3. At $T = 0$, the derivative $\partial n_{\text{tot}}/\partial\mu$ diverges at the phase transitions between the BEC and the empty phase and the BEC and the MI phase. The sharp transitions are "washed out" at finite temperatures.

The zero temperature mean-field results for the total particle density and the condensate density of the paired-fermion model and the slave boson model agree and are given in the eqs. (8.23) and (8.24). We find a total particle density which increases linearly with μ. In the dilute regime the condensate density is given by $n_0 = n_{\text{tot}} - \mathcal{O}(n_{\text{tot}}^2)$. If we neglect the terms of order n_{tot}^2, this is in agreement with Gross-Pitaevskii theory which assumes that all particles are condensed in this regime. At non-zero temperatures the phase boundaries of the empty phase and the MI are not well defined any more, like in the one-dimensional case. The region of BEC shrinks and the condensate density decreases. Non-zero temperature results of the paired-fermion model and the slave boson model are not identical, compare the figs. 8.2 and 9.2. For the slave boson model they depend on the free parameter s, which was introduced in eq. (9.10) for the convergence of the Φ integral, and reflects the ambiguity of the Hubbard-Stratonovich transformation.

For the hard-core Bose model, mean-field theory only gives qualitative results for the total density and the particle density, if one leaves the imaginary-time variable discrete with time step β/M. But then the mean-field results depend on β/M and vanish in the limit $M \to \infty$. The corrections which come from the Gaussian fluctuations are equivalent to an ideal Bose gas in the non-condensed phase, and in the BEC phase they lead to the results of Bogoliubov theory. In the N-component extension of the hard-core Bose model they are of the order $1/N$.

c) Excitation spectrum

The spectrum of quasiparticle excitations is found on the level of Gaussian fluctuations. For the hard-core Bose model, the paired-fermion model, and the slave boson model, the expressions for the quasiparticle spectra $E_{\mathbf{k}}$ are summarised in the subsequent tabular:

model	$E_{\mathbf{k}}$ in the BEC phase	$E_{\mathbf{k}}$ in the non-condensed phases
hard-core Bose	$\sqrt{\epsilon_{\mathbf{k}}\left(2(\mu+J)+\epsilon_{\mathbf{k}}\right)}$	$\epsilon_{\mathbf{k}} + \lvert\mu+J\rvert$
paired-fermion	$\sqrt{\epsilon_{\mathbf{k}}\left[J\left(1-\left(\frac{\mu}{J}\right)^2\right)+\left(\frac{\mu}{J}\right)^2\epsilon_{\mathbf{k}}\right]}$	$\epsilon_{\mathbf{k}} + \lvert\mu\rvert - J$
slave boson	$\sqrt{\epsilon_{\mathbf{k}}\left(2\,\frac{(s+J)^2}{s^2}\,\tilde{a}_4\,\lvert\Phi_0\rvert^2+\epsilon_{\mathbf{k}}\right)}$	$\epsilon_{\mathbf{k}} + (s+J)^2\tilde{a}_2/s^2$

Here, $\epsilon_{\mathbf{k}}$ is the free-particle dispersion relation in the optical lattice, given by eq. (4.7). We find a spectrum which is linear for small wave vectors $\mathbf{k}$ in the BEC phase, whereas the spectrum has a gap in the non-condensed phases. The gapless spectrum in the BEC phase is caused by a Goldstone mode due to a broken $U(1)$ phase symmetry. The spectrum for the hard-core Bose model is not temperature dependent. The result given for the paired-fermion model is only valid at zero temperature: The gapped spectrum is found both in the empty phase and in the MI phase. The result for the slave boson model depends implicitly on temperature via the coefficients $\tilde{a}_2$ and $\tilde{a}_4$ given in eqs. (9.26) and (9.27), and it also depends on the free parameter s.

We have shown that the zero temperature results of all three models inside the BEC phase and near the phase boundary to the empty phase ($\mu + J \ll J$), agree with the Bogoliubov result given in eq. (5.11). The only difference is that the chemical potential is shifted ($\mu \to \mu + J$), because the phase transition in Bogoliubov theory is given by $\mu = 0$ instead of $\mu = -J$ for the three hard-core systems. The region near the phase transition to the empty phase is the weakly interacting regime, therefore Bogoliubov theory is applicable there. The interaction constant was identified as $g \equiv 2a^3 J$.

The gapped spectrum in the MI that was found in the paired-fermion and slave bsosn model is of the form

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Delta \, . \tag{10.1}$$

We have shown that in the MI phase near the phase transition to the BEC phase, the gap is given by $\Delta = \mu - J$.

For the one-dimensional system, the excitation spectrum in the incommensurate phase can be found indirectly by means of the Feynman relation and is given in eq. (6.29). It is linear for small wave-vectors $\mathbf{k}$, like in the BEC phase of the three-dimensional systems discussed above.

d) Static structure factor

The static structure factor is defined as the Fourier transformation of the equal-time density-density CF, as it is defined in eq. (3.27). At zero temperature it is related to the quasiparticle excitation spectrum via the Feynman relation

$$S(\mathbf{q}) = \frac{Ja^2\mathbf{q}^2}{2d\, E_{\mathbf{q}}} \, ,$$

where the identification $\hbar^2/2m \equiv Ja^2/2d$ can be considered for a lattice system (in this case $m = m^*$ is the band mass). The quasiparticle spectrum for the three-dimensional system near the phase transition to the MI phase is plotted in the left hand graph of fig. 10.1. The corresponding static structure factor at zerotemperature is plotted in the right hand graph. The symmetrical case, i.e. the phase transition between the BEC and the empty phase, is equivalent. For the hard-core Bose model the density-density CF was calculated explicitly on the level of a Gaussian approximation. It shows

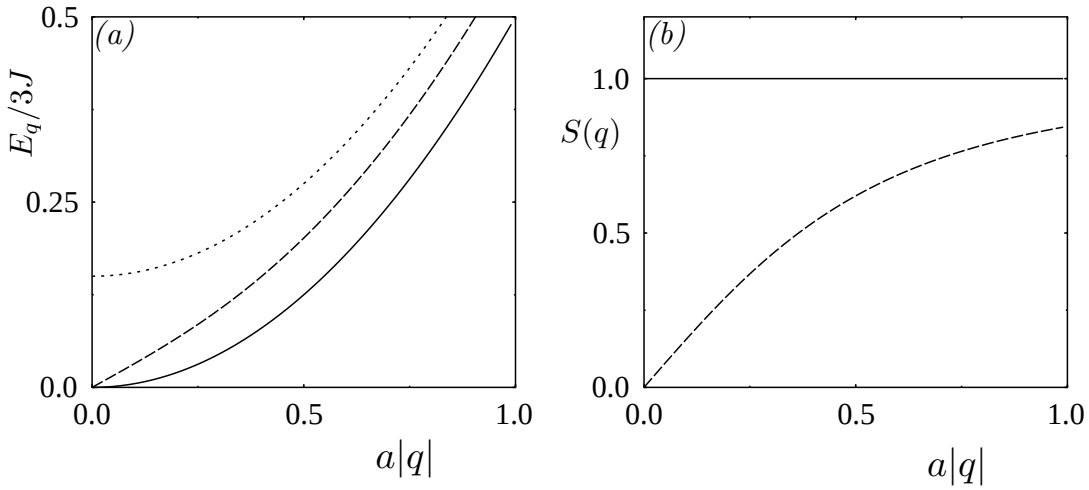

Figure 10.1: *(a)* Quasiparticle spectrum of a hard-core Bose gas in a three-dimensional lattice on the phase transition between the BEC and the MI (solid line), inside the BEC phase (dashed line), inside the MI phase (dotted line). *(b)* Corresponding static structure factor for the BEC phase.

an algebraic decay with $1/r^{d+1}$, where d is the dimension. The result for the static structure factor agrees with the Feynman relation. For the one-dimensional system the density-density CF, and therefore the static structure factor, were calculated exactly in the incommensurate phase, and agree with results from the literature. In the empty phase and the MI phase it vanishes, in agreement with the vanishing result found for the empty phase of the hard-core Bose model from the saddle point expansion.

For the paired-ferion model and the slave-boson model the density-density CF was not calculated explicitly, so the Feynman relation was assumed to be valid to find the expression for the static structure factor.

10.2 Excitation spectrum in the large-U of the Bose-Hubbard model

In the large-U limit of the Bose-Hubbard model, multiple occupation of lattice sites is prohibited because it cost a large amount of energy. Therefore one can assume that in this case, the bosons behave like hard-core bosons. However, this is not clear because the models which were presented here are very different from the Bose-Hubbard model.

The results for the excitation spectrum in the Mott-insulating phase from the paired-fermion model and the slave boson model are consistent with the spectrum that was found for the Bose-Hubbard model in the large-U limit. Inside the first Mott lobe,

which is the equivalent to the MI with filling $n_{\mathrm{tot}} = 1$ for hard-core bosons, the latter is given by the expression [35, 83, 91]

$$E_{\mathbf{k}}^{\mathrm{qp/qh}} = \pm\left(-\mu + \frac{U}{2} - \frac{J-\epsilon_{\mathbf{k}}}{2}\right) + \frac{1}{2}\sqrt{(J-\epsilon_{\mathbf{k}})^2 - 6U(J-\epsilon_{\mathbf{k}}) + U^2}\,, \tag{10.2}$$

which describes two branches: One ("+" sign) is assigned to quasiparticles and one ("−" sign) to quasiholes. It depends on the interaction parameter U. For our hard-core bosons, only the quasihole branch can exist, because the hard-core condition prohibits multiple occupation of lattice sites, in contrary to the Bose-Hubbard model, where multiple occupation is possible and allows the creation of particle-hole pairs. For large values of U the square root term can be written as

$$\frac{1}{2}\sqrt{(J-\epsilon_{\mathbf{k}})^2 - 6U(J-\epsilon_{\mathbf{k}}) + U^2} = \frac{U}{2} - \frac{3}{2}(J-\epsilon_{\mathbf{k}}) + \mathcal{O}\left(U^{-1}\right)\,,$$

such that we find for the two branches the large-U results

$$E_{\mathbf{k}}^{\mathrm{qp}} = \epsilon_{\mathbf{k}} + U - (\mu + 2J) + \mathcal{O}\left(U^{-1}\right)\,, \tag{10.3}$$

$$E_{\mathbf{k}}^{\mathrm{qh}} = \epsilon_{\mathbf{k}} + (\mu - J) + \mathcal{O}\left(U^{-1}\right)\,. \tag{10.4}$$

The gap of the quasiparticle branch is of the order of U, and in the $U \to \infty$ limit it goes to infinity, because the energy to occupy a site with two particles is infinitely large. On the other hand, the terms which are proportional to U cancel for the quasihole branch, and its $U \to \infty$ limit is identical to the result given in eq. (10.1). Particle-hole excitations cannot be created for hard-core bosons, so the creation of an elementary excitation is associated to removing a particle out of the Mott-insulator. Inside the empty phase, the same quasiparticle spectrum was found as for the Mott-insulator, due to the particle-hole symmetry. Here, the creation of an excitation is interpreted by putting an additional particle into the system.

In the BEC phase, two branches of the spectrum have been found, too [91]: Besides the Goldstone mode, which is linear for small wave vectors, also a mass mode (Higgs mode) with a gap was found. A calculation for the large-U limit shows, that the Goldstone mode agrees with the Bogoliubov spectrum that was found for the models discussed here. On the other hand, the gap of the mass mode is of the order of U and goes to infinity if $U \to \infty$, which explains why it has not been found for the hard-core bosons.

11 Conclusion

In this thesis, the many-particle problem of strongly interaction bosons in a lattice potential was investigated. Motivated by recent experiments on Bose-Einstein condensates in optical lattices which showed the existence of a Mott-insulator, four different models are presented, which allow the calculation of the phase diagram, and experimentally observable physical quantities like the total density and the condensate density, the quasiparticle spectrum, and the static structure factor. All these models have in common that they simulate a strong repulsive interaction by imposing a hard-core condition on the bosons, which prohibits a multiple occupation of lattice sites. They are defined by means of the functional integral method.

The first model is a special sublattice construction which describes non-interacting impenetrable fermions in a one-dimensional lattice. It was discussed in chapter 6. We exploited the well-known fact that such a fermionic system is equivalent to impenetrable bosons in one dimension, and that the static structure factors of the fermionic and the bosonic system are identical. As the fermions are non-interacting, the model can be integrated out exactly. We calculated the local particle density, the density-density correlation function and the static structure factor in a translational invariant system as well as in a system with a harmonic trap potential. In the translational invariant case, the static structure factor, which is experimentally accessible in Bragg scattering experiments, increases linearly for small wave vectors, until it reaches unity and remains constant. The density-density correlation function shows characteristic oscillations and decays like $1/r^2$.

The other three models were applied on a Bose gas in a three dimensional lattice. They were treated in mean-field theory. The first two, which were called the hard-core Bose model and the paired-fermion model, were constructed as fields of pairs of Grassmann variables in the chapters 7 and 8, respectively. They can be seen as interacting fermionic models. The third one, introduced in chapter 9, was based on a slave boson approach and was referred to as slave boson model. A Hubbard-Stratonovich transformation allows to integrate out the original fields in all three models. This transformation leads to new fields, which are connected to the condensate order parameter. A saddle point approximation provides both a mean-field solution and Gaussian fluctuations. The latter contain the information about quasiparticle excitations. For a three-dimensional lattice, the total particle density and the condensate density can be calculated in mean-field theory, and the quasiparticle spectrum and the static structure factor was calculated on the level of Gaussian fluctuations. The saddle point approximations of the three models

lead to different results.

Our results for the one-dimensional model, the paired-fermion model, and the slave boson model, show a particle hole symmetry with the symmetry axis $\mu = 0$. At zero temperature, they have a common phase diagram, with one phase boundary between the empty phase and the incommensurate phase, and one between the incommensurate phase and the Mott-insulating phase. If the temperature is non-zero, the empty phase and the Mott-insulator are affected by thermal fluctuations. While there is no Bose-Einstein condensation in the one-dimensional system, the incommensurate phase is a BEC in the paired-fermion and slave boson model in three dimensions. For the latter two models, the mean-field results for the total density and the condensate density agree exactly at zero temperature, at higher temperature they agree qualitatively. It was shown that they lead to the Gross-Pitaevskii result in the limit of low temperature, if the density is small compared to the lattice constant. At higher temperatures, we have shown that the slave boson model leads to a "renormalised" Gross-Pitaevskii equation with temperature dependent coefficients. A similar theory could in principle be derived on the mean-field level from the paired-fermion model as well. It could be compared to the renormalised Gross-Pitaevskii theory which was derived from the slave boson model.

The mean-field theory of the hard-core Bose model does not show the Mott-insulating phase. The reason can be understood when one considers the N-component extension of this model. In this case, the mean-field result is exact in the limit $N \to \infty$, and the Gaussian fluctuations give rise to $1/N$-corrections. With each tunneling process, the bosons can choose between one of the N degenerate internal states, and the hard-core interaction only affects bosons which are in the same internal state. This means, that the hard-core interaction becomes weak if N is large, and is not strong enough to establish a Mott-insulating state. Thus the mean-field theory of the hard-core Bose model is only sufficient to describe the weakly interacting regime.

The quasiparticle spectra which were found for all three-dimensional models, are gapless (Goldstone mode) in the BEC phase due to a broken $U(1)$ symmetry. In the dilute regime, they agree with the well-known Bogoliubov result. In the empty phase and the Mott-insulator, the quasiparticle spectrum is gapped. Our results agree with results which were derived for the Bose-Hubbard model, if the on-site interaction constant U is very large. The Goldstone mode in the BEC phase of the paired-fermion model was found as the quasiparticle pole of only one eigenvalue of the 4×4 quasiparticle Green's function. Additional mass modes may be found from the remaining eigenvalues.

At zero temperature, the elementary excitations are connected to the static structure factor via the Feynman relation $S(\mathbf{q}) = \epsilon_{\mathbf{q}}/E_{\mathbf{q}}$, where $\epsilon_{\mathbf{q}}$ is the free-particle spectrum and $E_{\mathbf{q}}$ the quasiparticle spectrum. In the empty phase and the Mott-insulator, the static structure factor vanishes because of the absence of density fluctuations.

A Finite summations and products

The following summations and products are necessary to calculate determinants and matrix elements, which arise when dealing with discrete imaginary-time functional integrals.

A.1 Finite products

An often used product is given by the identity

$$\prod_{n=1}^{M} \left(1 - a\, e^{\frac{2\pi \mathrm{i}}{M} n}\right) = 1 - a^M \,, \tag{A.1}$$

where a can be any complex number. This identity is easily shown to be true by using the Fundamental Theorem of Algebra: The factors on the left hand side contain the zeroes of the polynomial on the right hand side.

We now want to perform a product of the type

$$\prod_{n=1}^{M} \left(b - \cos\left(\frac{2\pi}{M} n\right)\right) \,, \quad |b| > 1 \,.$$

This can be verified to be equal to

$$\prod_{n=1}^{M} \left[\frac{1}{2}\left(b + \sqrt{b^2-1}\right)\left(1 - \left(b - \sqrt{b^2-1}\right) e^{\mathrm{i}\frac{2\pi}{M} n}\right)\left(1 - \left(b - \sqrt{b^2-1}\right) e^{-\mathrm{i}\frac{2\pi}{M} n}\right)\right] \,,$$

such that the identity (A.1) can be applied. As a result we find

$$\prod_{n=1}^{M} \left(b - \cos\left(\frac{2\pi}{M} n\right)\right) = 2^{-M} \left(\left(b + \sqrt{b^2-1}\right)^M + \left(b - \sqrt{b^2-1}\right)^M - 2\right) \,. \tag{A.2}$$

A.2 Finite sums

a) Bosonic sum.
For bosonic systems, which have a periodic structure in the imaginary time variable, we

have to perform sums of the type

$$\sum_{n=1}^{M} \frac{1}{M} \frac{e^{-\frac{2\pi i}{M} nm}}{1 - a\, e^{\frac{2\pi i}{M} n}} \,.$$

This sum is performed by finding the common denominator, which is given by the experession in eq. (A.1). The numerator then is

$$\text{numerator} = \sum_{n=1}^{M} e^{-\frac{2\pi i}{M} nm} \prod_{k \neq n} \left(1 - a\, e^{+\frac{2\pi i}{M} k}\right)$$

where

$$\prod_{k \neq n} \left(1 - a\, e^{\frac{2\pi i}{M} k}\right) = \frac{1 - a^M}{1 - a\, e^{\frac{2\pi i}{M} n}} = 1 + a\, e^{\frac{2\pi i}{M} n} + a^2 e^{\frac{2\pi i}{M} 2n} + \ldots + a^{M-1} e^{\frac{2\pi i}{M} (M-1)n} \,.$$

Therefore we find

$$\text{numerator} = \sum_{n=1}^{M} e^{-\frac{2\pi i}{M} nm} \sum_{l=1}^{M} a^{l-1} e^{\frac{2\pi i}{M} (l-1)n} = \sum_{n,l=1}^{M} a^{l-1} e^{-\frac{2\pi i}{M} n(m-l+1)} =$$

$$M \sum_{l=1}^{M} a^{l-1} \delta'_{l,m+1}, \quad \text{where } \delta'_{l,k} := \sum_{j=-\infty}^{\infty} \delta_{l,k+jM} \,.$$

With the restriction $m = -(M-1), \ldots, M-1$ the "enhanced" Kronecker symbol δ' contributes for the two cases

$$\begin{array}{ll} l = m + 1 & \text{if} \quad m \geq 0 \\ l = M + m + 1 & \text{if} \quad m < 0 \,. \end{array}$$

Finally, this leads to the components of the inverse matrix:

$$\sum_{n=1}^{M} \frac{1}{M} \frac{e^{-\frac{2\pi i}{M} nm}}{1 - a\, e^{\frac{2\pi i}{M} n}} = \frac{1}{1 - a^M} \times \begin{cases} a^m & \text{if} \quad m \geq 0 \\ a^{M+m} & \text{if} \quad m < 0 \end{cases} \,. \tag{A.3}$$

b) Fermionic sum.
For fermionic systems, which have an anti-periodic structure in the imaginary time variable, we have to perform sums of the type

$$\sum_{n=1}^{M} \frac{1}{M} \frac{e^{-\frac{2\pi i}{M} (n-\frac{1}{2}) m}}{1 - a\, e^{\frac{2\pi i}{M} (n-\frac{1}{2})}} = \frac{1}{1 + a^M} \times \begin{cases} a^m & \text{if} \quad m \geq 0 \\ -a^{M+m} & \text{if} \quad m < 0 \end{cases} \,. \tag{A.4}$$

This sum differs from the sum given in eq. (A.3) only by the substitution $a \to a\, e^{-\pi \mathrm{i} m/M}$ and a multiplication by the factor $e^{\pi \mathrm{i} m/M}$, so the result can be verified easily.

c) Sums with cosines.
The following two sums require the condition $|b| > 1$:

$$\sum_{n=1}^{M} \frac{1}{M} \frac{1}{\cos\left(\frac{2\pi}{M} n\right) - b} = \frac{1}{\sqrt{b^2-1}} \frac{\left(b - \sqrt{b^2-1}\right)^M + \left(b + \sqrt{b^2-1}\right)^M + 2}{\left(b - \sqrt{b^2-1}\right)^M - \left(b + \sqrt{b^2-1}\right)^M} \tag{A.5}$$

$$\sum_{n=1}^{M} \frac{1}{M} \frac{\cos\left(\frac{2\pi}{M} n\right)}{\cos\left(\frac{2\pi}{M} n\right) - b} = \frac{1}{\sqrt{b^2-1}} \frac{\left(b - \sqrt{b^2-1}\right)^{M-1} + \left(b + \sqrt{b^2-1}\right)^{M-1} + 2b}{\left(b - \sqrt{b^2-1}\right)^M - \left(b + \sqrt{b^2-1}\right)^M} \tag{A.6}$$

To perform these two sums the following identities were used:

$$\frac{1}{\cos(x) - \frac{a^2+1}{2a}} = \frac{2a^2}{a^2-1} \left[\frac{1}{e^{\mathrm{i}x} - a} - \frac{1}{a} \frac{1}{a\, e^{\mathrm{i}x} - 1} \right]$$

$$\frac{\cos(x)}{\cos(x) - \frac{a^2+1}{2a}} = \frac{a^2}{a^2-1} \left[\frac{1}{a\, e^{\mathrm{i}x} - 1} - \frac{1}{a} \frac{1}{e^{\mathrm{i}x} - a} - \frac{1}{a} \frac{1}{e^{-\mathrm{i}x} - a} + \frac{1}{a\, e^{-\mathrm{i}x} - 1} \right]$$

All separate terms can be traced back to the sum given in eq. (A.3).

d) Sum in eq. (6.11).
Make the following substitutions:

$$a := -\left(1 - \frac{\beta}{M}\mu\right) e^{\frac{\pi i}{M}} \quad ; \quad b = \frac{\beta}{M} J e^{\frac{\pi i}{2M}} \cos\frac{k}{2} \,,$$

$$f(z) := \frac{z+a}{(z+a)^2 - b^2 z} \,.$$

With these definitions, the sum is given as

$$C(k) = -\lim_{M\to\infty} \sum_{l=1}^{M} \frac{1}{M} e^{\frac{\pi \mathrm{i}}{M}} f\left(e^{\frac{2\pi \mathrm{i}}{M} l}\right) \,.$$

The roots of the denominator of $f(z)$ are

$$z^{\pm} = \frac{b^2}{2} - a \pm \frac{b}{2}\sqrt{b^2 - 4a} \,.$$

We perform an expansion into partial fraction and find

$$f(z) = \frac{A}{z - z^+} + \frac{B}{z - z^-} = \frac{(A+B)z - (Az^- + Bz^+)}{(z - z^+)(z - z^-)}$$

with

$$A = \frac{1}{2} + \frac{b}{2\sqrt{b^2-4a}} \quad ; \quad B = \frac{1}{2} - \frac{b}{2\sqrt{b^2-4a}} \, .$$

To perform the sum, we use the following identity which can be traced back to eq. (A.3):

$$\sum_{l=1}^{M} \frac{1}{M} \frac{1}{e^{\frac{2\pi i}{M} l} - z^{\pm}} = -\frac{1}{z^{\pm}} \frac{1}{1-\left(\frac{1}{z^{\pm}}\right)^M}$$

$$\Longrightarrow -\sum_{l=1}^{M} \frac{1}{M} e^{\frac{\pi \mathrm{i}}{M}} f\left(e^{\frac{2\pi \mathrm{i}}{M} l}\right) = \left[\frac{A}{z^+} \frac{1}{1-\left(\frac{1}{z^+}\right)^M} + \frac{B}{z^-} \frac{1}{1-\left(\frac{1}{z^-}\right)^M}\right] e^{\frac{\pi i}{M}} \, .$$

The limit $M \to \infty$ can now be performed, by the help of the identities

$$\lim_{M\to\infty} (z^{\pm})^M = e^{\pi i} \lim_{M\to\infty} \left(1 + \left(\pm J \cos\frac{k}{2} - \mu\right)\frac{\beta}{M} + \mathcal{O}\left(\frac{1}{M^2}\right)\right)^M = -e^{\beta\left(\pm J \cos\frac{k}{2} - \mu\right)}$$

$$\lim_{M\to\infty} z^{\pm} = 1 \quad ; \quad \lim_{M\to\infty} A, B = \frac{1}{2} \, .$$

The result is given in eq. (6.12).

e) Sum in eq. (8.15).

We define

$$a := 1 + (\mathrm{i}\varphi + \chi)(\mathrm{i}\varphi^* + \chi^*) \, , \quad b := 1 - \left(\frac{\beta\mu}{M}\right)^2 \, ,$$

$$f(z) = \frac{1}{a - 2z + bz^2} \, .$$

The roots of the denominator of $f(z)$ are

$$z^{\pm} = \frac{1}{b}\left(1 \pm \sqrt{1-ab}\right) \, .$$

An expansion into partial fraction leads to

$$f(z) = A\left(\frac{1}{z-z^+} - \frac{1}{z-z^-}\right) \, , \quad \text{where} \quad A = \frac{1}{2\sqrt{1-ab}} \, .$$

To perform the sum, we use the following identity which can be traced back to eq. (A.4):

$$\sum_{l=1}^{M} \frac{1}{M} \frac{1}{e^{\frac{2\pi i}{M}\left(l+\frac{1}{2}\right)} - z^{\pm}} = -\frac{1}{z^{\pm}} \frac{1}{1+\left(\frac{1}{z^{\pm}}\right)^M}$$

$$\Longrightarrow -\sum_{l=1}^{M} \frac{1}{M} f\left(e^{\frac{2\pi \mathrm{i}}{M}\left(l+\frac{1}{2}\right)}\right) = A\left[\frac{1}{z^+} \frac{1}{1+\left(\frac{1}{z^+}\right)^M} - \frac{1}{z^-} \frac{1}{1+\left(\frac{1}{z^-}\right)^M}\right] \, .$$

B Gaussian integrals and expectation values

B.1 Gaussian integrals

(a) **Real variables**
The $n \times n$ matrix A shall be symmetric and positive.

$$\int \exp\left[-\frac{1}{2}\sum_{j,k=1}^{n}\phi_j A_{jk}\phi_k + \sum_{j=1}^{n}\phi_j J_j\right]\left(\prod_{j=1}^{n}\frac{\mathrm{d}\phi_j}{(2\pi)^{1/2}}\right)$$

$$= [\det A]^{-1/2}\exp\left[\frac{1}{2}\sum_{j,k=1}^{n} J_j A^{-1}_{jk} J_k\right] \tag{B.1}$$

(b) **Complex conjugate variables**
The $n \times n$ matrix H shall be self-adjoint and positive.

$$\int \exp\left[-\sum_{j,k=1}^{n}\phi^*_j H_{jk}\phi_k + \sum_{j=1}^{n}(J^*_j\phi_j + J_j\phi^*_j)\right]\left(\prod_{j=1}^{n}\frac{\mathrm{d}\phi^*_j\mathrm{d}\phi_j}{2\pi i}\right)$$

$$= [\det H]^{-1}\exp\left[\sum_{j,k=1}^{n} J^*_j H^{-1}_{jk} J_k\right] \tag{B.2}$$

(c) **conjugate Grassmann-Variables**
The $n \times n$-Matrix H shall be self-adjoint.

$$\int \exp\left[-\sum_{j,k=1}^{n}\bar{\psi}_j H_{jk}\psi_k + \sum_{j=1}^{n}(J^*_j\psi_j + J_j\bar{\psi}_j)\right]\left(\prod_{j=1}^{n}\mathrm{d}\bar{\psi}_j\mathrm{d}\psi_j\right)$$

$$= [\det H]\,\exp\left[\sum_{j,k=1}^{n} J^*_j H^{-1}_{jk} J_j\right] \tag{B.3}$$

B.2 Expectation values and Wick's theorem

An expectation value of an expression in terms of real/complex/Grassmann variables is defines as

$$\langle \textit{expression} \rangle = \frac{\int \textit{expression} \exp\Big[\dots\Big]\mathcal{D}\Big(\dots\Big)}{\int \exp\Big[\dots\Big]\mathcal{D}\Big(\dots\Big)} ,$$

where the exponent and the integration measure are due to eqs. (B.1), (B.2), or (B.3) respectively, with $J_j \equiv 0$. The **second order expectation values** provide the matrix element of the (inverse) matrix A or H, respectively:

$$\begin{array}{ll} \text{Real variables:} & \langle \phi_j \phi_k \rangle = \frac{1}{2} A^{-1}_{jk} \\ \text{Complex conjugate variables:} & \langle \phi^*_j \phi_k \rangle = H^{-1}_{jk} \\ \text{Conjugate Grassmann variables:} & \langle \bar{\psi}_j \psi_k \rangle = H_{jk} \end{array} \tag{B.4}$$

Forth order expectation values can be calculated via the application of Wick's theorem [8, 9]. It can be split into products of second-order expectation values and a sum has to be performed over all possible pairings (including a sign for Grassmann variables):

$$\begin{array}{ll} \text{Real var.:} & \langle \phi_j \phi_k \phi_l \phi_m \rangle = \langle \phi_j \phi_k \rangle \langle \phi_l \phi_m \rangle + \langle \phi_j \phi_l \rangle \langle \phi_k \phi_m \rangle + \langle \phi_j \phi_m \rangle \langle \phi_k \phi_l \rangle \\ \text{C. conj. var.:} & \langle \phi^*_j \phi^*_k \phi_l \phi_m \rangle = \langle \phi^*_j \phi_m \rangle \langle \phi^*_k \phi_l \rangle + \langle \phi^*_j \phi_l \rangle \langle \phi^*_k \phi_m \rangle \\ \text{Conj. Gr. var.:} & \langle \bar{\psi}_j \bar{\psi}_k \psi_l \psi_m \rangle = \langle \bar{\psi}_j \psi_m \rangle \langle \bar{\psi}_k \psi_l \rangle - \langle \bar{\psi}_j \psi_l \rangle \langle \bar{\psi}_k \psi_m \rangle \end{array} \tag{B.5}$$

C Coherent states for bosons, fermions, and hard-core bosons

The functional integral representation for bosonic and fermionic systems is constructed of coherent states [9]. It shall be demonstrated that an analogous procudere can be performed for a system of hard-core bosons, by defining coherent states for the hard-core operators by a nilpotent field as defined by eq. (7.1). Here we denote bosonic operators by $\hat{a}_\alpha^+$, $\hat{a}_\alpha$, fermionic operators by $\hat{c}_\alpha^+$, $\hat{c}_\alpha$, and hard-core operators by $\hat{b}_\alpha^+$, $\hat{b}_\alpha$. The commutation relations are:

$$\left[\hat{a}_\alpha, \hat{a}_{\alpha'}^+\right]_- = \delta_{\alpha\alpha'} \,, \tag{C.1}$$

$$\left[\hat{c}_\alpha, \hat{c}_{\alpha'}^+\right]_+ = \delta_{\alpha\alpha'} \,, \tag{C.2}$$

$$\left[\hat{b}_\alpha, \hat{b}_{\alpha'}^+\right]_- = 0 \;\text{ if } \alpha \neq \alpha' \,, \quad \hat{b}_{\mathbf{r}}^2 = (\hat{b}_{\mathbf{r}}^+)^2 = 0 \,. \tag{C.3}$$

The vacuum state, i.e. the state containing no particle, we call $|0\rangle$. We define coherent states for

- bosons by means of complex field variables ϕ_α^*, ϕ_α:

$$|\phi\rangle = e^{\sum_\alpha \phi_\alpha \hat{a}_\alpha^+} |0\rangle \,, \quad \langle\phi| = \langle 0| \, e^{\sum_\alpha \phi_\alpha^* \hat{a}_\alpha} \,. \tag{C.4}$$

- fermions by means of conjugate Grassmann variables $\bar{\psi}_\alpha$, ψ_α, where we require, that the Grassmann variables anticommute with the fermionic operators:

$$|\psi\rangle = e^{-\sum_\alpha \psi_\alpha \hat{c}_\alpha^+} |0\rangle = \prod_\alpha \left(1 - \psi_\alpha \hat{c}_\alpha^+\right) |0\rangle \,,$$

$$\langle\psi| = \langle 0| \, e^{\sum_\alpha \bar{\psi}_\alpha \hat{c}_\alpha} = \langle 0| \prod_\alpha \left(1 + \bar{\psi}_\alpha \hat{c}_\alpha\right) \,. \tag{C.5}$$

- hard-core bosons by means of nilpotent commutating variables $\bar{\eta}_\alpha$, η_α:

$$|\eta\rangle = e^{\sum_\alpha \eta_\alpha \hat{b}_\alpha^+} |0\rangle = \prod_\alpha \left(1 + \eta_\alpha \hat{b}_\alpha^+\right) |0\rangle \,,$$

$$\langle\eta| = \langle 0| \, e^{\sum_\alpha \bar{\eta}_\alpha \hat{b}_\alpha} = \langle 0| \prod_\alpha \left(1 + \bar{\eta}_\alpha \hat{b}_\alpha\right) \,. \tag{C.6}$$

For the construction of the coherent state functional integral, the following properties are relevant. They can be checked by using the previous definitions and the integration properties of complex, Grassmannian and nilpotent variables:

- Coherent states are eigenvalues of annihilation operators:

$$\hat{x}_\alpha|\xi\rangle = \xi_\alpha|\xi\rangle \ , \quad \langle\xi|\hat{x}_\alpha^+ = \langle\xi|\bar{\xi}_\alpha \ , \tag{C.7}$$

  where $\hat{x} = \hat{a}$, $\xi = \phi$, $\bar{\xi} = \phi^*$ for bosons, $\hat{x} = \hat{c}$, $\xi = \psi$, $\bar{\xi} = \bar{\phi}$ for fermions, $\hat{x} = \hat{b}$, $\xi = \eta$, $\bar{\xi} = \bar{\eta}$ for hard-core bosons[1].

- Scalar product, where the operator $\hat{X}$ is built of bosonic, fermionic, or hard-core operators, respectively:

$$\langle\xi|\hat{X}(\hat{x}^+,\hat{x})|\xi'\rangle = e^{\sum_\alpha \bar{\xi}_\alpha\xi'_\alpha} X(\bar{\xi}_\alpha,\xi'_\alpha) \ , \tag{C.8}$$

  where $\hat{x}$, ξ, $\bar{\xi}$ have to be chosen as mentioned above.

- Closure relation (the unity operator is denoted by $\mathbf{1}$):

$$\mathbf{1} = \int e^{-\sum_\alpha \phi^*_\alpha\phi_\alpha} |\phi\rangle \langle\phi| \prod_\alpha \frac{\mathrm{d}\phi^*_\alpha \mathrm{d}\phi_\alpha}{2\pi\mathrm{i}} \tag{C.9}$$

$$\mathbf{1} = \int e^{-\sum_\alpha \bar{\psi}_\alpha\psi_\alpha} |\psi\rangle \langle\psi| \prod_\alpha \mathrm{d}\bar{\psi}_\alpha \mathrm{d}\psi_\alpha \tag{C.10}$$

$$\mathbf{1} = \int e^{+\sum_\alpha \bar{\eta}_\alpha\eta_\alpha} |\eta\rangle \langle\eta| \prod_\alpha \mathrm{d}\bar{\eta}_\alpha \mathrm{d}\eta_\alpha \ . \tag{C.11}$$

- Trace of an operator $\hat{X}$:

$$\mathrm{Tr}\ \hat{X}(\hat{a}^+_\alpha,\hat{a}_\alpha) = \int e^{-\sum_\alpha \phi^*_\alpha\phi_\alpha} \langle\phi|\hat{X}|\phi\rangle \prod_\alpha \frac{\mathrm{d}\phi^*_\alpha \mathrm{d}\phi_\alpha}{2\pi\mathrm{i}} \tag{C.12}$$

$$\mathrm{Tr}\ \hat{X}(\hat{c}^+_\alpha,\hat{c}_\alpha) = \int e^{-\sum_\alpha \bar{\psi}_\alpha\psi_\alpha} \langle -\psi|\hat{X}|\psi\rangle \prod_\alpha \mathrm{d}\bar{\psi}_\alpha \mathrm{d}\psi_\alpha \tag{C.13}$$

$$\mathrm{Tr}\ \hat{X}(\hat{b}^+_\alpha,\hat{b}_\alpha) = \int e^{+\sum_\alpha \bar{\eta}_\alpha\eta_\alpha} \langle\eta|\hat{X}|\psi\rangle \prod_\alpha \mathrm{d}\bar{\eta}_\alpha \mathrm{d}\eta_\alpha \tag{C.14}$$

Using these identities, the functional integral of the grand canonical partition function

$$Z = \mathrm{Tr}\ e^{-\beta(\hat{H}(\hat{x}^+_\alpha,\hat{x}_\alpha)-\mu\hat{N}(\hat{x}^+_\alpha,\hat{x}_\alpha))}$$

[1] Note: Here, the symbol ξ has nothing to do with the generating field in eq. (7.6).

with the Hamiltonian $\hat{H}$ is constructed in the following manner: We apply the relation for the trace and insert the closure relation $M-1$ times. Introducing the discrete-imaginary-time index $n = 1, \ldots, M$ we have:

$$Z = \int e^{\sigma_1 \sum_{\alpha,n} \bar{\xi}_{\alpha,n}\xi_{\alpha,n}} \langle \sigma_2 \bar{\xi}_1 | e^{-\frac{\beta}{M}(\hat{H}-\mu\hat{N})} | \xi_M \rangle \prod_{n=2}^{M} \langle \bar{\xi}_n | e^{-\frac{\beta}{M}(\hat{H}-\mu\hat{N})} | \xi_{n-1} \rangle \prod_{\alpha,n} \frac{\mathrm{d}\bar{\xi}_\alpha \mathrm{d}\xi_\alpha}{\mathcal{N}} \,, \tag{C.15}$$

where $\sigma_1 = -1$ for bosons and fermions and $+1$ for hard-core bosons, $\sigma_2 = +1$ for bosons and hard-core bosons and -1 for fermions, and $\mathcal{N} = 2\pi\mathrm{i}$ for bosons and 1 for fermions and hard-core bosons. The minus sign inside the scalar product in the fermionic trace gives rise to the anti-periodicity of the fermionic field variables. The different sign in the exponent of the hard-core bosonic trace is the reason that the diagonal term in the action for hard-core bosons is different from bosonic and fermionic actions.

The operator in the exponent $\hat{H}(\hat{x}_\alpha^+, \hat{x}_\alpha) - \mu\hat{N}(\hat{x}_\alpha^+, \hat{x}_\alpha)$ can be replaced by its normal ordered from by making an error of the order $(\beta/M)^2$ which vanishes for $M \to \infty$. Applying the eigenvalue property and the product property yields

$$Z = \lim_{M\to\infty} \int e^{-A(\bar{\xi},\xi)} \prod_{n=1}^{M} \prod_{\alpha} \frac{\mathrm{d}\bar{\xi}_{\alpha,n} \mathrm{d}\xi_{\alpha,n}}{\mathcal{N}} \tag{C.16}$$

with the action

$$A(\bar{\xi},\xi) = \frac{\beta}{M} \sum_{n=1}^{M} \left\{ \sum_{\alpha} \sigma_1 \bar{\xi}_{\alpha,n+1} \left[\frac{M}{\beta} \left(\xi_{\alpha,n+1} - \xi_{\alpha,n} \right) - \mu\xi_{\alpha,n} \right] + H(\xi^*_{\alpha,n+1}, \xi_{\alpha,n}) \right\} \tag{C.17}$$

and the boundary condition $\xi_{\alpha,1} = \sigma_2 \xi_{\alpha,M+1}$, $\bar{\xi}_{\alpha,1} = \sigma_2 \bar{\xi}_{\alpha,M+1}$.

D Correlation functions for the hard-core Bose model

We expand the expressions inside the angled brackets of the three expectation values given in eqs. (7.34), (7.36) and (7.39) For simplicity we write

$$\tilde{\mu} = \frac{\beta(\mu + J)}{M} , \quad f_{\mathbf{r}} = \delta\varphi_{\mathbf{r}} + \mathrm{i}\delta\chi_{\mathbf{r}} , \quad \bar{f}_{\mathbf{r}} = \delta\varphi^*_{\mathbf{r}} + \mathrm{i}\delta\chi^*_{\mathbf{r}} ,$$

where we have dropped the imaginary time index $n = 0$. We neglect all terms of higher order than $\tilde{\mu}^1$. For the trivial solution, we find

$$\begin{aligned} C_1(\mathbf{r},\mathbf{r}) &\approx \left\langle 1 - f_{\mathbf{r}}\bar{f}_{\mathbf{r}} \right\rangle \\ C_1(\mathbf{r},\mathbf{r}') &\approx \left\langle f_{\mathbf{r}}\bar{f}_{\mathbf{r}'} \right\rangle \\ C_2(\mathbf{r},\mathbf{r}';\mathbf{r}',\mathbf{r}) &\approx \left\langle 1 - f_{\mathbf{r}}\bar{f}_{\mathbf{r}} - f_{\mathbf{r}'}\bar{f}_{\mathbf{r}'} \right\rangle . \end{aligned}$$

For the non-trivial solution, i.e. in the broken $U(1)$ symmetry case, we find

$$\begin{aligned} C_1(\mathbf{r},\mathbf{r}) &\approx \left\langle 1 - \tilde{\mu} - \sqrt{\tilde{\mu}}(f_{\mathbf{r}} + \bar{f}_{\mathbf{r}}) + (-1 + 3\tilde{\mu}) f_{\mathbf{r}}\bar{f}_{\mathbf{r}} + \tilde{\mu}(f^2_{\mathbf{r}} + \bar{f}^2_{\mathbf{r}}) \right\rangle \\ C_1(\mathbf{r},\mathbf{r}') &\approx \Big\langle \tilde{\mu} + \sqrt{\tilde{\mu}}(f_{\mathbf{r}} + \bar{f}_{\mathbf{r}'}) - 2\tilde{\mu}(f_{\mathbf{r}}\bar{f}_{\mathbf{r}} + f_{\mathbf{r}'}\bar{f}_{\mathbf{r}'}) - \tilde{\mu}(f^2_{\mathbf{r}} + \bar{f}^2_{\mathbf{r}'}) \\ &\quad -\tilde{\mu}(f_{\mathbf{r}}f_{\mathbf{r}'} + \bar{f}_{\mathbf{r}}\bar{f}_{\mathbf{r}'}) + (1 - 3\tilde{\mu}) f_{\mathbf{r}}\bar{f}_{\mathbf{r}'} \Big\rangle \\ C_2(\mathbf{r},\mathbf{r}';\mathbf{r}',\mathbf{r}) &\approx \Big\langle (1 - 2\tilde{\mu}) - \sqrt{\tilde{\mu}}(f_{\mathbf{r}} + \bar{f}_{\mathbf{r}} + f_{\mathbf{r}'} + \bar{f}_{\mathbf{r}'}) + \tilde{\mu}(f^2_{\mathbf{r}} + \bar{f}^2_{\mathbf{r}} + f^2_{\mathbf{r}'} + \bar{f}^2_{\mathbf{r}'}) \\ &\quad +(-1 + 4\tilde{\mu})(f_{\mathbf{r}}\bar{f}_{\mathbf{r}} + f_{\mathbf{r}'}\bar{f}_{\mathbf{r}'}) + \tilde{\mu}(f_{\mathbf{r}}f_{\mathbf{r}'} + \bar{f}_{\mathbf{r}}\bar{f}_{\mathbf{r}'} + f_{\mathbf{r}}\bar{f}_{\mathbf{r}'} + \bar{f}_{\mathbf{r}}f_{\mathbf{r}'}) \Big\rangle . \end{aligned}$$

The expectation values which are linear in the field fluctuations vanish: $\langle f_{\mathbf{r}} \rangle = \langle \bar{f}_{\mathbf{r}} \rangle = 0$. The expectations values which are quadratic in $f_{\mathbf{r}}$ and $\bar{f}_{\mathbf{r}}$, are given by the functions in eqs. (7.40) and (7.41), and can be calculated as linear combinations of expectations values with respect to the fluctuations of the real fields $\delta\phi^{\gamma}_{\mathbf{r}}$:

$$\begin{aligned} F_1(\mathbf{r} - \mathbf{r}') &= \langle f_{\mathbf{r}} f_{\mathbf{r}'} \rangle = \langle \bar{f}_{\mathbf{r}} \bar{f}_{\mathbf{r}'} \rangle \\ &= \left\langle (\delta\phi^1_{\mathbf{r}} + \mathrm{i}\delta\phi^2_{\mathbf{r}} + \mathrm{i}\delta\phi^3_{\mathbf{r}} - \delta\phi^4_{\mathbf{r}})(\delta\phi^1_{\mathbf{r}'} + \mathrm{i}\delta\phi^2_{\mathbf{r}'} + \mathrm{i}\delta\phi^3_{\mathbf{r}'} - \delta\phi^4_{\mathbf{r}'}) \right\rangle \\ F_2(\mathbf{r} - \mathbf{r}') &= \langle f_{\mathbf{r}} \bar{f}_{\mathbf{r}'} \rangle = \langle \bar{f}_{\mathbf{r}} f_{\mathbf{r}'} \rangle \\ &= \left\langle (\delta\phi^1_{\mathbf{r}} + \mathrm{i}\delta\phi^2_{\mathbf{r}} + \mathrm{i}\delta\phi^3_{\mathbf{r}} - \delta\phi^4_{\mathbf{r}})(\delta\phi^1_{\mathbf{r}'} + \mathrm{i}\delta\phi^2_{\mathbf{r}'} - \delta\phi^3_{\mathbf{r}'} - \mathrm{i}\delta\phi^4_{\mathbf{r}'}) \right\rangle \end{aligned}$$

On the level of Gaussian fluctuations, these expectation values are given by the matrix elements of inverse of the matrix $\hat{\mathcal{G}}^{-1}$ given in eq. (7.25):

$$\left\langle \delta\phi^{\gamma}_{\mathbf{r}} \delta\phi^{\gamma'}_{\mathbf{r}'} \right\rangle = \frac{1}{2} \hat{\mathcal{G}}^{\gamma\gamma'}_{\mathbf{r}\mathbf{r}';nm}$$

For the Fourier transforms of the functions F_1 and F_2 we find for the trivial solution the expressions

$$F_1^{\mathrm{tr}}(\mathbf{k}) = 0 \tag{D.1}$$

$$\begin{aligned} F_2^{\mathrm{tr}}(\mathbf{k}) &= \lim_{M\to\infty} \frac{1}{M} \sum_{n=1}^{M} \frac{\tilde{b}_{\mathbf{k}} \left(\cos\left(\frac{2\pi}{M} n\right) - \tilde{b}_{\mathbf{k}} \right)}{-2\tilde{b}_{\mathbf{k}} \cos\left(\frac{2\pi}{M} n\right) + 1 + \tilde{b}_{\mathbf{k}}^2} \\ &= \frac{1}{2} \coth\left(\frac{\beta}{2} (\epsilon_{\mathbf{k}} - (\mu + J)) \right) - \frac{1}{2} , \end{aligned} \tag{D.2}$$

which vanish completely at zero temperature. For the non-trivial solution we find

$$\begin{aligned} F_1^{\mathrm{nt}}(\mathbf{k}) &= \lim_{M\to\infty} \frac{1}{M} \sum_{n=1}^{M} \frac{\tilde{b}_{\mathbf{k}}^2 \tilde{\mu}}{2\tilde{b}_{\mathbf{k}} \cos\left(\frac{2\pi}{M} n\right) - 1 - 2\tilde{\mu} - \tilde{b}_{\mathbf{k}}^2 (1 + \tilde{\mu})} \\ &= -\frac{\mu + J}{2E_{\mathbf{k}}} \coth\left(\frac{\beta}{2} E_{\mathbf{k}} \right) \end{aligned} \tag{D.3}$$

$$\begin{aligned} F_2^{\mathrm{nt}}(\mathbf{k}) &= \lim_{M\to\infty} \frac{1}{M} \sum_{n=1}^{M} \frac{\tilde{b}_{\mathbf{k}} \left(\tilde{b}_{\mathbf{k}} - (1 + 2\tilde{\mu}) \cos\left(\frac{2\pi}{M} n\right) \right)}{2\tilde{b}_{\mathbf{k}} \cos\left(\frac{2\pi}{M} n\right) - 1 - 2\tilde{\mu} - \tilde{b}_{\mathbf{k}}^2 (1 + \tilde{\mu})} \\ &= \frac{\epsilon_{\mathbf{k}} + (\mu + J)}{2E_{\mathbf{k}}} \coth\left(\frac{\beta}{2} E_{\mathbf{k}} \right) - \frac{1}{2} \end{aligned} \tag{D.4}$$

where $\tilde{b}_{\mathbf{k}}$ is given in eq. (7.30), $E_{\mathbf{k}}$ is the Bogoliubov quasiparticle spectrum in eq. (7.33), $\epsilon_{\mathbf{k}}$ in eq. (4.7), and the sums are performed by help of the identities (A.5) and (A.6). The back transformation gives

$$F_{1,2}^{\mathrm{tr,nt}}(\mathbf{r} - \mathbf{r}') = \int F_{1,2}^{\mathrm{tr,nt}}(\mathbf{k}) \, \mathrm{e}^{-\mathrm{i}\mathbf{k}(\mathbf{r}-\mathbf{r}')} \, \frac{\mathrm{d}^d k}{(2\pi)^2} . \tag{D.5}$$

In the limit $M \to \infty$, the results are

$$C_1(\mathbf{r}, \mathbf{r}) = 1 - F_2^{\mathrm{tr,nt}}(\mathbf{r} = \mathbf{r}') \tag{D.6}$$

$$C_1(\mathbf{r}, \mathbf{r}') = F_2^{\mathrm{tr,nt}}(\mathbf{r} - \mathbf{r}') \tag{D.7}$$

$$C_2(\mathbf{r}, \mathbf{r}'; \mathbf{r}', \mathbf{r}) = 1 - 2\, F_2^{\mathrm{tr,nt}}(\mathbf{r} = \mathbf{r}') \tag{D.8}$$

D.1 Decay of the density-density CF

The decay of the density-density CF given in eq. (7.45) is investigated in $d = 1, 2, 3$ dimensions. For convenience we write $c := \sqrt{2(\mu + J)}$. We use a cut-off at $|\mathbf{q}| = Q$ for the integrals.

- **One dimension:**

$$D(r) = \int_{-Q}^{Q} \frac{|q|}{c} e^{\mathrm{i}qr} \,\mathrm{d}q = \frac{2}{cr^2} \int_0^{Qr} q' \cos(q') \mathrm{d}q' \sim \frac{1}{r^2}$$

  The anti-symmetrical part which is $\sim \sin(q')$ does not contribute.

- **Two dimensions** with polar coordinates (q, ϕ):

$$D(r) = \int_0^Q \mathrm{d}q\, q \int_0^{2\pi} \mathrm{d}\phi \frac{q}{c} e^{\mathrm{i}qr\cos\phi} = \frac{1}{cr^3} \int_0^{2\pi} \mathrm{d}\phi \frac{1}{\cos^3\phi} \int_0^{rQ} q'^2 \cos(q') \mathrm{d}q' \sim \frac{1}{r^3}$$

- **Three dimensions** with spherical coordinates (q, θ, ϕ):

$$D(r) = \int_0^Q \mathrm{d}q\, q^2 \int_0^{2\pi} \mathrm{d}\phi \int_1^{-1} \mathrm{d}(\cos\theta) \frac{q}{c} e^{\mathrm{i}qr\cos\theta}$$

$$= \frac{2\pi}{cr^3} \int_1^{-1} \mathrm{d}(\cos\theta) \frac{1}{\cos^4\phi} \int_0^{rQ} q'^3 \cos(q') \mathrm{d}q' \sim \frac{1}{r^4}$$

E Calculations to the slave-boson model

E.1 Integration of the constraint

We perform the integration of the complex fields b and e in eq. (9.13). The integral factorises such that it can be performed for each lattice site $\mathbf{r}$ independently. Therefore we will drop the index $\mathbf{r}$ here temporarily and evaluate the expression

$$\int \exp\left\{-\beta s\varphi^2 - \beta(e,b)\begin{pmatrix} 2s\varphi+s & s\Phi \\ s\Phi^* & -\mu \end{pmatrix}\begin{pmatrix} e^* \\ b^* \end{pmatrix}\right\}\delta(|b|^2+|e|^2-1)\mathrm{d}e^*\mathrm{d}e\,\mathrm{d}b^*\mathrm{d}b\,. \tag{E.1}$$

The eigenvalues of the 2×2 matrix are

$$\lambda_\pm = \beta s\left(\varphi+\frac{1}{2}\right) - \beta\frac{\mu}{2} \pm \beta\sqrt{\left[\left(\varphi+\frac{1}{2}\right)s+\frac{\mu}{2}\right]^2 + s^2|\Phi|^2}\,.$$

A unitary transformation can be applied to the vector (e,b) such that the matrix has diagonal form. This does not affect the constraint, because the expression $|b|^2+|e|^2=1$ remains unchanged after a unitary transformation. Therefore the integral is equal to

$$\begin{aligned}
&\int \mathrm{d}e^*\mathrm{d}e\,\mathrm{d}b^*\mathrm{d}b\exp\left[-\beta s\varphi^2-\lambda_1|e|^2-\lambda_2|b|^2\right]\delta(|b|^2+|e|^2-1)\\
&\quad= (2\pi)^2\frac{1}{2}\int_0^1 \mathrm{d}\rho\,\rho\exp\left[-\beta s\varphi^2-\lambda_1\rho^2-\lambda_2\left(1-\rho^2\right)\right]\\
&\quad= 2\pi^2 e^{-\beta s\varphi^2}\,\frac{\mathrm{e}^{-\lambda_1}-\mathrm{e}^{-\lambda_2}}{\lambda_1-\lambda_2}\\
&= 4\pi^2\exp\left[-\beta s\varphi^2-\beta s\left(\varphi+\frac{1}{2}\right)+\beta\frac{\mu}{2}\right]\frac{\sinh\left[\beta\sqrt{\left[\left(\varphi+\frac{1}{2}\right)s+\frac{\mu}{2}\right]^2+s^2|\Phi|^2}\right]}{\beta\sqrt{\left[\left(\varphi+\frac{1}{2}\right)s+\frac{\mu}{2}\right]^2+s^2|\Phi|^2}}\,.
\end{aligned}$$

After performing the shift $\varphi+1/2\to\varphi$ and using the index $\mathbf{r}$ again, the integral (E.1) gives the result

$$\int_{-\infty}^{\infty}\mathrm{d}\varphi_{\mathbf{r}}\,\frac{\sinh\left[\beta\sqrt{\left(\varphi_{\mathbf{r}}s+\frac{\mu_{\mathbf{r}}}{2}\right)^2+s^2|\Phi_{\mathbf{r}}|^2}\right]}{\beta\sqrt{\left(\varphi_{\mathbf{r}}s+\frac{\mu_{\mathbf{r}}}{2}\right)^2+s^2|\Phi_{\mathbf{r}}|^2}}e^{-\beta s\varphi_{\mathbf{r}}^2+\frac{\beta\mu_{\mathbf{r}}}{4}}\,. \tag{E.2}$$

E.2 Condensate density and total particle density

Condensate density.
In a Bose system in an optical lattice, which is described by a complex field $\phi_{\mathbf{r}}(\tau)$, the condensate density is defined by the expression (3.25) via the concept of off-diagonal long range order. In classical approximation, the field does not depend on imaginary time τ, and in the slave-boson approach, we replace

$$\phi^*_{\mathbf{r}} \to b^*_{\mathbf{r}} e_{\mathbf{r}} \; ; \quad \phi_{\mathbf{r}} \to e^*_{\mathbf{r}} b_{\mathbf{r}} \; ,$$

thus we use the definition

$$n_0 = \lim_{\mathbf{x}-\mathbf{x}'\to\infty} \langle b^*_{\mathbf{x}} e_{\mathbf{x}} e^*_{\mathbf{x}'} b_{\mathbf{x}'} \rangle \; . \tag{E.3}$$

for the condensate density. Here, the expectation value is defined with respect the functional integral (9.14) by

$$\langle \cdots \rangle = \frac{1}{Z_{\mathrm{sb}}} \int \cdots \exp[\ldots] \; \mathcal{D}[\Phi^*, \Phi, \varphi] \, \mathcal{D}[b, b^*, e, e^*] \; . \tag{E.4}$$

We are interested in the connection between the correlation function $\langle \Phi_{\mathbf{x}} \Phi^*_{\mathbf{x}'} \rangle$ and the condensate density. For this purpose we integrate out the field Φ to transform the correlation function of the field Φ back to a correlation function of the fields b and e. Therefore, we write

$$\hat{v}_{\mathbf{r}\mathbf{r}'} := \frac{s\delta_{\mathbf{r}\mathbf{r}'} - \hat{J}_{\mathbf{r}\mathbf{r}'}}{s^2}$$

for simplicity and perform the integration

$$\beta^2 s^2 \int \Phi_{\mathbf{x}} \Phi^*_{\mathbf{x}'} \exp\left[\beta \sum_{\mathbf{r},\mathbf{r}'} \Phi^*_{\mathbf{r}} \hat{v}^{-1}_{\mathbf{r}\mathbf{r}'} \Phi_{\mathbf{r}'} + \beta s \sum_{\mathbf{r}} \Phi_{\mathbf{r}} b^*_{\mathbf{r}} e_{\mathbf{r}} + \beta s \sum_{\mathbf{r}} \Phi^*_{\mathbf{r}} e^*_{\mathbf{r}} b_{\mathbf{r}} \right] \prod_{\mathbf{r}} \mathrm{d}\Phi_{\mathbf{r}} \mathrm{d}\Phi^*_{\mathbf{r}} =$$

$$\frac{\partial}{\partial(b^*_{\mathbf{x}} e_{\mathbf{x}})} \frac{\partial}{\partial(b_{\mathbf{x}'} e^*_{\mathbf{x}'})} \int \exp\left[\beta \sum_{\mathbf{r},\mathbf{r}'} \Phi^*_{\mathbf{r}} \hat{v}^{-1}_{\mathbf{r}\mathbf{r}'} \Phi_{\mathbf{r}'} + \beta s \sum_{\mathbf{r}} \Phi_{\mathbf{r}} b^*_{\mathbf{r}} e_{\mathbf{r}} + \beta s \sum_{\mathbf{r}} \Phi^*_{\mathbf{r}} e^*_{\mathbf{r}} b_{\mathbf{r}} \right] \prod_{\mathbf{r}} \mathrm{d}\Phi_{\mathbf{r}} \mathrm{d}\Phi^*_{\mathbf{r}} =$$

$$\frac{\partial}{\partial(b^*_{\mathbf{x}} e_{\mathbf{x}})} \frac{\partial}{\partial(b_{\mathbf{x}'} e^*_{\mathbf{x}'})} \det\left(\frac{\hat{v}}{\beta}\right) \exp\left[\beta s^2 \sum_{\mathbf{r},\mathbf{r}'} b^*_{\mathbf{r}} e_{\mathbf{r}} \hat{v}_{\mathbf{r}\mathbf{r}'} e^*_{\mathbf{r}'} b_{\mathbf{r}'} \right] =$$

$$\beta s^2 \det\left(\frac{\hat{v}}{\beta}\right) \left[\hat{v}_{\mathbf{x}\mathbf{x}'} + \beta s^2 \sum_{\mathbf{r},\mathbf{r}'} b^*_{\mathbf{r}} e_{\mathbf{r}} e^*_{\mathbf{r}'} b_{\mathbf{r}'} \hat{v}_{\mathbf{r}\mathbf{x}} \hat{v}_{\mathbf{x}'\mathbf{r}'} \right] \exp\left[\beta s^2 \sum_{\mathbf{r},\mathbf{r}'} b^*_{\mathbf{r}} e_{\mathbf{r}} \hat{v}_{\mathbf{r}\mathbf{r}'} e^*_{\mathbf{r}'} b_{\mathbf{r}'} \right] \; .$$

Since we are interested in the limit $\mathbf{x}-\mathbf{x}' \to \infty$, and the matrix $\hat{J}_{\mathbf{x}\mathbf{x}'}$ includes nearest-neighbour hopping only, the term $\hat{v}_{\mathbf{x}\mathbf{x}'}$ vanishes. This yields for far distant lattice sites $\mathbf{x}, \mathbf{x}'$ the expression

$$\langle \Phi^*_{\mathbf{x}} \Phi_{\mathbf{x}'} \rangle = s^2 \sum_{\mathbf{r},\mathbf{r}'} \langle b^*_{\mathbf{r}} e_{\mathbf{r}} e^*_{\mathbf{r}'} b_{\mathbf{r}'} \rangle \, \hat{v}_{\mathbf{r}\mathbf{x}} \hat{v}_{\mathbf{x}'\mathbf{r}'} \; .$$

Further we can assume that $\langle b^*_{\mathbf{r}} e_{\mathbf{r}} e^*_{\mathbf{r}'} b_{\mathbf{r}'} \rangle = \langle b^*_{\mathbf{x}} e_{\mathbf{x}} e^*_{\mathbf{x}'} b_{\mathbf{x}'} \rangle$ for $\mathbf{r}, \mathbf{x}$ and $\mathbf{r}', \mathbf{x}'$ nearest neighbours. Using

$$\sum_{\mathbf{r}} \hat{v}_{\mathbf{r}\mathbf{x}} = \sum_{\mathbf{r}'} \hat{v}_{\mathbf{x}'\mathbf{r}'} = \frac{s+J}{s^2} \; ,$$

we get

$$\lim_{\mathbf{x}-\mathbf{x}'\to\infty} \langle \Phi^*_{\mathbf{x}} \Phi_{\mathbf{x}'} \rangle = \frac{(s+J)^2}{s^2} \lim_{\mathbf{x}-\mathbf{x}'\to\infty} \langle b^*_{\mathbf{x}} e_{\mathbf{x}} e^*_{\mathbf{x}'} b_{\mathbf{x}'} \rangle$$

and therefore

$$n_0 = \frac{s^2}{(s+J)^2} \lim_{\mathbf{x}-\mathbf{x}'\to\infty} \langle \Phi^*_{\mathbf{x}} \Phi_{\mathbf{x}'} \rangle \; .$$

Total particle density.
The total particle density at site $\mathbf{r}$ is given as

$$n_{\mathbf{r}} = 1 - \left\langle |e_{\mathbf{r}}|^2 \right\rangle \; , \tag{E.5}$$

where e is the field associated to empty sites. Expectation values are defined by means of eq. (E.3) with respect to the functional integral (9.14). It is possible to express the expectation value of the complex field e in terms of an expectation value of the real field φ. To achieve that, let us regard the integration over the fields b, e, and φ. After performing the substitution $\varphi + 1/2 \to \varphi$ and dropping the index $\mathbf{r}$, we have

$$\begin{aligned} &\int \mathrm{d}\varphi \, \mathrm{e}^{-\beta s \left(\varphi - \frac{1}{2}\right)^2} \int \mathcal{D}[b, b^*, e, e^*] \, |e|^2 \exp\left\{ -\beta (e, b) \begin{pmatrix} 2s\varphi & s\Phi \\ s\Phi^* & -\mu \end{pmatrix} \begin{pmatrix} e^* \\ b^* \end{pmatrix} \right\} \\ &\quad = -\frac{1}{2s\beta} \int \mathrm{d}\varphi \, \mathrm{e}^{-\beta s \left(\varphi - \frac{1}{2}\right)^2} \frac{\partial}{\partial \varphi} \int \mathcal{D}[b, b^*, e, e^*] \, \exp\Big\{ \dots \Big\} \; . \end{aligned}$$

Partial integration leads to

$$\frac{1}{2s\beta} \int \mathrm{d}\varphi \left[-2\beta s \left(\varphi - \frac{1}{2} \right) \right] \mathrm{e}^{-\beta s \left(\varphi - \frac{1}{2}\right)^2} \int \mathcal{D}[b, b^*, e, e^*] \, \exp\Big\{ \dots \Big\} \; .$$

Therefore we find

$$\left\langle |e|^2 \right\rangle = \left\langle - \left(\varphi - \frac{1}{2} \right) \right\rangle \; .$$

Together with eq. (E.5) we find for the local total particle density the expression

$$n_{\mathbf{r}} = \langle \varphi_{\mathbf{r}} \rangle + \frac{1}{2} \; . \tag{E.6}$$

E.3 Zero temperature limit

We want to integrate out the function Z' (we drop the index $\mathbf{r}$) given in eq. (9.17) for zero temperature, i.e. in the limit $\beta \to \infty$. For simplicity we write $\tilde{\beta} := \beta s$ and perform the limit $\beta \to \infty$ instead. Further we write $a := \mu/2s$, and $x := |\Phi|^2$. The function Z' we write as

$$Z' = \frac{1}{2\tilde{\beta}}(Z_- - Z_+) \,,$$

where

$$Z_\pm = \int_{-\infty}^{\infty} \frac{e^{-\tilde{\beta} f_\pm(\varphi,x)}}{\sqrt{(\varphi+a)^2+x}} \,\mathrm{d}\varphi$$

and

$$f_\pm(\varphi,x) = \varphi^2 \pm \sqrt{(\varphi+a)^2+x} \,.$$

In the limit $\tilde{\beta} \to \infty$ we can calculate the φ-integral $Z_\pm$ exactly by means of a saddle-point integration. This is done by expanding the functions $f_\pm$ in second order about their minimum with respect to φ. We need partial derivatives

$$\begin{aligned} \frac{\partial f_\pm(\varphi,x)}{\partial\varphi} &= 2\varphi \pm \frac{\varphi+a}{\sqrt{(\varphi+a)^2+x}} \\ \frac{\partial^2 f_\pm(\varphi,x)}{\partial\varphi^2} &= 2 \pm \frac{x}{[(\varphi+a)^2+x]^{\frac{3}{2}}} \,. \end{aligned}$$

We determine the extrema of $f_\pm$:

$$\frac{\partial f_\pm(\varphi_0,x)}{\partial\varphi} = 0 \quad \Rightarrow \quad \sqrt{(\varphi_0+a)^2+x} = \mp\frac{\varphi_0+a}{2\varphi_0} \,, \tag{E.7}$$

which is equivalent to

$$x = (\varphi_0+a)^2\left(\frac{1}{4\varphi_0^2}-1\right) \,. \tag{E.8}$$

Thus the saddle point approximation for large values of $\tilde{\beta}$ is

$$\begin{aligned} Z_\pm &\approx \int_{-\infty}^{\infty} \frac{e^{-\tilde{\beta}\left[f_\pm(\varphi_0,x)+\frac{1}{2}\frac{\partial^2 f_\pm}{\partial\varphi^2}(\varphi_0,x)(\varphi-\varphi_0)^2\right]}}{\sqrt{(\varphi_0+a)^2+x}} \,\mathrm{d}\varphi \\ &= \sqrt{\frac{\pi}{(\varphi_0+a)^2+x}} \frac{e^{-\tilde{\beta} f_\pm(\varphi_0,x)}}{\sqrt{\frac{\tilde{\beta}}{2}\frac{\partial^2 f_\pm(\varphi_0,x)}{\partial\varphi^2}}} \,. \end{aligned}$$

From eq. (E.7) we get

$$f_\pm(\varphi_0) = \varphi_0^2 - \frac{1}{2} - \frac{a}{2\varphi_0} \,; \quad \frac{\partial^2 f_\pm(\varphi_0)}{\partial\varphi^2} = 2 - \frac{8x(\varphi_0)\varphi_0^3}{(\varphi_0+a)^3} \,,$$

where x itself depends on φ_0 independently via eq. (E.8). For given x there are two solutions for φ_0, but only the one which is the absolute minimum contributes to Z' for large values of $\tilde{\beta}$. Therefore:

$$\log Z' = \log(\varphi_0) - \log(\varphi_0 + a) - \frac{1}{2}\log\left(\frac{\partial^2 f_\pm(\varphi_0)}{\partial\varphi^2}\right) - \tilde{\beta} f_\pm(\varphi_0) + \text{const}\,.$$

The term that is proportional to $\tilde{\beta}$ dominates all the others, and in the limit $\tilde{\beta} \to \infty$ we find the *exact* result

$$\lim_{\tilde{\beta}\to\infty} \frac{1}{\tilde{\beta}} \log Z' = -f_\pm(\varphi_0)$$

$$\Rightarrow \quad \lim_{\tilde{\beta}\to\infty} \frac{1}{\tilde{\beta}} \frac{\partial}{\partial x} \log Z' = -\left[\frac{\mathrm{d}f_\pm(\varphi_0)}{\mathrm{d}\varphi_0}\right] \frac{\mathrm{d}\varphi_0}{\mathrm{d}x}\,.$$

The derivative of φ_0 with respect to x we get from eq. (E.8) by means of the implicit function theorem:

$$\frac{\mathrm{d}\varphi_0}{\mathrm{d}x} = \frac{-2\varphi_0^3}{(\varphi_0 + a)(4\varphi_0^3 + a)}\,.$$

Therefore:

$$\lim_{\tilde{\beta}\to\infty} \frac{1}{\tilde{\beta}} \frac{\partial}{\partial x} \log Z' = \frac{\varphi_0}{\varphi_0 + a}\,.$$

Together with the mean-field equation (9.22), we find the zero temperature result in the condensed phase (i.e. where $x > 0$):

$$\frac{s}{s+J} - \frac{\varphi_0}{\varphi_0 + a} = 0 \quad \Rightarrow \quad \varphi_0 = \frac{\mu}{2J}\,.$$

For the order parameter we find from eq. (E.8) in the condensed phase:

$$|\Phi|^2 = x = \frac{1}{4}\left(\frac{s+J}{Js}\right)^2 \left(J^2 - \mu^2\right)\,.$$

Thus the condensate density by the definition in eq. (9.18) is:

$$n_0 = \frac{s^2}{(s+J)^2}|\Phi|^2 = \begin{cases} \frac{1}{4}\left(1 - \frac{\mu^2}{J^2}\right) & \text{if } -J < \mu < J \\ 0 & \text{else}\,, \end{cases} \tag{E.9}$$

and because of $\langle\varphi\rangle = \varphi_0$ the total particle density by the definition (9.19) is:

$$n_{\text{tot}} = \varphi_0 + \frac{1}{2} = \begin{cases} 0 & \text{if } \mu \le -J \\ \frac{1}{2}\left(1 - \frac{\mu}{J}\right) & \text{if } -J < \mu < J \\ 1 & \text{if } J \le \mu\,. \end{cases} \tag{E.10}$$

To determine the coefficient $\tilde{a}_4$ in eq. (9.27), we need the second derivative of $\log Z$ with respect to x:

$$\begin{aligned}\lim_{\tilde{\beta}\to\infty} \frac{1}{\tilde{\beta}} \frac{\partial^2}{\partial x^2} \log Z' &= \left[\frac{\mathrm{d}}{\mathrm{d}\varphi} \lim_{\tilde{\beta}\to\infty} \frac{1}{\tilde{\beta}} \frac{\partial}{\partial x} \log Z'\right] \frac{\mathrm{d}\varphi_0}{\mathrm{d}x} \,, \\ &= \frac{1}{s} \frac{-\mu\varphi_0^3}{(\varphi_0+a)^3(4\varphi_0^3+a)} \,.\end{aligned}$$

With the above solution this yields

$$\lim_{\beta\to\infty} \frac{1}{\beta} \frac{\partial^2}{\partial x^2} \log Z' = 2J \frac{s^4}{(s+J)^4} \left[1 - 4\,\frac{s}{s+J}\, n_0\right] \,. \tag{E.11}$$

With these results we also find the zero temperature expressions for the renormalised coefficients (9.42) and (9.43):

$$\mu_\mathrm{R} = -(s+J) + \frac{(s+J)^2}{s+|\mu|} \,; \quad g_\mathrm{R} = 2a^3 J \,. \tag{E.12}$$

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Lebenslauf

Name:	Christopher Moseley
Geburtsdatum:	15. Juni 1976
Geburtsort:	Groß-Gerau (Hessen)
Staatsangehörigkeit:	deutsch

1983	Grundschule Groß-Zimmern (Hessen)
1984	Umzug nach Mering (Bayern) Grundschule Mering
1987-1996	Rudolf-Diesel-Gymnasium Augsburg
1993	Umzug nach Augsburg
1996	Abitur
1996/97	Zivildienst in Augsburg
WS 1997	Immatrikulation an der Universität Augsburg im Fach Physik (Diplom)
1999	Vordiplom
Jun. 2003	Diplomablschluss
seit Sept. 2003	Doktorand an der Universität Augsburg bei Prof. Dr. Klaus Ziegler zum Thema Bose-Einstein-Kondensation