BEC in Optical Lattices: Beyond the Bogoliubov Approximation

Diploma Thesis by
Pascal Mattern

Supervisor: Prof. Dr. Dr. h.c. mult. Hagen Kleinert

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Chapter 1

Introduction

"*From a certain temperature on, the molecules 'condense' without attractive forces; that is, they accumulate at zero velocity. The theory is pretty, but is there some truth to it?*"

Albert Einstein, Letter to Ehrenfest 1924

1.1 What is a BEC?

In general, particles in a quantum-mechanical physical system can assume infinitely many different states. One might ask the question whether it would be possible for all particles to be in the *same* state and what this would mean for such a degenerate system. Quantum Field Theory shows that there are two kind of particles: only those particles with an integer spin, called *bosons*, are allowed to populate one state multiple times. The other kind of particles are called fermions, of which only one can be in a specific quantum state. We remark that in 3 (or more) dimensions only these two distinctions between particles occur, while in 2D-systems (quasi-)particles called Anyons can exist, which for example are needed to explain the fractional quantum Hall effect.
The typical quantum system has one well-defined ground state, and a particle in this state has the least possible energy. So, obviously, the system needs to be cooled down in order to have many particles in the ground state. Interestingly, formation of BEC sets in at temperatures considerably higher than the energy of the first excited state [1], showing that at this critical temperature T_C actually something very interesting happens.
A phase transition to such a *macroscopic population* of one single state at very low temperatures was predicted in 1924 for ideal Bose gases by Satyendranath Bose [2] and Albert Einstein [3]. Such a system possesses an extremely high coherence which motivates a very descriptive visualization as a *macroscopic matter wave*: at low temperatures, the wave-like character of the atoms dominates their behavior, and their wavelength grows. At some point, the waves start to overlap and we can no longer distinguish between the atoms but instead have to think of the whole condensate as a giant matter wave. In short, a BEC allows us to observe quantum-mechanical features on a macroscopic level. We remark that a pair of two fermions is again a bosonic particle. In a neutral atom, we have the same number of electrons (spin = 1/2) and protons (spin = 1/2). Therefore the number of neutrons (also spin=1/2) determines whether

the atom is a boson or a fermion: isotopes with an even number of neutrons are bosonic, those with an odd number fermionic, so in theory, every element could be in a state of BEC.

In a physical system, depending on the temperature, the particles will populate the different states, with the probability for states of higher energy exponentially lower than those with lower energies, the distribution function being the *Bose-Einstein* or *Fermi distribution*, respectively, and in classical physics or as an approximation in Quantum Mechanics, the *Boltzmann distribution*. At zero temperature, all bosons should be in the ground state (or the ground states, if they are degenerate). It became a challenge for experimental physicists to create a system with a low enough temperature. As it turned out, this was actually a very daunting task, during the completion of which several methods had to be invented and several Nobel Prizes were awarded for these. The Nobel Prize for Physics in 2001 was jointly awarded to Eric Cornell and Carl Wieman (University of Colorado) as well as Wolfgang Ketterle (MIT) for the creation of the first BEC in 1995.

So, not until 70 years after its original prediction, Bose-Einstein condensation was first observed in a gas consisting of around 2000 spin-polarized Rb^{87} atoms, which were enclosed in a quadrupole trap, cf. [4]. The transition temperature for that experiment lies at about $170 * 10^{-9}$ K, a temperature which could not be realized before. For BEC's with other atoms, the needed temperatures are of similar order, for spin-polarized Li^7 atoms for example, $T_C = 400 * 10^{-9}$ K.
One might at first raise the objection that at such low temperatures the alkali atoms should form a solid; this is indeed a problem, however, a metastable gaseous state can be maintained within the trap even at temperatures in the nanokelvin range. In the initial experiments the condensed state could be kept for about ten seconds. Solidification is basically a three-body-process, so a low density should help to extend the lifetime of the BEC.

1.2 Why are BEC's interesting?

Physics as an empiric science obviously needs the experiment to confirm its theoretical models. So, although the BEC-transition had been predicted many decades ago, it was still a huge breakthrough to finally see its actual appearance in nature. Furthermore, BEC's could be applied in a multitude of fields, such as the construction of a *quantum computer* which uses quantum logic (with so-called qubits) instead of the classical 0-1 transistors. A group at the Max-Planck-Institute for Quantum Optics (MPQ) is currently conducting experiments of this nature [5].

Since a BEC allows for the creation of UV-light or even X-rays, i.e. EM-waves with a considerably lower wavelength than what could be achieved earlier, called *atom-laser* [6], many more practical uses will be found, for example in the production of extremely small circuits on semiconductors. When a BEC of Cesium was created for the first time in 2002 ([7]), this opened up new possibilities for measuring gravitational fields very accurately (Cesium is a prime candidate since it has a large mass) as well as help with the defining of our fundamental unit of time cf. [8].

In general, a BEC in an optical lattice behaves like a perfect (without impurities) solid state body with a very high tunability of the system parameters which makes it very attractive to work with.

To simulate the effects of a strong magnetic field with the electrically neutral BEC-atoms, a group in Munich recently developed a method by using a Raman Laser (in addition to the lasers needed for the optical lattice) see [9]. This opens new possibilities to observe the behavior in extremely strong magnetic fields.

As in solid state bodies, in a BEC in an optical lattice, band structures will appear. These can be manipulated by superimposing phase-shifted lasers and can then be used to realize such interesting phenomena like the Klein-tunneling [10].

There is indeed a wide range of applications for the theory of BEC, ranging from the extremely small (the Higgs boson in the vacuum) to the extremely large (matter in the core of a neutron star). It is no surprise that this field of research has attracted a lot of attention over the last years and that we have chosen it to be the subject of this thesis.

1.3 Overview of this diploma thesis

After this introductory chapter we proceed directly to BEC's in optical lattices in **chapter 2**. We introduce and explain the Bose-Hubbard Hamiltonian and how the phase transition from the superfluid to the Mott-insulator takes place. A very short and, owing to the theoretical nature of this thesis, incomplete, overview of the most important experimental methods to create a BEC is also given.

As the starting point of our calculations in **chapter 3** we use the approximation that the wave function of the system is essentially a classical state, namely the ground state with a small correction, i.e. we start in the superfluid state. Our aim is to calculate the value for U/J where the phase transition from the SF to the MI state takes place. This is done by observing the ground state density n_0: when it reaches zero, the system is in the Mott-insulator state. The correlation of U/J and n_0 is plotted by eliminating the chemical potential.

In **chapter 4**, in order to increase the magnitude of the interactions that should lead to the insulator state, we include the next order in the interactions and represent them diagrammatically by Feynman Diagrams.

We use these in **chapter 5** by taking the zero temperature limit and again looking for the critical value of U/J including the second order.

After showing that this path leads to problems, we try another way: instead of solving the two fundamental equations by reinserting and eliminating as before, we try a purely numerical calculation of the original equations with a self-written program thereby avoiding the aforementioned problems. **Chapter 6** shows the result, while the program and the result of some unwieldy derivations can be found in the **Appendix**.

A short summary of this work is given in **chapter 7**.

Chapter 2

BEC in optical lattices

"To coldly go where no one has gone before."
Charles Seife, in an article about BEC

In this thesis, we will examine BEC's in optical lattices. "Optical" meaning that a (1-,2- or 3-dimensional) lattice of laser-light intensity minima and maxima is created, which due to the Stark-Effect means that the atoms will be drawn to either the maxima or minima and repelled by the other, respectively. We therefore get the two limiting cases:

- a very weak laser field, i.e. extremely shallow potential wells, means that the atoms are able to move freely within the BEC (as mentioned, interactions between the atoms themselves are typically very weak). This state is called "superfluid", and like a superfluid it has a linear excitation spectrum without a gap.

- as the laser intensity is raised, the atoms become more and more trapped at the intensity extrema. When they are highly localized, we speak of the BEC being in a "Mott-insulator state". No excitations are possible for energies too low to allow the atoms to escape the potential wells.

As mentioned earlier, the phase transition that appears between these two extremes is what we will investigate in this thesis, namely the one starting from the superfluid state and ending in the Mott-insulator state. The other direction has been the topic of several works, cf. [11], [12].

2.1 Theoretical basics

We will now investigate BEC's in optical cubic lattices from a theorist's point of view. The first successful experiment where a BEC could be confined in an optical lattice took place in 1997 at MIT [13].

2.1.1 Bose-Hubbard-Hamiltonian

A reasonable starting point for our calculations is the **Bose-Hubbard-Hamiltonian**, well-known from Solid State Physics.

For example in [11] (in German) or in the seminal paper [14] the Bose-Hubbard Hamiltonian has been shown to be a special case for the general Hamiltonian for interacting bosons:

$$\hat{H} = \int d^3x \hat{\Psi}^\dagger(\mathbf{x}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}} \right] \hat{\Psi}(\mathbf{x}) + \frac{1}{2} \int \int d^3x_1 d^3x_2 \hat{\Psi}^\dagger(\mathbf{x}_1)\hat{\Psi}^\dagger(\mathbf{x}_2) V_{\text{int}}(\mathbf{x}_1, \mathbf{x}_2)\hat{\Psi}(\mathbf{x}_1)\hat{\Psi}(\mathbf{x}_2) \tag{2.1}$$

We will therefore not do a step-by-step derivation but instead just list the underlying assumptions:

- Only two-particle contact interaction
  Due to the low density of atoms in a BEC it is generally assumed that the interaction between the particles is of the form:

  $$V_{\text{int}} = \frac{4\pi\hbar^2 a_s}{m}\delta(\mathbf{x}_1 - \mathbf{x}_2) \ , \tag{2.2}$$

  with a_s being the s-wave (i.e. lowest order) scattering length. This is valid to a high degree of precision in a BEC because of the low particle density. Obviously, this enormously facilitates all of our calculations and is a reason why a BEC is so attractive from a theorist's point of view. We refer to a recent work [15] where more realistic interactions are examined.

- High localization
  For highly localized particles it is more suitable to work with a basis that already has this property. These are the Wannier functions, described below. Also, it is assumed that if a particle is annihilated, it can only appear ("hop to") at a neighboring lattice site. Effects of beyond nearest-neighbor tunneling due to finite temperatures are the subject of [16].

- Lowest Band
  Since we work at very low temperatures, it is reasonable to assume that the bosons do not have enough energy to overcome the band gap. Therefore, as mentioned earlier, we only use the Wannier functions for the lowest energy band. The changes when including the other excited bands are discussed in [17].

- Periodicity
  The external potential is assumed to be periodical, which is a given for the potential created by the lasers but the influence of the harmonic trap is completely ignored. In, for example, [18] the influence of the trapping potential is examined.

We now write down the Bose-Hubbard-Hamiltonian:

$$\boxed{\hat{H} = \frac{1}{2}U \sum_i \hat{c}_i^\dagger \hat{c}_i^\dagger \hat{c}_i \hat{c}_i - J \sum_{<i,j>} \hat{c}_i^\dagger \hat{c}_j - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i} \tag{2.3}$$

The sum is to be calculated over all lattice sites i, and $\hat{c}_i$ denotes the (bosonic) annihilation operator at the lattice site i. The chevrons under the sum $< i, j >$ denote a summation of only nearest neighbor sites i and j.

What do the different parts in (2.3) mean? The first term, called the interaction term, describes an attractive force between atoms at the same site i. By using the commutation rules for bosonic

annihilation and creation operators, we can also write this part as $U\hat{n}(\hat{n}-1)$. Obviously, for zero or one particle at one lattice site, no interaction energy should arise and we indeed see that the contribution of this term to the Hamiltonian yields zero for these cases. The next term, the so-called hopping term, describes the lowering of the energy by a moving (hopping) of one particle from site j to a neighboring site i.

These two processes compete with each other to lower the energy, depending on the parameters U and J and we can distinguish between the two cases where one of them dominates the Hamiltonian:

if $U \gg J$, the interactions between the bosons keep them in their respective lattice sites, they will not hop, i.e. we have the Mott-insulator state.

If on the other hand, $J \gg U$, the hopping is highly favored, the system is therefore in the superfluid state.

We mentioned that it is very attractive to work with a BEC in an optical lattice because the parameters can be changed very easily over a wide range. What is the relationship between the adjustable laser strength V_0 defined below in (2.13) and U or J?

Very often, the assumption of a harmonic potential (quadratic with a maximum at the lattice sites) is made which very much simplifies the calculations. One should, however, use the Wannier-functions, as mentioned above. Thus, the bosonic creation and annihilation operators are expanded in the basis of the Wannier-functions $w(\mathbf{x}-\mathbf{x}_i)$:

$$\hat{\Psi}^\dagger = \sum_i \hat{c}_i^\dagger w(\mathbf{x}-\mathbf{x}_i)^*, \hat{\Psi} = \sum_i \hat{c}_i w(\mathbf{x}-\mathbf{x}_i) \tag{2.4}$$

The Wannier functions have long been used in the study of solid state physics. They are calculated via a Fourier transformation of the Bloch functions:

$$w(x-x_i) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} dq u_q(x) e^{-iqx_i} \tag{2.5}$$

This is a 1-D Wannier-function, with $u_q(x)$ being a Bloch-function and a the lattice constant.

They are highly localized at the lattice sites $\mathbf{x}_i$ (in contrast to Bloch functions which are delocalized over the whole lattice), which makes them a suitable basis for our optical lattice. Obviously, each energy band will in general have a different Wannier function, so if we would not restrict ourselves to the lowest band only, they should be marked with an additional parameter for the band index.

The Wannier functions are not uniquely defined by Eq. 2.5, because each of the wavefunctions $u_q(x)$ could get a different phase factor which would not have an impact on each of the Bloch functions but on the Wannier function it would indeed.

There is, however, for each band one uniquely determined *maximally localized Wannier function* with the property that it is real, symmetric and decreasing exponentially [19].

A thorough numerical calculation of U and V by using Wannier functions can be found in [20]. It turns out that that U depends polynomially on V_0 and J depends exponentially on V_0. Dividing eq. 2.3 by J, we see that the influence of the laser strength seems only to manifest itself via U/J, which will stay true for our further calculations in this thesis. But, this is not necessarily

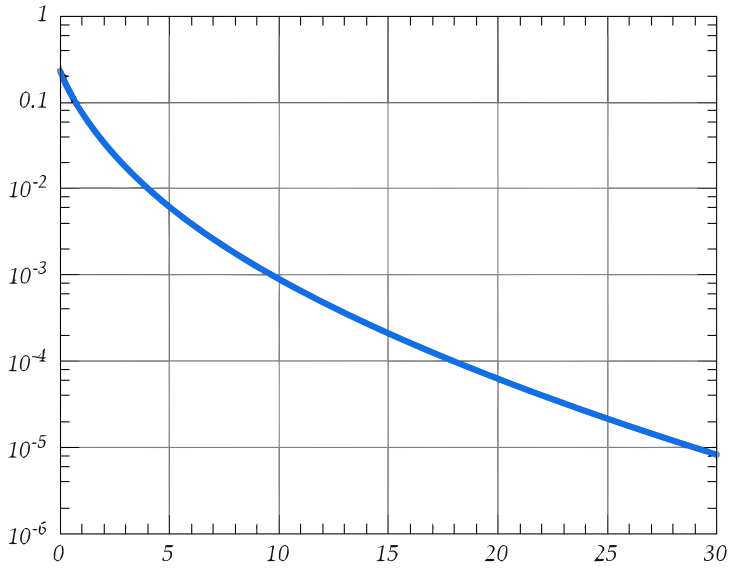


Figure 2.1: J/U over V_r taken from [20]

always the case, since through Feshbach resonances it is possible to change the s-wave scattering length a_s, thereby influencing the particle interaction.

V_r stands for the laser potential V_0 in units of the recoil energy $E_R = \frac{\hbar^2\pi^2}{2a^2m}$, with a being the lattice spacing. Changing a_s would lead to a scaling of the y-axis with the factor a/a_s.

As mentioned, the two obvious choices for the starting point of further calculations are the strong-coupling case where the hopping-term is introduced as a perturbation and the superfluid phase in which the interaction is small.

2.1.2 Phase transitions

A very broad and fascinating area of physics is concerned with *phase transitions*. A well-known everyday example is the evaporation or the solidification of liquid water: depending on external variables, such as pressure and temperature, the system can assume different states, or phases, in this case liquid, gaseous and solid. This diploma thesis will examine the phase transition from the superfluid state to the Mott-insulator state of a BEC in an optical lattice, depending on the externally adjustable laser strength. Common to all phase transitions is a discontinuity in a derivative of the appropriate thermodynamic potential, which were therefore classified according to when the first discontinuity appears (Ehrenfest classification). This has proven to be too restrictive since there are examples for logarithmic and exponential singularities. Today, one usually only differentiates between first-order phase transitions where at least one partial derivative of a thermodynamic potential are discontinous, and second-order (or continous) phase transitions.

The *order parameter* of a theory is a variable (in our case a scalar) defined such that it is zero for one phase and nonzero in the other. For a BEC, the order parameter is the particle density for the ground state, n_0 (actually, it is its squareroot). Another prominent example is the energy gap Δ in superconductors.

Some assumptions have to be made as to how the order parameter appears in the thermody-

namic potential. Some that have had much success are the *Landau theory* and the Φ^4-theory. A very thorough treatment of the latter topic can be found in [21].

Within the Landau theory, the grand-canonical potential Ω is expanded with respect to the order parameter Ψ up to fourth order. For symmetry reasons, only even powers appear.

$$\Omega = a\Psi^4 + b\Psi^2 + c \tag{2.6}$$

We can calculate the order parameter by demanding that Ω has a minimum:

$$\frac{\partial\Omega}{\partial\Psi} = 4a\Psi^3 + 2b\Psi = 0 \tag{2.7}$$

and

$$\frac{\partial^2\Omega}{\partial\Psi^2} = 12a\Psi^2 + 2b > 0 \tag{2.8}$$

In our coming calculations we will also derive the grand-canonical potential, but with respect to n_0 which is actually Ψ^2. Of course, this will also give us the minimum of Ω:

$$\frac{\partial\Omega}{\partial\Psi^2} = \frac{\partial\Omega}{\partial\Psi}\frac{\partial\Psi}{\partial\Psi^2} = \frac{\partial\Omega}{\partial\Psi}\frac{1}{2\Psi} \tag{2.9}$$

And, for $\Psi \neq 0$, both derivatives have the same set of solutions.

In this thesis, we will not analyze the regular phase transition to a BEC, but the phase transition of a BEC in an optical lattice.Experimentally, the phase transition in an optical lattice was first observed in 2002 [22]. This Mott-superfluid-transition is called a quantum phase transition, the difference to the general phase transition being that it also takes place at zero temperature due to quantum fluctuations.

The change to the superfluid state in He^4 is obviously also a phase transition. One might ask whether this is not another example of a Bose-Einstein condensate. Calculating T_C, we get 3.14K, close enough to the experimental value $T_\lambda = 2.18$K for the so-called *lambda-point* where superfluidity sets in. We now know that the reasonable assumption of a BEC was not entirely correct. The fraction of the condensate at 0K is only about 1/12th, owing to the very strong interactions in Helium. Furthermore, in 1972 He^3 could be cooled down enough to about 2 millikelvin to exhibit a superfluid state (this feat was awarded the Nobel Prize in Physics in 1996 to David Lee, Robert Richardson and Douglas Osheroff). Since He^3 consists of fermions, this cannot be a pure Bose Einstein condensate, for only through the strong correlations between the atoms they are able to form pairs, which then are bosons able to condensate in the ground state. Much research has been done concerning the BCS-BEC crossover, which is achieved by the use of Feshbach resonances [23].

2.2 Experimental realization

In this chapter we give an overview of the experimental methods used to create a Bose-Einstein-Condensate and the difficulties that had to be overcome. Since this thesis will emphasize theoretical calculations, just a rough overview will be provided. The methods used have become even more refined during these last years, and we cannot explore all the details here.

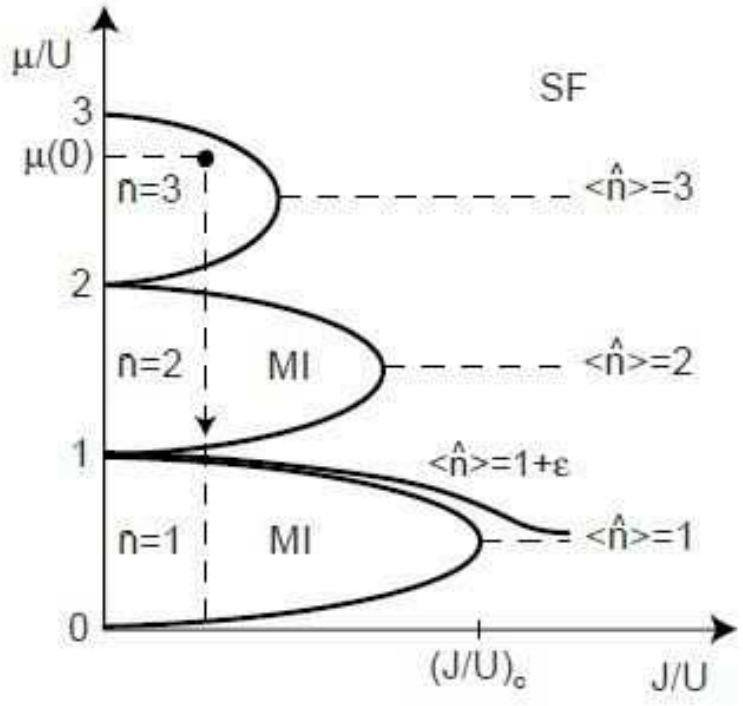


Figure 2.2: Phase diagram for T= 0 [24]. Only for integer density n there is a Mott insulator (MI) phase, a small deviation ϵ means the system always has a small part of particles that can move freely, a sign for the superfluid state (SF). The dashed line shows how changing the chemical potential (which is in general space-dependent) means passing through several different phases.

As we already mentioned, the theoretical prediction of the occurrence of BEC took place many decades before it could finally be experimentally realized. The main obstacle was to achieve temperatures low enough to allow for a macroscopic population of the ground state, though at the same time not allowing the atoms to solidify in the process. At the start of every BEC, a gas has to be produced by heating the atoms which gain enough thermic energy that they can leave the solid. Obviously, they then have a very high kinetic energy, which in the following steps must be reduced in order to observe a BEC.

The basic principle here is that of *Doppler cooling*, so named because it exploits the Doppler-shift of relative motion: due to the high velocity of the still hot particles, the frequency needed for a transition between states is red-shifted. This can be used so that only particles around a certain velocity absorb a photon from an external laser. After a very short time, the particle transitions back to its former state by emitting again a photon. The difference is that during the absorbtion the particle receives momentum from the photon which leads to a deceleration while the emission spreads over all angels, i.e. no net momentum change occurs. More on Laser Cooling can, for example, be found in [25]. For sodium, for example, a temperature as low as 240μK can be reached by the Doppler mechanism alone.

Additionally, in a magneto-optical trap (MOT) an inhomogeneous magnetic field is superimposed over the laser field for optical cooling. Due to the Zeeman-shift, the energy levels of the particles change depending on their distance from the center of the trap in such a way that the chance for absorbing a photon increases with the distance, resulting in a net force towards the center, thereby trapping the particles.

The last and deciding step in creating a BEC is the *evaporative cooling* [26]. The basic idea is that, as temperature is a measure for the mean energy per particle, the temperature must decrease if the particles with the highest energy are removed.

The condition for an induced transition is:

$$g\mu_B B = \hbar\omega \ , \tag{2.10}$$

with g the g-factor, μ_B the Bohr magneton and and ω the frequency of the field. The potential seen by a particle in a magnetic field is

$$V = m_F g\mu_B B \tag{2.11}$$

so by adjusting the spin state it is possible to change a particle from a low field seeking one to a high field seeking one, which results in the particle leaving the trap. By lowering the magnetic field, more particles will leave so trap so one can adjust the desired temperature (but accepting that always particles are lost) until BEC can be achieved. This typically takes only several seconds.

The BEC is then loaded into an optical lattice, for the 3D case generated by six counterpropagating lasers, creating standing waves in every direction. 1D or 2D optical lattices are also possible to realize [27]. Also, a trapping potential is present to prevent loss. Under the assumptions that there is no interference (this can be done by taking orthogonal polarization vectors as well as a tiny offset for the wavelengths) and neglecting the trapping potential, the laser intensity is simply the sum

$$I = I_0 \sum_{i=1}^{d} \sin^2(\frac{2\pi}{\lambda} x_i) \tag{2.12}$$

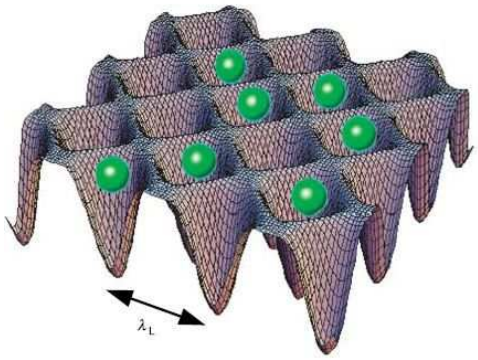


Figure 2.3: Particles in the potential of an optical lattice [28].

(with λ being the laser wavelength) .

Perturbation theory for an external electric field acting as the perturbation (Stark effect) shows that there is a linear correlation between I and the potential. With these assumptions, the potential for the optical lattice reads:

$$V = V_0 \sum_{i=1}^{d} \sin^2(\frac{2\pi}{\lambda} x_i) \tag{2.13}$$

We still haven't answered the question how the existence of a BEC can actually be seen. Apart from indirect features like the existence of a gap in the MI state, there is a visually appealing way by creating time-of-flight (TOF) pictures. This means that the trap is switched off completely and the particles expand freely. Neglecting gravity, the time Δt a particle needs to cover the distance Δr is related to the wave vector $\mathbf{k}$ simply as:

$$\hbar k = p = mv = m\frac{\Delta r}{\Delta t} \tag{2.14}$$

By measuring the distance and the time, one can therefore observe how many particles are in each $\mathbf{k}$-state. For $T < T_C$ one should begin to see a peak for $\mathbf{k} = 0$ which gets more and more pronounced as the temperature is lowered.

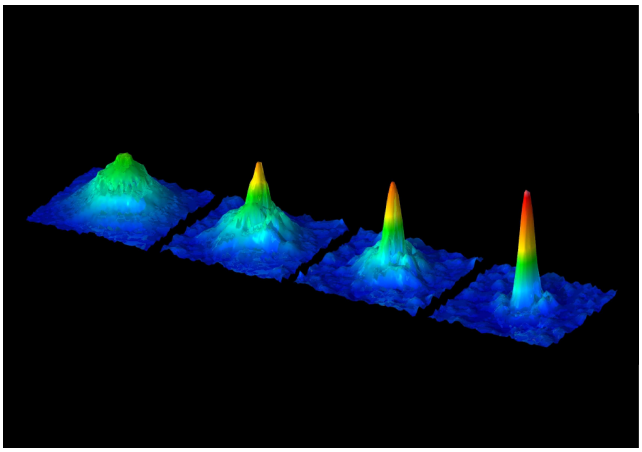


Figure 2.4: TOF picture of the formation of a BEC at the MPQ.

Chapter 3

Effective Hamiltonian for the Bogoliubov Approximation

"*More is different.*"
Aphorism by P.W. Anderson

In this chapter we will study the Bogoliubov approximation [29] [30] , which is a suitable ansatz for the case that the optical lattice depth is sufficiently low, so that we can assume that the BEC is essentially described by a macroscopic wave function plus a (small) correction term..

3.1 Bogoliubov Approximation

We call N_S the number of lattice sites in the optical lattice we are studying, and write $\hat{c}_i^\dagger$ for the creation operator which creates one particle at the lattice site with the coordinates $\mathbf{r}_i$.

Statistical calculations with bosons at very low temperatures necessitate a special treatment of the ground state $\mathbf{k} = 0$, which is macroscopically populated in the experiments we discuss here. It is therefore suitable to Fourier-transform the creation and annihilation operators:

$$\hat{c}_i = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} \ , \tag{3.1}$$

$$\hat{c}_i^\dagger = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger e^{i\mathbf{k}\cdot\mathbf{r}_i} \ . \tag{3.2}$$

The inverse relations are

$$\hat{a}_{\mathbf{k}} = \frac{1}{\sqrt{N_s}} \sum_{i} \hat{c}_i e^{i\mathbf{k}\cdot\mathbf{r}_i} \ , \tag{3.3}$$

$$\hat{a}_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N_s}} \sum_{i} \hat{c}_i^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}_i} \ . \tag{3.4}$$

Note that the definitions are normalized in such a way that $\sum_i \hat{c}_i^\dagger \hat{c}_i = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}$, which means that the sum of all particle number operators taken over all sites $\mathbf{r}_i$ equals the sum of all particle number operators taken over all possible values for $\mathbf{k}$. This sum obviously yields the value N,

the number of all particles, when applied to any state. In our calculations we shall make use of the following representation of the Dirac Delta-function:

$$\sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} = N_S \delta_{\mathbf{k},\mathbf{k}'} \ . \tag{3.5}$$

With that, we can prove the above statement:

$$\sum_i \hat{c}_i^\dagger \hat{c}_i = \sum_i \frac{1}{N_S} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger e^{i\mathbf{k}\cdot\mathbf{r}_i} \sum_{\mathbf{k}'} \hat{a}_{\mathbf{k}'} e^{-i\mathbf{k}'\cdot\mathbf{r}_i} = \frac{1}{N_S} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \sum_{\mathbf{k}'} \hat{a}_{\mathbf{k}'} \left(N_S \delta_{\mathbf{k},\mathbf{k}'}\right) = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \ . \tag{3.6}$$

The Fourier components are operators which satisfy the ordinary commutation relations:

$$[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}] = [\hat{a}_{\mathbf{k}}^\dagger, \hat{a}_{\mathbf{k}'}^\dagger] = 0 \ , \tag{3.7}$$

and

$$\left[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}^\dagger\right] = \delta_{\mathbf{k},\mathbf{k}'} \ . \tag{3.8}$$

Eq. (3.7) is easy to prove, because $\hat{a}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}'}$ consist of sums of $\hat{c}_i$'s, which commute pairwise due to the standard commutation relation $[\hat{c}_i, \hat{c}_j] = 0$. Likewise, all $\hat{c}_i^\dagger$'s commute because $[\hat{c}_i^\dagger, \hat{c}_j^\dagger] = 0$. The last missing commutation relation describes a mixed pair of creation and annihilation operators:

$$\left[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}^\dagger\right] = \frac{1}{N_S} \left[\sum_i \hat{c}_i e^{i\mathbf{k}\cdot\mathbf{r}_i}, \sum_j \hat{c}_j^\dagger e^{-i\mathbf{k}'\cdot\mathbf{r}_j}\right] = \frac{1}{N_S} \delta_{i,j} \sum_{i,j} e^{-(\mathbf{k}\cdot\mathbf{r}_i - \mathbf{k}'\cdot\mathbf{r}_j)} \left[\hat{c}_{\mathbf{i}}, \hat{c}_{\mathbf{j}}^\dagger\right] = \left[\hat{c}_{\mathbf{i}}, \hat{c}_{\mathbf{i}}^\dagger\right] \delta_{\mathbf{k},\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'} \ . \tag{3.9}$$

Plugging (3.1) and (3.2) in the Bose-Hubbard Hamiltonian (2.3) thus yields:

$$\begin{aligned} \hat{H} = & \frac{1}{2} U \frac{1}{N_S^2} \sum_i \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \sum_{\mathbf{k}''} \sum_{\mathbf{k}'''} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}'}^\dagger \hat{a}_{\mathbf{k}''} \hat{a}_{\mathbf{k}'''} e^{i\mathbf{r}_i\cdot(\mathbf{k}+\mathbf{k}'-\mathbf{k}''-\mathbf{k}''')} \\ & - J \frac{1}{N_S} \sum_{<i,j>} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{r}_i - \mathbf{k}'\cdot\mathbf{r}_j} - \mu \frac{1}{N_S} \sum_i \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{r}_i - \mathbf{k}'\cdot\mathbf{r}_i} \ . \end{aligned} \tag{3.10}$$

This expression can be simplified as follows: We discuss here only the case of a cubic lattice with the lattice constant a, so that in the sum over next neighbors the sum over j just becomes $\mathbf{r}_j = \mathbf{r}_i \pm a\mathbf{e}_p$ with p as a unit vector denoting the direction the neighbored lattice site lies. Therefore the Hamiltonian can be written as:

$$\begin{aligned} \hat{H} = & \frac{1}{2} U \frac{1}{N_S^2} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \sum_{\mathbf{k}''} \sum_{\mathbf{k}'''} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}'}^\dagger \hat{a}_{\mathbf{k}''} \hat{a}_{\mathbf{k}'''} \sum_i e^{\mathbf{r}_i\cdot(\mathbf{k}+\mathbf{k}'-\mathbf{k}''-\mathbf{k}''')} \\ & - J \frac{1}{N_S} \sum_i \sum_{\mathbf{k}} \sum_{\mathbf{k}'} e^{i\mathbf{r}_i\cdot(\mathbf{k}-\mathbf{k}')} \sum_{p=\pm 1,2,\ldots d} e^{ia\mathbf{k}'\cdot\mathbf{e}_p} - \mu \frac{1}{N_S} \sum_i \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}'} e^{i\mathbf{r}_i\cdot(\mathbf{k}-\mathbf{k}')} \ . \end{aligned} \tag{3.11}$$

By using the Euler-relation and the formula for the Delta-function (3.5), this gives:

$$\hat{H} = \frac{1}{2}\frac{U}{N_S}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''}\sum_{\mathbf{k}'''}\hat{a}^\dagger_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}'}\hat{a}_{\mathbf{k}''}\hat{a}_{\mathbf{k}'''}\delta_{(\mathbf{k}+\mathbf{k}'),(\mathbf{k}''+\mathbf{k}''')} - \sum_{\mathbf{k}}\left[\mu + \sum_{p=1}^{d} 2J\cos(k_p a)\right]\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} \ . \quad (3.12)$$

In the following, the starting point for our calculations will be the superfluid phase, so that almost all atoms in the trap occupy the ground state. If the laser strength is increased, one observes a behavior typical of a second order phase transition, and the corresponding order parameter can be shown to be $\sqrt{N_0}$. We will see that this is approximately equal to the expectation values of the creation and the annihilation operator for the ground state, $<\hat{a}_0>$ and $<\hat{a}_0^\dagger>$, respectively: Indeed, since it follows from the definition of the expectation functional applied to an operator $\hat{A}$ in the grand-canonical ensemble,

$$<\hat{A}>= \frac{\mathrm{tr}\left(e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\hat{A}\right)}{\mathrm{tr}\left(e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\right)}^{1} \ , \quad (3.13)$$

that it is linear (the trace operator tr<.> is linear!), we have $<\hat{a}_0^\dagger\hat{a}_0>=<\hat{n}_0>= N_0$
and $<\hat{a}_0\hat{a}_0^\dagger>=<\hat{a}_0^\dagger\hat{a}_0 + [\hat{a}_0, \hat{a}_0^\dagger]>=<\hat{a}_0^\dagger\hat{a}_0 - 1>= N_0 - 1 \approx N_0$, since in the superfluid phase $N_0 \gg 1$.

Furthermore, the expectation value of the hermitian conjugated operator is just the complex conjugate of the operator's expectation value:
$<\hat{O}^\dagger>=<\hat{O}>^*$, so that we obtain $<\hat{a}_0>=<\hat{a}_0^\dagger>= \sqrt{N_0}$. In the deep superfluid regime, we may thus assume that it is justified to write $\hat{a}_0 = \sqrt{N_0} + \delta\hat{a}_0$ and likewise for the creation operator, in both cases the deviation from the mean value $\sqrt{N_0}$ is supposed to be small, so that we can neglect higher orders.

In the next step, we sort the terms by their order in the fluctuations $\delta\hat{a}_0$ and $\delta\hat{a}_0^\dagger$. The zeroth order terms are called Gross-Pitaevskii contributions, the first order terms vanish as we will soon see, the second order ones are called Bogoliubov terms and the higher orders are neglected for now. As the title of this thesis suggests, we will later also need the higher order terms, so we here list all orders.

We introduce here the dispersion relation

$$\epsilon_{\mathbf{k}} = 2J\sum_{p=1}^{d} 1 - \cos(k_p a) \ . \quad (3.14)$$

This choice of the sign for the dispersion relation is chosen so that in the limiting case $a \to 0$ we actually get the free dispersion $\epsilon_{\mathbf{k}} \propto k^2$: Taylor expansion at $a = 0$ up to second order yields: $\epsilon_{\mathbf{k}} \propto \sum_{p=1}^{d} 1-(1-{k_p}^2)+O(a^3) \propto k^2$, which is the expected quadratic dispersion. Furthermore, we have $\epsilon_0 = 0$, so that the energy scale starts at zero and never gets negative.

With the abbreviation $z = 2d$, z being the number of nearest neighbors, we can also write $\epsilon_{\mathbf{k}} = Jz - 2J\sum_{p=1}^{d}\cos(k_p a)$.

[1]The term $-\mu\hat{N}$ is already included in our Hamiltonian (2.3), so this term will not appear again in the following calculations.

We sort the orders by writing $\sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} = \hat{a}_0 + \sum_{\mathbf{k}\neq 0} \hat{a}_{\mathbf{k}}$.

0^{th} order:
All sums are replaced by $\sqrt{N_0}$ so only one term remains in this order:

$$H^0_{\text{int}} = \frac{1}{2} U N_S N_0^2 + N_0(-Jz - \mu) = \frac{1}{2} U n_0 N_0 + N_0(-Jz - \mu) \tag{3.15}$$

1^{st} order:
Only one sum (= one fluctuation about N_0) remains. There is no contribution from the quartic sum since in the $\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''}$ we have one $\mathbf{k} \neq 0$ and all others are zero, so all terms in first order vanish. So we only have

$$-\sum_{\mathbf{k}} \left[\mu + \sum_{p=1}^{d} 2J\cos(k_p a) \right] \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} \tag{3.16}$$

2^{nd} order:

$$\begin{aligned} H^{(2)}_{\text{int}} = \frac{1}{2} U n_0 \Bigg\{ & \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \sum_{\mathbf{k}'} \hat{a}^\dagger_{\mathbf{k}'} + \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \sum_{\mathbf{k}''} \hat{a}_{\mathbf{k}''} + \sum_{\mathbf{k}'} \hat{a}^\dagger_{\mathbf{k}'} \sum_{\mathbf{k}''} \hat{a}_{\mathbf{k}''} \\ & + \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \sum_{\mathbf{k}'''} \hat{a}_{\mathbf{k}'''} + \sum_{\mathbf{k}'} \hat{a}^\dagger_{\mathbf{k}'} \sum_{\mathbf{k}'''} \hat{a}_{\mathbf{k}'''} + \sum_{\mathbf{k}''} \hat{a}_{\mathbf{k}''} \sum_{\mathbf{k}'''} \hat{a}_{\mathbf{k}'''} \Bigg\} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''} + \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) \hat{a}_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \end{aligned} \tag{3.17}$$

3^{rd} and 4^{th} order:

$$\begin{aligned} H^{(3)}_{\text{int}} = \frac{1}{2} \frac{U}{N_S} \sqrt{N_0} \Bigg\{ & \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \sum_{\mathbf{k}'} \hat{a}^\dagger_{\mathbf{k}'} \sum_{\mathbf{k}''} \hat{a}_{\mathbf{k}''} + \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \sum_{\mathbf{k}'} \hat{a}^\dagger_{\mathbf{k}'} \sum_{\mathbf{k}'''} \hat{a}_{\mathbf{k}'''} \\ & + \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \sum_{\mathbf{k}''} \hat{a}_{\mathbf{k}''} \sum_{\mathbf{k}'''} \hat{a}_{\mathbf{k}'''} + \sum_{\mathbf{k}'} \hat{a}^\dagger_{\mathbf{k}'} \sum_{\mathbf{k}''} \hat{a}_{\mathbf{k}''} \sum_{\mathbf{k}'''} \hat{a}_{\mathbf{k}'''} \Bigg\} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''} \ . \end{aligned} \tag{3.18}$$

The first two and the last two terms are equal after renaming the summation indices, since this change also does not affect the δ.

$$H^{(4)}_{\text{int}} = \frac{1}{2} \frac{U}{N_S} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''} \sum_{\mathbf{k}} \hat{a_{\mathbf{k}}}^\dagger \sum_{\mathbf{k}'} \hat{a_{\mathbf{k}'}}^\dagger \sum_{\mathbf{k}''} \hat{a_{\mathbf{k}''}} \sum_{\mathbf{k}'''} \hat{a_{\mathbf{k}'''}} \tag{3.19}$$

As mentioned, our effective Hamiltonian will only include terms up to second order in the fluctuations about $\sqrt{N_0}$, the higher orders will only play a role in later chapters, where we will perform a perturbation expansion.

We can simplify $\hat{H}^{(2)}$: renaming indices, the second and third as well as the fourth and fifth term are equal

$$\hat{H_{\text{eff}}} = N_0 \left(\frac{1}{2} U n_0 - \mu - zJ \right) + \eta \left[{\sum_{\mathbf{k}}}' \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} (\epsilon_k - Jz - \mu + 2Un_0) + \frac{1}{2} U n_0 {\sum_{\mathbf{k}}}' \hat{a}_{\mathbf{k}} \hat{a}_{\text{-}\mathbf{k}} + \hat{a}^\dagger_{\text{-}\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \right] \tag{3.20}$$

Here η represents an artificial smallness to keep track of the order of the fluctuations. As soon as we need quantitative results, we will set $\eta = 1$.

The aim of the Bogoliubov transformation is to achieve a diagonal Hamiltonian in new creation and annihilation operators $\hat{b_{\mathbf{k}}}$ and $\hat{b_{\mathbf{k}}}^{\dagger}$, which depend linearly on the old ones. To this end we make the following ansatz:

$$\begin{aligned} \hat{b}_{\mathbf{k}} &= u_{\mathbf{k}} \cdot \hat{a}_{\mathbf{k}} + v_{\mathbf{k}} \cdot \hat{a}^{\dagger}_{-\mathbf{k}} \ , \\ \hat{b}^{\dagger}_{-\mathbf{k}} &= v^{*}_{\mathbf{k}} \cdot \hat{a}_{\mathbf{k}} + u^{*}_{\mathbf{k}} \cdot \hat{a}^{\dagger}_{-\mathbf{k}} \ . \end{aligned} \tag{3.21}$$

By taking the hermitian conjugate of the first equation and replacing $\mathbf{k}$ with -$\mathbf{k}$ we see by comparing to the second equation that the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ must not depend on the sign of $\mathbf{k}$:

$$\begin{aligned} u_{\mathbf{k}} &= u_{-\mathbf{k}} \ , \\ v_{\mathbf{k}} &= v_{-\mathbf{k}} \ . \end{aligned} \tag{3.22}$$

Since we have shown in Eqs. (3.7) and (3.8) that $\hat{a}_{\mathbf{k}}$ and $\hat{a}^{\dagger}_{\mathbf{k}}$ obey the standard commutation laws for creation and annihilation operators, we obtain

$$\begin{aligned} [\hat{b}_{\mathbf{k}}, \hat{b}^{\dagger}_{\mathbf{k}'}] = [u_{\mathbf{k}}\hat{a}_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^{\dagger}_{-\mathbf{k}}, v^{*}_{\mathbf{k}'}\hat{a}_{\mathbf{k}'} + u^{*}_{\mathbf{k}'}\hat{a}^{\dagger}_{-\mathbf{k}'}] &= u_{\mathbf{k}}u^{*}_{\mathbf{k}'}[\hat{a}_{\mathbf{k}}, \hat{a}^{\dagger}_{-\mathbf{k}'}] + v_{\mathbf{k}}v^{*}_{\mathbf{k}'}[\hat{a}^{\dagger}_{-\mathbf{k}}, \hat{a}_{\mathbf{k}'}] \\ &= u_{\mathbf{k}}u^{*}_{\mathbf{k}'}\delta_{\mathbf{k},\mathbf{k}'} - v_{\mathbf{k}}v^{*}_{\mathbf{k}'}\delta_{\mathbf{k},\mathbf{k}'} = (|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2)\delta_{\mathbf{k},\mathbf{k}'} \ , \end{aligned} \tag{3.23}$$

and see that, in order to retain the standard commutator relations, it is necessary that

$$|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1 \ . \tag{3.24}$$

This is also sufficient, since the remaining commutation relations are automatically fulfilled:

$$[\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}] = [u(\mathbf{k})\hat{a}_{\mathbf{k}} + v(\mathbf{k})\hat{a}^{\dagger}_{-\mathbf{k}}, u(\mathbf{k}')\hat{a}_{\mathbf{k}'} + v(\mathbf{k}')\hat{a}^{\dagger}_{-\mathbf{k}'}] = [u_{\mathbf{k}}a_{\mathbf{k}}, v_{\mathbf{k}'}a^{\dagger}_{-\mathbf{k}'}] + [v_{\mathbf{k}}a^{\dagger}_{-\mathbf{k}}, u_{\mathbf{k}'}a_{\mathbf{k}'}] = 0 \ , \tag{3.25}$$

since in our sums the case $\mathbf{k} = 0$ is excluded, so that always $\mathbf{k} \neq -\mathbf{k}$.

Correspondingly, we obtain

$$[\hat{b}^{\dagger}_{\mathbf{k}}, \hat{b}^{\dagger}_{\mathbf{k}'}] = [v^{*}_{\mathbf{k}'}\hat{a}_{\mathbf{k}} + u^{*}_{\mathbf{k}}\hat{a}^{\dagger}_{\text{-}\mathbf{k}}, v^{*}_{\mathbf{k}'}\hat{a}_{\mathbf{k}'} + u^{*}_{\mathbf{k}'}\hat{a}^{\dagger}_{\text{-}\mathbf{k}'}] = [v^{*}_{\mathbf{k}'}\hat{a}_{\mathbf{k}}, u^{*}_{\mathbf{k}'}\hat{a}^{\dagger}_{\text{-}\mathbf{k}'}] + [u^{*}_{\mathbf{k}}\hat{a}^{\dagger}_{\text{-}\mathbf{k}}, v^{*}_{\mathbf{k}'}\hat{a}_{\mathbf{k}'}] = 0 \tag{3.26}$$

with the same reasoning as above.

We now impose further conditions for the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ by requiring that the Hamiltonian (3.20) takes on a diagonal form like

$$\hat{H}_{\text{eff}} = \alpha + {\sum_{\mathbf{k}}}' (\hbar\omega_{\mathbf{k}} + \beta) + {\sum_{\mathbf{k}}}' \hbar\omega_{\mathbf{k}}\hat{b}^{\dagger}_{\mathbf{k}}\hat{b}_{\mathbf{k}} \ . \tag{3.27}$$

In the following steps, we will frequently use that the identity $\sum_{\mathbf{k}} f(\mathbf{k}) = \sum_{\mathbf{k}} f(\mathbf{\text{-}k})$ is valid for any function f and, since our sums exclude $\mathbf{k} = 0$, we see from Eq. (3.8) that we can write: $a_{-\mathbf{k}} a_{\mathbf{k}}^\dagger = a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}$.

Our effective Hamiltonian (3.20) thus has the alternative representation

$$\hat{H}_{\text{eff}} = N_0(\frac{1}{2}Un_0 - \mu - zt) + \frac{1}{2}\eta \Bigg[\sum_{\mathbf{k}}{}' (\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) + \sum_{\mathbf{k}}{}' Un_0 \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{\text{-}k}} + Un_0 \hat{a}_{\mathbf{\text{-}k}}^\dagger \hat{a}_{\mathbf{k}}^\dagger + (\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + (\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) \hat{a}_{\mathbf{\text{-}k}} \hat{a}_{\mathbf{\text{-}k}}^\dagger \Bigg] . \tag{3.28}$$

Now we use the inverse relations to (3.21),

$$\begin{aligned} \hat{a}_{\mathbf{k}} &= u_{\mathbf{k}}^* \hat{b}_{\mathbf{k}} - v_{\mathbf{k}} \hat{b}_{\mathbf{\text{-}k}}^\dagger \\ \hat{a}_{-\mathbf{k}}^\dagger &= -v_{\mathbf{k}}^* \hat{b}_{\mathbf{k}} + u_{\mathbf{k}} \hat{b}_{\mathbf{\text{-}k}}^\dagger \ , \end{aligned} \tag{3.29}$$

and insert them in (3.44). Sorting by the different products of the new creation and annihilation operators, we obtain:

$$\hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} : \frac{1}{2} \left[(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) |u_{\mathbf{k}}|^2 - Un_0 v_{\mathbf{k}}^* u_{\mathbf{k}} - Un_0 u_{\mathbf{k}}^* v_{\mathbf{k}} + \epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) |v_{\mathbf{k}}|^2 \right] , \tag{3.30}$$

$$\hat{b}_{\mathbf{\text{-}k}} \hat{b}_{\mathbf{\text{-}k}}^\dagger : \frac{1}{2} \left[(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) |u_{\mathbf{k}}|^2 - Un_0 v_{\mathbf{k}}^* u_{\mathbf{k}} - Un_0 u_{\mathbf{k}}^* v_{\mathbf{k}} + (\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) |v_{\mathbf{k}}|^2 \right] , \tag{3.31}$$

$$\hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}^\dagger : -\frac{1}{2} \left[2(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) u_{\mathbf{k}} v_{\mathbf{k}} - Un_0 v_{\mathbf{k}}^2 - Un_0 u_{\mathbf{k}}^2 \right] , \tag{3.32}$$

$$\hat{b}_{\mathbf{\text{-}k}} \hat{b}_{\mathbf{k}} : -\frac{1}{2} \left[2(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) u_{\mathbf{k}}^* v_{\mathbf{k}}^* - Un_0 v_{\mathbf{k}}^{*2} - Un_0 u_{\mathbf{k}}^{*2} \right] . \tag{3.33}$$

We see that the last two equations are just complex conjugated to each other, if we remember (3.1) and (3.22), but this is not quite true for (3.30) and (3.31), as we have to commute $\hat{b}_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}^\dagger$. Since we demand that the $\hat{b}_{\mathbf{k}}$'s only appear in terms of the form $\hbar\omega_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}$, we have reduced the number of equations to two, and additionally still the condition (3.24) :

$$-\frac{1}{2} \left[2(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) u_{\mathbf{k}} v_{\mathbf{k}} - Un_0 v_{\mathbf{k}}^2 - Un_0 u_{\mathbf{k}}^2 \right] = 0 . \tag{3.34}$$

$$\frac{1}{2} \left[(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) |u_{\mathbf{k}}|^2 - Un_0 v_{\mathbf{k}}^* u_{\mathbf{k}} - Un_0 u_{\mathbf{k}}^* v_{\mathbf{k}} + \epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) |v_{\mathbf{k}}|^2 \right] = \hbar\omega_{\mathbf{k}} . \tag{3.35}$$

Since we have more variables than equations, we cannot expect a unique solution, however, that is not necessary at this point. First of all, we remark that a global phase factor cannot change the Hamiltonian since it has U(1)-symmetry. Yet, we can answer the question how the phases of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are related relative to each other. This can be seen from Eq. 3.35, where the left-hand side must yield a real result. By writing $u_{\mathbf{k}} = |u_{\mathbf{k}}| e^{i\phi_{u_k}}$ and $v_{\mathbf{k}} = |v_{\mathbf{k}}| e^{i\phi_{v_k}}$ we

see that after an arbitrary phase-shift the energy stays real iff $\phi_{u_k} - \phi_{v_k} = 0$ [2] or, equivalently, $\phi_{u_k} = \phi_{v_k}$. Later, we will proof that this also stays true for the second order terms. If we assume at this point that the phase is arbitrary, the obvious choice is to make $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ real.

Now we can solve the above equations. First of all, $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$ implies that we can write $u_{\mathbf{k}} = \cosh x$ and $v_{\mathbf{k}} = \sinh(x)$. Equation 3.34 is of the form

$$2\alpha(\cosh x \sinh x) - \beta(\cosh^2 x + \sinh^2 x) = 0 \ . \tag{3.36}$$

We rearrange this to

$$\frac{\beta}{\alpha} = 2\frac{\cosh x \sinh x}{\cosh^2 x + \sinh^2 x} = 2\frac{\frac{\sinh x}{\cosh x}}{1 + \frac{\sinh^2 x}{\cosh^2 x}} = 2\frac{\tanh x}{1 + \tanh^2 x}, \tag{3.37}$$

which, by an addition theorem, is equal to $\tanh 2x$. Using the following trigonometric identities,

$$\cosh^2 x = \frac{1}{2}(\cosh 2x + 1) = \frac{1}{2}\left(\frac{1}{\sqrt{1 - \tanh^2 2x}} + 1\right) = \frac{1}{2}\left(\frac{1}{\sqrt{1 - \frac{\beta^2}{\alpha^2}}} + 1\right) \tag{3.38}$$

$$= \frac{1}{2}\left(\frac{\alpha}{\sqrt{\alpha^2 - \beta^2}} + 1\right) \ . \tag{3.39}$$

we can now solve 3.35:

$$\hbar\omega_{\mathbf{k}} = \alpha(\cosh^2 x + \sinh^2 x) - 2\beta(\sinh x \cosh x) = \alpha(\frac{\alpha}{\sqrt{\alpha^2 - \beta^2}}) - \frac{\beta^2}{\alpha}\frac{\alpha}{\sqrt{\alpha^2 - \beta^2}} \tag{3.40}$$

$$= \frac{\alpha^2 - \beta^2}{\sqrt{\alpha^2 - \beta^2}} = \sqrt{\alpha^2 - \beta^2}, \tag{3.41}$$

where we have used (3.36) to eliminate $\sinh x \cosh x$.

Writing out α and β yields:

$$|u_{\mathbf{k}}|^2 = |v_{\mathbf{k}}|^2 + 1 = \frac{1}{2}\left(\frac{\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0}{\hbar\omega} + 1\right) \tag{3.42}$$

with the dispersion relation

$$\hbar\omega_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - Jz - \mu + Un_0)^2 + 2Un_0(\epsilon_{\mathbf{k}} - Jz - \mu + Un_0)} \ . \tag{3.43}$$

At last, we now can write down our diagonal effective Hamiltonian. We must not forget to include $\frac{1}{2}\hbar\omega_{\mathbf{k}}$, which arises due to the commutation performed in (3.31).

$$\boxed{\hat{H}_{\text{eff}} = N_S\left(\frac{1}{2}Un_0^2 - \mu n_0 - Jzn_0\right) + \frac{1}{2}{\sum_{\mathbf{k}}}' [\hbar\omega_{\mathbf{k}} - (\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0)] + {\sum_{\mathbf{k}}}' \hbar\omega_{\mathbf{k}}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}}} \tag{3.44}$$

[2] The difference may also be a multiple of 2π, we neglect this ambiguity.

3.2 The condensate density

We are ultimately interested in a relationship between the condensate density n_0 and the experimentally adjustable parameters U and J. Obviously, the number of all atoms must equal the sum over the expectation values of all $\hat{n}_{\mathbf{k}}$:

$$N = N_0 + \sum_{\mathbf{k}}{}' < \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} > \tag{3.45}$$

For calculating a trace we may use any basis, so in (3.45)we will choose one that is well-suited. Due to the fact that there are only one-particle contributions in our Hamiltonian (3.44), the occupancy number representation $|n_{\alpha_1}, n_{\alpha_2} \cdots >$ yields such a basis, since their elements are eigenstates to $\hat{H}$ and to the new occupancy number operator $b^\dagger_{\mathbf{k}} b_{\mathbf{k}}$. The fact that all states used for the trace are eigenstates to $\hat{H}$ simplifies the expectation value, since we can just apply $\hat{H}$ in the denominator and the numerator and cancel the resulting eigenvalues. It just remains to calculate $\mathrm{tr}(\hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}})$. To this end, we express the old creation and annihilation operators by the new ones via (3.29) and get:

$$N = N_0 + \eta \left[\sum_{\mathbf{k}}{}' < |u_{\mathbf{k}}|^2 \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + |v_{\mathbf{k}}|^2 \hat{b}_{-\mathbf{k}} \hat{b}^\dagger_{-\mathbf{k}} - v^*_{\mathbf{k}} u^*_{\mathbf{k}} \hat{b}_{-\mathbf{k}} \hat{b}_{\mathbf{k}} - v_{\mathbf{k}} u_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}^\dagger_{-\mathbf{k}} > \right] . \tag{3.46}$$

The action of $\hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} = \hat{n}_{\mathbf{k}}$ is obvious:

$$< n_{\mathbf{k}_1}, \ldots | \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} | n_{\mathbf{k}_1}, \cdots > = < n_{\mathbf{k}_1}, \ldots | n_{\mathbf{k}} | n_{\mathbf{k}_1}, \cdots > = n_{\mathbf{k}} \ . \tag{3.47}$$

Now, the first term in the sum is trivial, because the trace is a sum of its eigenstates. The second term likewise, if we commute the operators, which gives an additional factor $|v_{\mathbf{k}}|^2$. The third and fourth term yield the expectation value zero, because they produce states with different $n_{\mathbf{k}}$'s in the bra- and ket-vectors, which are orthogonal.

We introduce the particle density per site n:
$n = \frac{N}{N_S}$

$$n = n_0 + \eta < \left[\frac{1}{N_S} \sum_{\mathbf{k}}{}' |u_{\mathbf{k}}|^2 \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + |v_{\mathbf{k}}|^2 (\hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + 1) \right] > \ . \tag{3.48}$$

We insert (3.42) and remember that $< \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} >$ is described by the Bose distribution. Now we have our result,

$$\boxed{n = n_0 + \eta \frac{1}{N_S} \left[\sum_{\mathbf{k}}{}' \frac{\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0}{\hbar \omega_{\mathbf{k}}} \cdot \left(\frac{1}{e^{\beta \hbar \omega_{\mathbf{k}}} - 1} + \frac{1}{2} \right) - \frac{1}{2} \right] .} \tag{3.49}$$

Since the experiments which we aim to explain are carried out at extreme low temperatures of the order of $10^{-8} K$, it is only natural to examine in particular the limit $T \to 0$. This is easily

done, since $T \to 0$ means $\beta \to \infty$ and therefore $e^{-\beta\hbar\omega} \to 0$. In the zero-temperature limit we thus have:

$$n = n_0 + \eta \frac{1}{N_S} \left[\sum_{\mathbf{k}}{}' \frac{1}{2} \frac{(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0)}{\hbar\omega_{\mathbf{k}}} - \frac{1}{2} \right] . \tag{3.50}$$

For a numerical evaluation, we take the $\mathbf{k}$'s to be sufficiently dense so that we may regard them as quasi-continuous. This allows us to change the sum to an integral via the general formula:

$$\sum_{\mathbf{k}} f(\mathbf{k}) \longmapsto \int_{\mathbf{k}} \rho(\mathbf{k}) f(\mathbf{k}) d\mathbf{k} . \tag{3.51}$$

Here $\rho(\mathbf{k})$ denotes the density of states in $\mathbf{k}$-space. Using periodic boundary conditions, the states have a distance of $\frac{2\pi}{a}$ in every direction, so that one state occupies a volume of $\left(\frac{2\pi}{a}\right)^d$, which gives a density of $\rho(\mathbf{k}) = \left(\frac{a}{2\pi}\right)^d$. Like in solid-state physics (the optical lattice has obviously many similarities to the free electron model), we project all states in $\mathbf{k}$-space onto the first Brillouin zone $\bigotimes_{i=1}^{d} \left(-\frac{\pi}{a}\overrightarrow{e}_i, \frac{\pi}{a}\overrightarrow{e}_i\right)$.

Since we have originally just one state in a volume of the Brillouin zone, the density becomes much larger if we only take the integral from $-\pi/a$ to $+\pi/a$, namely by the factor N_S, the number of unit cells in $\mathbf{k}$-space. We thus get:

$$n = n_0 + \eta \left[\frac{1}{N_S} \int_{-\pi/a}^{\pi/a} N_S \left(\frac{a}{2\pi}\right)^d \left(\frac{1}{2} \frac{(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0)}{\hbar\omega_{\mathbf{k}}} - \frac{1}{2} \right) d^d\mathbf{k} \right] . \tag{3.52}$$

For simplicity we introduce the dimensionless variable $\mathbf{q} := \frac{a}{2\pi}\mathbf{k}$ and get the following expression that we will solve numerically:

$$\boxed{n = n_0 + \eta \int_{-\frac{1}{2}}^{\frac{1}{2}} \left[\frac{1}{2} \frac{\left(\epsilon_{\left(\frac{2\pi}{a}\mathbf{q}\right)} - Jz - \mu + 2Un_0\right)}{\hbar\omega_{\left(\frac{2\pi}{a}\mathbf{q}\right)}} - \frac{1}{2} \right] d^d\mathbf{q} .} \tag{3.53}$$

3.3 The grand-canonical potential and self-consistency

In this section we check whether our whole idea of diagonalizing and neglecting higher terms in the Hamiltonian is consistent with the basic rules of thermodynamics. In particular, we verify that we can also calculate the particle density n by differentiating the grand-canonical potential with respect to μ. The partition function Z is defined as $\mathrm{tr}(e^{-\beta\hat{H}})$, where $\hat{H}$ is our effective Hamiltonian (3.44). The so-called effective potential V_{eff} is then calculated by $-\frac{1}{\beta}\ln Z$. This is not yet the grand-canonical potential, since we still have a dependency upon n_0, which is itself a function of μ. This dependency must be eliminated. At first we get

$$V_{\text{eff}} = -\frac{1}{\beta} \ln \mathrm{tr} \left\{ e^{-\beta N_S (\frac{1}{2}Un_0^2 - \mu n_0 - Jzn_0) + \eta \left[\frac{1}{2} \sum_{\mathbf{k}}{}' (\hbar\omega_{\mathbf{k}} - (\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0)) + \sum_{\mathbf{k}}{}' \hbar\omega_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \right]} \right\} . \tag{3.54}$$

Like before, the appropriate basis for the calculation of the trace is the number occupancy basis. The terms without operators can simply be taken out of the trace, so for now we will look only at the last sum:

$$-\frac{1}{\beta}\ln \mathrm{tr}\left(e^{\sum_{\mathbf{k}}{}' -\beta\hbar\omega_{\mathbf{k}}\hat{b}^{\dagger}_{\mathbf{k}}\hat{b}_{\mathbf{k}}}\right) = -\frac{1}{\beta}\ln\left(\sum_{n_{\mathbf{k}1}} e^{-\beta n_{\mathbf{k}_1}}\right)\left(\sum_{n_{\mathbf{k}2}} e^{-\beta n_{\mathbf{k}_2}}\right)\cdots = -\frac{1}{\beta}\ln\prod_{\mathbf{k}}{}'\left(\sum_{n_{\mathbf{k}i}} e^{-\beta n_{\mathbf{k}i}}\right)$$
$$= -\frac{1}{\beta}\ln\prod_{\mathbf{k}}{}'\frac{1}{1-e^{-\beta\hbar\omega_{\mathbf{k}}}}\ , \tag{3.55}$$

where in the last step we have used the formula for the geometric series. By using the known properties of the logarithm can now write down the final result for the effective potential:

$$V_{\text{eff}} = N_S\left(\frac{1}{2}Un_0^2 - \mu n_0 - Jzn_0\right) \tag{3.56}$$
$$+\eta\left[\frac{1}{2}\sum_{\mathbf{k}}{}'\left(\hbar\omega_{\mathbf{k}} - (\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0)\right) + \frac{1}{\beta}\sum_{\mathbf{k}}{}'\ln\left(1-e^{-\beta\hbar\omega_{\mathbf{k}}}\right)\right]\ . \tag{3.57}$$

As said before, V_{eff} is not a thermodynamic potential, yet it will become the grand-canonical potential Ω at the extremum with respect to n_0: Solving $\frac{\partial V_{\text{eff}}}{\partial n_0} = 0$ yields $n_{0_{\text{extr}}}$ and $V_{\text{eff}}(n_0 = n_{0_{\text{extr}}}, \mu, T, V)$ is $\Omega(\mu, T, V)$. This we will calculate in the next step.

$$\frac{\partial V_{\text{eff}}}{\partial n_0} = N_S(-Jz - \mu + Un_0) \tag{3.58}$$
$$+\eta\left[\frac{1}{2}\sum_{\mathbf{k}}{}'\left(-2U + \frac{\partial\hbar\omega_{\mathbf{k}}}{\partial n_0}\right) + \frac{1}{\beta}\sum_{\mathbf{k}}{}'\frac{1}{1-e^{-\beta\hbar\omega_{\mathbf{k}}}}\left(-e^{-\beta\hbar\omega_{\mathbf{k}}}\right)(-\beta)\frac{\partial\hbar\omega_{\mathbf{k}}}{\partial n_0}\right] \tag{3.59}$$

By looking at (3.43), we can calculate that

$$\frac{\partial\hbar\omega_{\mathbf{k}}}{\partial n_0} = \frac{U(2\epsilon_{\mathbf{k}} - 2Jz - 2\mu + 3Un_0)}{\hbar\omega_{\mathbf{k}}}\ , \tag{3.60}$$

which we plug in and get:

$$0 = N_S(-Jz - \mu + Un_0) + \eta\left\{U\sum_{\mathbf{k}}{}'\left[\frac{(2\epsilon_{\mathbf{k}} - 2Jz - 2\mu + 3Un_0)}{\hbar\omega_{\mathbf{k}}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}}-1}\right) - 1\right]\right\}\ . \tag{3.61}$$

One important result from this equation is that, in the lowest order in η, we can write

$$n_0 = \frac{Jz + \mu}{U} + O(\eta)\ . \tag{3.62}$$

We now re-insert this result in (3.61), and since we disregard orders of η higher than one, we can just insert the lowest order for n_0 in those terms that already are of first order in η.

$$n_0 = \frac{Jz+\mu}{U} - \eta\left[\frac{1}{N_S}\sum_{\mathbf{k}}{}' \frac{(2\epsilon_{\mathbf{k}} + Jz + \mu)}{\hbar\omega_{\mathbf{k}}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}}-1}\right) - 1\right] + O(\eta^2)\ . \tag{3.63}$$

This result must be inserted in Eq.(3.57) in order to obtain the grand-canonical potential Ω up to first order in η:

$$\Omega = -\frac{N_S}{2U}(Jz+\mu)^2 + \frac{\eta}{2}\sum_{\mathbf{k}}{}'\left(\hbar\omega_{\mathbf{k}}^{(0)} - \epsilon_{\mathbf{k}} - Jz - \mu\right) + \frac{1}{\beta}\sum_{\mathbf{k}}{}' \ln\left(1 - e^{-\beta\hbar\omega_{\mathbf{k}}^{(0)}}\right]\ . \tag{3.64}$$

Here and in the following, we will often omit the $O(\eta^2)$, because we do not need to emphasize every time that we neglect higher orders in η. Inserting (**??**) in (3.43) results in the zeroth order of $\hbar\omega_{\mathbf{k}}$.

$$\begin{aligned}\hbar\omega_{\mathbf{k}}{}^{(0)} &= \sqrt{(\epsilon_{\mathbf{k}} + \mu - \mu)^2 + 2\left[(Jz+\mu)^2 - (zJ+\mu)(-\epsilon_{\mathbf{k}} - Jz + \mu)\right]} \\ &= \sqrt{\epsilon_{\mathbf{k}}^2 + 2\epsilon_{\mathbf{k}}(Jz+\mu)}\ .\end{aligned} \tag{3.65}$$

For checking the self-consistency we now need the particle density n which we get with the help of the grand-canonical potential: $n = -\frac{1}{N_S}\frac{\partial\Omega}{\partial\mu}$.

With very similar calculations as before, we get:

$$\frac{\partial\hbar\omega_{\mathbf{k}}^{(0)}}{\partial\mu} = \frac{\epsilon_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}^{(0)}}\ , \tag{3.66}$$

and therefore:

$$n = \frac{(Jz+\mu)}{U} + \frac{1}{N_S}\eta\left[\sum_{\mathbf{k}}{}' \frac{(-\epsilon_{\mathbf{k}})}{\hbar\omega_{\mathbf{k}}^{(0)}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}^{(0)}}-1}\right) + \frac{1}{2}\right]\ . \tag{3.67}$$

To see the equivalence to (3.49), we insert the equation (3.63) for n_0 and subtract:

$$n - n_0 = \frac{(Jz+\mu)}{U} - \frac{(Jz+\mu)}{U} + \eta\frac{1}{N_S}\left[\sum_{\mathbf{k}}{}' \frac{-\epsilon_{\mathbf{k}} + Jz + 2\epsilon_{\mathbf{k}} + \mu}{\hbar\omega_{\mathbf{k}}^{(0)}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}^{(0)}}-1}\right) - 1 + \frac{1}{2}\right] \tag{3.68}$$

$$= \eta\frac{1}{N_S}\left[\sum_{\mathbf{k}}{}' \frac{1}{\hbar\omega_{\mathbf{k}}^{(0)}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}^{(0)}}-1}\right)(\epsilon_{\mathbf{k}} + Jz + \mu) - \frac{1}{2}\right] \tag{3.69}$$

We are almost done, we just remember that according to (3.62) we have in zeroth order $2(Jz+\mu) = 2Un_0$, so that

$$n - n_0 = \eta\frac{1}{N_S}\left[\sum_{\mathbf{k}}{}' \frac{1}{\hbar\omega_{\mathbf{k}}^{(0)}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}^{(0)}}-1}\right)(\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0) - \frac{1}{2}\right]\ . \tag{3.70}$$

We see that we have indeed gotten the same result as in (3.49) in two different ways, which shows the inner consistency of the Bogoliubov approximation. We can now eliminate the chemical potential μ, which we achieve by substituting Eq. (**??**) in (**??**), which yields

$$n - n_0 = \eta \frac{1}{N_S} \left[\sum_{\mathbf{k}}{}' \frac{1}{\hbar\omega_{\mathbf{k}}} \left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} \right) (\epsilon_{\mathbf{k}} + Un_0) - \frac{1}{2} \right] , \tag{3.71}$$

and we likewise get for the integral in (3.53):

$$\boxed{n = n_0 + \eta \int_{-\frac{1}{2}}^{\frac{1}{2}} \left[\frac{1}{2} \frac{(\epsilon_{\left(\frac{2\pi}{a}\mathbf{q}\right)} + Un_0)}{\hbar\omega_{\left(\frac{2\pi}{a}\mathbf{q}\right)}} - \frac{1}{2} \right] d^d\mathbf{q} \, ,} \tag{3.72}$$

a result also obtained in [29].

We now check whether our result (3.71) gives the correct results in the limit $\frac{U}{J} \to 0$, which should of course result in the model for free Bosons. At first we take the temperature to be zero, so we consider $n - n_0 = \eta \left[\sum_{\mathbf{k}}{}' \frac{1}{\hbar\omega_{\mathbf{k}}} \frac{1}{2} (-\epsilon_{\mathbf{k}} + 2Jz + Un_0) - \frac{1}{2} \right]$. Now we only examine the expression in the sum. We can easily perform the limit:

$$\begin{aligned} \frac{U}{J} n_0 + \frac{\epsilon_{\mathbf{k}}}{J} &\overset{\frac{U}{J}\to 0}{\longrightarrow} \frac{\epsilon_{\mathbf{k}}}{J} \\ \sqrt{\left(\frac{U}{J} n_0 + \frac{\epsilon_{\mathbf{k}}}{J} \right)^2 + 2\frac{U}{J} n_0 \left(\frac{U}{J} n_0 + \frac{\epsilon_{\mathbf{k}}}{J} \right)} &\overset{\frac{U}{J}\to 0}{\longrightarrow} \sqrt{\left(\frac{\epsilon_{\mathbf{k}} + Jz}{J} \right)^2} \end{aligned} \tag{3.73}$$

We now insert the definition (3.14) of $\epsilon_{\mathbf{k}}$ and thus get

$$\frac{2\sum_{p=1}^{d} (1 - \cos(k_p a))}{\left| 2\sum_{p=1}^{d} (1 - \cos(k_p a)) \right|} \, . \tag{3.74}$$

Since $|\cos| \leq 1$, the enumerator is positive, so the fraction just gives the value $+1$. We also see that in the sum we have the values $+\frac{1}{2}$ and $-\frac{1}{2}$ which cancel each other out, therefore the result, as expected for Bosons at zero temperature, states that $n = n_0$, i.e. all Bosons occupy the ground state.

Next, we examine the case of a finite temperature. We encounter the same fraction as before, which again gives the value $+1$, and so the result is

$$n = n_0 + \eta \sum_{\mathbf{k}}{}' \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} \, , \tag{3.75}$$

which is just the Bose-Einstein distribution, so again the correct limit is obtained.

3.4 Plots for T = 0

After having shown the inner consistency of our ansatz, we now turn to a plot of Eq. (3.53). In order to do that, we have to have μ eliminated, which we already did in Eq. (3.72), which

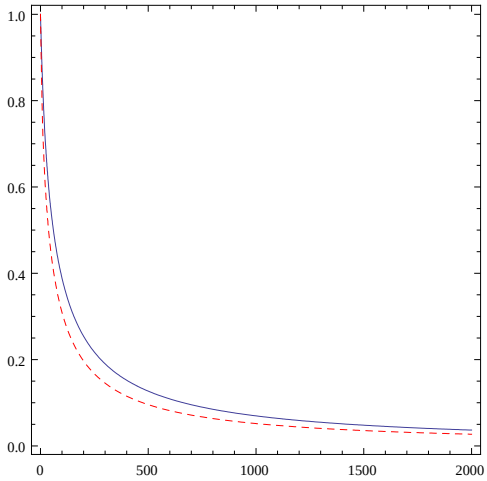


Figure 3.1: The condensate density n_0 relative to n versus $\frac{U}{J}$ in $d = 3$ dimensions. The solid line represents n=1, the dashed line stands for $n = 0.5$.

we plot by numerical calculations. The Bogoliubov approach will be a good model in the deep superfluid regime, since there most of the atoms populate the ground state. That in turn means we do not make great errors when neglecting higher orders of η, which was introduced as the deviation from the case that all atoms assume the state $\mathbf{k} = 0$. In the figure we plot the condensate fraction $\frac{n_0}{n}$ versus $\frac{U}{J}$. We expect that for $\frac{U}{J} = 0$, all atoms occupy the ground state, so the condensate fraction should be equal to one. For higher values of $\frac{U}{J}$, the condensate fraction decreases monotonically, until it (hopefully) reaches zero at a value we will call $\frac{U}{J}_{\text{crit}}$. Monte-Carlo calculations [31] which have been shown to agree very well with the experimental results [32] predict the critical value to be at about 29.

In Fig. (3.1) we plot the three-dimensional case with two different values for n. The plots show that our theory unfortunately does not predict the quantum phase transition we hoped for. As said before, the Bogoliubov approach will provide the best results in the deep superfluid phase, and the phase transition seems to be beyond its area of validity. Indeed, we can see that this must be the case: the phase transition is defined by the value of $\frac{U}{J}$ where $n_0 = 0$. Inserting that yields $\hbar\omega = \epsilon_{\mathbf{k}}$ which means the whole integrand in 3.72 becomes zero and we get $n = 0$, therefore obviously no phase transition takes place within the simplifications of our model.

It is therefore necessary to modify our theory so that its scope reaches farther into the Mott-insulator regime.

3.5 Popov approximation

The Popov approximation is an application of variational perturbation theory to expand the area of validity of the Bogoliubov approach in the hopes of finding a phase transition at high values of U/J. We follow an earlier work in our research group [33], who used the Path-Integral formalism but, stemming from an operator-ordering ambiguity in this formalism, did not get the same result we did.

To this end, we make a variational ansatz for μ by setting

$$\mu = M + \eta\Delta \ , \tag{3.76}$$

and replacing μ in Ω with again neglecting terms of higher order in η than one. We will call the result $\tilde{\Omega}$. Again, in the terms that already are in first order of η, we just need to insert the zeroth order for μ.

$$\begin{aligned}\tilde{\Omega} = &-\frac{N_S}{2U}\left(J^2z^2 + 2JzM + 2Jz\eta\Delta + 2M\eta\Delta + M^2\right) \\ &+ \eta\sum_{\mathbf{k}}{}' \left[\frac{\hbar\tilde{\omega}_{\mathbf{k}}^{(0)} - \epsilon_{\mathbf{k}} - 2Jz - M}{2} + \frac{1}{\beta}\ln\left(1 - e^{-\beta\hbar\tilde{\omega}^{(0)}}\right)\right] + O\left(\eta^2\right) \ .\end{aligned} \tag{3.77}$$

Here $\tilde{\omega}^{(0)}$ is just $\omega^{(0)}$ with μ replaced by M. We get rid of any remaining dependency on Δ by inserting the relation (3.76) again via $\Delta = \frac{\mu - M}{\eta}$:

$$\begin{aligned}\tilde{\Omega} = &-\frac{N_S}{2U}\left(J^2z^2 - M^2 + 2Jz\mu + 2M\mu\right) \\ &+ \eta\sum_{\mathbf{k}}{}' \left[\frac{\hbar\tilde{\omega}_{\mathbf{k}}^{(0)} - \epsilon_{\mathbf{k}} - 2Jz - M}{2} + \frac{1}{\beta}\ln\left(1 - e^{-\beta\hbar\tilde{\omega}^{(0)}}\right)\right] + O\left(\eta^2\right) \ .\end{aligned} \tag{3.78}$$

In order to eliminate the dependancy of $\tilde{\omega}_{\mathbf{k}}^{(0)}$ on M we differentiate $\tilde{\Omega}$ with respect to M, set the result equal to zero and insert the solution, which is M_{extr}:

$$0 = \frac{\partial\tilde{\Omega}}{\partial M} = \frac{N_S}{U}\left(M - \mu\right) + \eta\left[\sum_{\mathbf{k}}{}' \frac{(\epsilon_{\mathbf{k}})}{\hbar\tilde{\omega}_{\mathbf{k}}^{(0)}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\tilde{\omega}_{\mathbf{k}}^{(0)}} - 1}\right) - \frac{1}{2}\right] \ . \tag{3.79}$$

Obviously, under the sum just the same terms as in Eq. (3.67) arise, because the operations are the same with the replacement $\mu \longmapsto M$.

We solve Eq. (3.79) for M_{extr}, which gives:

$$M_{\text{extr}} = \mu - \frac{U}{N_S}\eta\left[\sum_{\mathbf{k}}{}' \frac{(\epsilon_{\mathbf{k}})}{\hbar\tilde{\omega}_{\mathbf{k}}^{(0)}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\tilde{\omega}_{\mathbf{k}}^{(0)}} - 1}\right) - \frac{1}{2}\right] \ . \tag{3.80}$$

In the next step, we calculate $n\left(M\right)$ using $N = nN_S = -\frac{\partial\Omega}{\partial\mu}$. The chain rule and the fact that $\Omega = \tilde{\Omega}\left(M\right)|_{M=M_{\text{extr}}}$ allows to rewrite this as:

$$nN_S = -\frac{\partial\Omega}{\partial\mu} = -\left.\frac{\partial\tilde{\Omega}\left(\mu, M_{\text{extr}}\left(\mu\right)\right)}{\partial\mu}\right|_{M=M_{\text{extr}}} = \left.\left(-\frac{\partial\tilde{\Omega}}{\partial\mu} - \frac{\partial\tilde{\Omega}}{\partial M_{\text{extr}}}\frac{\partial M_{\text{extr}}}{\partial\mu}\right)\right|_{M=M_{\text{extr}}} \ . \tag{3.81}$$

But from the definition in Eq. (3.79) we see that $\frac{\partial\tilde{\Omega}}{\partial M} = 0$, when $M = M_{\text{extr}}$, so

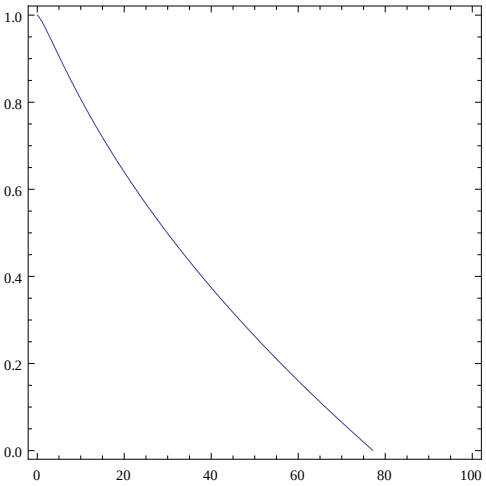


Figure 3.2: The condensate density n_0 relative to n versus $\frac{U}{J}$ in the Popov-approximation for $n = 1$.

$$nN_S = -\frac{\partial\Omega}{\partial\mu} = -\frac{\partial\tilde{\Omega}}{\partial\mu}\bigg|_{M=M_{\text{extr}}} \overset{3.78}{=} \frac{N_S}{U}\left(Jz + M_{\text{extr}}\right) \ . \tag{3.82}$$

We now need also $n_0\left(M_{\text{extr}}\right)$ in order to write down an improved Eq. (3.63). That means, we will again use the variational ansatz (3.76), this time in Eq. (3.63), which yields:

$$n_0 = \frac{Jz+\mu}{U} - \eta\frac{1}{N_S}{\sum_{\mathbf{k}}}'\left[\frac{\left(2\epsilon_{\mathbf{k}} + Jz + M\right)}{\hbar\tilde{\omega}_{\mathbf{k}}^{(0)}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\tilde{\omega}_{\mathbf{k}}^{(0)}} - 1}\right) - 1\right] \ , \tag{3.83}$$

where in terms that already are of first order in η, we just needed to substitute $\mu \longmapsto M$. Now we use Eq. (3.80) to eliminate the chemical potential μ which yields:

$$n_0 = \frac{Jz+M}{U} - \eta\frac{1}{N_S}{\sum_{\mathbf{k}}}'\left[\frac{\left(\epsilon_{\mathbf{k}} + Jz + M\right)}{\hbar\tilde{\omega}_{\mathbf{k}}^{(0)}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\tilde{\omega}_{\mathbf{k}}^{(0)}} - 1}\right) - \frac{1}{2}\right] \ . \tag{3.84}$$

Now, we want to eliminate the parameter M, which is done by inserting Eq.(3.82) for M:

$$\begin{aligned} n_0 &= \frac{Jz + (Un - Jz)}{U} - \eta\frac{1}{N_S}{\sum_{\mathbf{k}}}'\left[\frac{\left(\epsilon_{\mathbf{k}} + Jz + Un - Jz\right)}{\hbar\tilde{\omega}_{\mathbf{k}}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\tilde{\omega}_{\mathbf{k}}} - 1}\right) - \frac{1}{2}\right] \\ &= n - \eta\frac{1}{N_S}{\sum_{\mathbf{k}}}'\left[\frac{\left(\epsilon_{\mathbf{k}} + Un\right)}{\hbar\tilde{\omega}_{\mathbf{k}}}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\tilde{\omega}_{\mathbf{k}}} - 1}\right) - \frac{1}{2}\right] \ . \end{aligned} \tag{3.85}$$

By comparing this result to (3.71), we see that the result of the Popov-approximation is almost identical to the result we got before, except that we replaced $n_0 \longmapsto n$ in the sum, i.e. the condensate density with the particle density.

This result could have been obtained much easier, since we could have seen from Eq.(3.49) that $n_0 = n + O\left(\eta\right)$, which, when re-inserted would have yielded Eq.(3.85). We plot our newfound results, and see that the Popov approximation has indeed succeeded in introducing a quantum

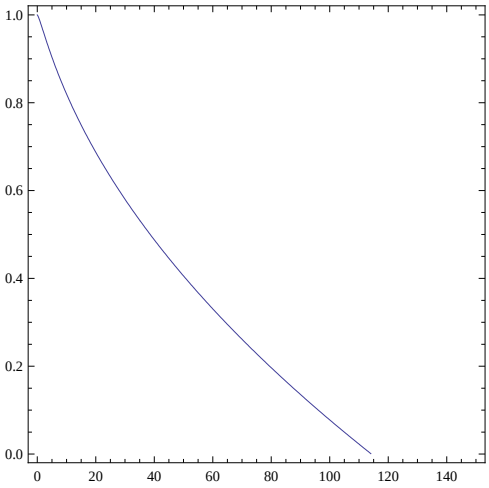


Figure 3.3: The condensate density n_0 relative to n versus $\frac{U}{J}$ in the Popov-approximation for $n = 2$.

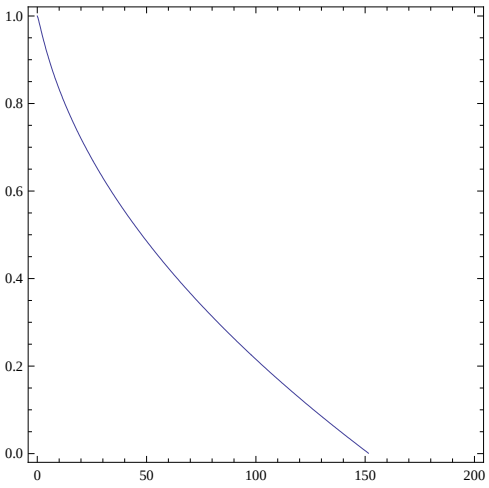


Figure 3.4: The condensate density n_0 relative to n versus $\frac{U}{J}$ in the Popov-approximation for $n = 3$.

phase transition. Looking back at fig. (2.2) we can also see the qualitatively correct behavior: for greater n, J/U_{crit} becomes smaller, i.e. U/J_{crit} becomes larger. Encouraged by this positive result, we now go to one order higher, in order to come closer to the expected value of 29 (as mentioned above) for $n = 1$.

Chapter 4

Beyond the Bogoliubov approximation: second order

"*If we are facing in the right direction, all we have to do is keep on walking.*"
Buddhist Saying

As the title of this thesis suggests, we will not stop with the level of approximation we did thus far but want to investigate also how to include higher orders. The terms of third (3.18) and fourth (3.19) order in the fluctuations represent the perturbation V to our diagonalized Hamiltonian.

4.1 How perturbation theory for T $\neq 0$ works

Quantum theory in the operator formalism is usually expressed in one of three choices: the Schrödinger picture, in which the time evolution of the system manifests itself in the states, whereas the operators can only be explicitly time-dependent. The Heisenberg picture turns this around, here the states are time-invariant. For our purposes, we will use the Dirac (or interaction) picture which already assumes that the Hamiltonian can be separated into a free, time-independent part $\hat{H}_0$ and a perturbation $\hat{V}$: $\hat{H} = \hat{H}_0 + \hat{V}$. The time evolution of the states is governed by $\hat{V}$, whereas that of the operators depends only on $\hat{H}_0$ via $\hat{A}_D(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{A}e^{-\frac{i}{\hbar}\hat{H}_0 t}$, where $\hat{A}$ denotes the operator in the Schrödinger picture. At $t = 0$ both pictures coincide. How this is accomplished in detail can be found in every standard textbook, e.g. [34]. As we had seen in the introduction, all interesting properties of a macroscopic system can be calculated by the respective thermodynamic potential. We now give a short derivation for the perturbation expansion of the grand-canonical potential in imaginary time:

The perturbation manifests itself twice in Ω, in the perturbation series of the time-evolution operator $\hat{U}$ and in the factor $e^{-\beta\hat{H}}$. We will see that it is much simpler to introduce the *Wick-rotation* $\tau = it$. In the Dirac-picture, the time-evolution operator $\hat{U}$ obeys the following equation of motion:

$$-\hbar\frac{\partial\hat{U}(\tau,\tau')}{\partial\tau} = \hat{V}(\tau)\hat{U}(\tau,\tau') \tag{4.1}$$

with the initial condition $\hat{U}(\tau,\tau) = \mathbb{1}$.

Formal integration and n-times iteration of the result yields with setting $\tau' = 0$:

$$\hat{U}(\tau,0)^{(n)} = \sum_{k=0}^{n} \frac{1}{k!} \left(\frac{-1}{\hbar}\right)^k \int_0^\tau d\tau_1 \dots d\tau_k \hat{T}\left(\hat{V}(\tau_1)\dots\hat{V}(\tau_k)\right) \ , \tag{4.2}$$

where $\hat{T}$ is the time-ordering operator [1], which sorts the operators in its argument with decreasing time from left to right.

From the explicit form of the Dirac time-evolution operator

$$\hat{U}(\tau,\tau') = e^{\frac{\hat{H}_0}{\hbar}\tau} e^{-\frac{\hat{H}_0}{\hbar}(\tau-\tau')} e^{-\frac{\hat{H}_0}{\hbar}\tau'} \tag{4.3}$$

and setting $\tau' = 0$,it can easily be seen that $e^{-\frac{1}{\hbar}\hat{H}\tau} = e^{-\frac{1}{\hbar}\hat{H}_0\tau}\hat{U}(\tau,0)$. By setting $\tau = \hbar\beta$, we get for the partition function:

$$Z = \mathrm{tr}\left(e^{-\beta\hat{H}}\right) = \mathrm{tr}\left(e^{-\beta\hat{H}_0}U(\hbar\beta,0)\right) \tag{4.4}$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-1}{\hbar}\right)^n \int_0^\tau d\tau_1 \dots d\tau_n \mathrm{tr}\{e^{-\beta\hat{H}_0}\hat{T}\left(\hat{V}(\tau_1)\dots\hat{V}(\tau_n)\right)\} \ . \tag{4.5}$$

This series conveniently sorts by the order in the perturbation $\hat{V}$ and is the starting point for further calculations in $T > 0$ perturbation theory.

4.2 The Wick theorem

In second quantization all operators are expressed by creation and annihilation operators. The problem to tackle now is thus how the time-ordered product of several annihilation and creation operators in the Dirac-picture looks like. An invaluable help when evaluation the time-ordered product is the *Wick-theorem* ([35], [36]). It states that the expectation value of a time-ordered product of creation and annihilation operators is equal to the expectation value of the time-ordered product of all possible pairs of creation and annihilation operators (one such pair is called a contraction). Usually, the Hamiltonian conserves the particle number, therefore only the pairs with one creation and one annihilation operator contribute. The expression $-\langle\hat{T}\left(\hat{a}_{\mathbf{k}}(\tau)\hat{a}_{\mathbf{k}'}(\tau')\right)\rangle$ is called the *free Green function* $G_{\mathbf{k}}(\tau,\tau')$ and is a fundamental quantity that will appear when we apply the Wick theorem. We remember that in the Dirac-picture the time-dependence is of the form

$$\hat{O}(\tau) = e^{\frac{1}{\hbar}\hat{H}_0\tau}\hat{O}e^{-\frac{1}{\hbar}\hat{H}_0\tau} \ . \tag{4.6}$$

Using $[\hat{b}_{\mathbf{k}}, \hat{n}_{\mathbf{k}'}] = [\hat{b}_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}\hat{b}_{\mathbf{k}}] = \hat{b}_{\mathbf{k}'}[\hat{b}_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}] + [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}]\hat{b}^\dagger_{\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'}\hat{b}_{\mathbf{k}} + 0$ and, similarly $[\hat{b}^\dagger_{\mathbf{k}}, \hat{n}_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}\hat{b}^\dagger_{\mathbf{k}}$, we can show that for an Hamiltonian of the form $\hat{H}_0 = \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}\hat{n}_{\mathbf{k}}$ we have

$$\hat{b}_{\mathbf{k}}(\tau) = e^{-\frac{1}{\hbar}\hbar\omega_{\mathbf{k}}\tau}\hat{b}_{\mathbf{k}}$$

[1] We remark that we use this definition since we will only work with bosons, for fermions the sign of the permutation needed to yield the correct time ordering must be included.

and

$$\hat{b}^\dagger_{\mathbf{k}}(\tau) = e^{\frac{1}{\hbar}\hbar\omega_{\mathbf{k}}\tau}\hat{b}^\dagger_{\mathbf{k}} \ , \tag{4.7}$$

so the time-dependence appears in such a way that the usual commutation rules are kept i.e. we can still speak of these operators as construction and annihilation operators.

Proof: We show that

$$\hat{b}_{\mathbf{k}}(\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'})^n = (\hbar\omega_{\mathbf{k}} + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'})^n\hat{b}_{\mathbf{k}} \tag{4.8}$$

for $n \in \mathbb{N}$.

For $n = 1$, this follows from the remark above:

$$\hat{b}_{\mathbf{k}}\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'} = [\hat{b}_{\mathbf{k}}, \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'}] + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'}\hat{b}_{\mathbf{k}} = \hbar\omega_{\mathbf{k}}\hat{b}_{\mathbf{k}} + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'}\hat{b}_{\mathbf{k}} \tag{4.9}$$

The induction step follows similarly:

$$\hat{b}_{\mathbf{k}}(\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'})^{n+1} = \hat{b}_{\mathbf{k}}(\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'})^n\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'} = (\hbar\omega_{\mathbf{k}} + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'})^n\hat{b}_{\mathbf{k}}\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'} \tag{4.10}$$

$$= (\hbar\omega_{\mathbf{k}} + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'})^{n+1}\hat{b}_{\mathbf{k}} \qquad \checkmark \tag{4.11}$$

We can use this to see

$$\hat{b}_{\mathbf{k}}(\tau) = e^{\frac{\tau}{\hbar}\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}}\hat{b}_{\mathbf{k}}e^{-\frac{\tau}{\hbar}\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}} = e^{\frac{\tau}{\hbar}\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}}\hat{b}_{\mathbf{k}}\sum_{n=0}^{\infty}\frac{1}{n!}\frac{-\tau}{\hbar}^n(\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'})^n \tag{4.12}$$

$$= e^{-\frac{\tau}{\hbar}\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}}\sum_{n=0}^{\infty}\frac{1}{n!}\left[-\frac{\tau}{\hbar}(\hbar\omega_{\mathbf{k}} + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'})\right]^n = e^{-\frac{\tau}{\hbar}\omega_{\mathbf{k}}}\hat{b}_{\mathbf{k}} \ , \tag{4.13}$$

where we used in the last step that $\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\hat{n}_{\mathbf{k}'}$ commutes with c-numbers so we can use that $e^{\frac{\tau}{\hbar}\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}}e^{-\frac{\tau}{\hbar}\sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}} = 1$.

(4.7) can be proven in a similar fashion, alternatively we remember that the property of two operators being Hermitian is time-independent.

We will later need $\hat{a}_{\mathbf{k}}(\tau)$ and $\hat{a}_{\mathbf{k}}(\tau)$, so we calculate these too. Luckily, their time-dependence is very similar:

$$\hat{a}_{\mathbf{k}}(\tau) = e^{\frac{1}{\hbar}\hat{H}_0\tau}\hat{a}_{\mathbf{k}}e^{-\frac{1}{\hbar}\hat{H}_0\tau} = e^{\frac{1}{\hbar}\hat{H}_0\tau}\left(u_{\mathbf{k}}\hat{b}_{\mathbf{k}} - v_{\mathbf{k}}\hat{b}^\dagger_{\text{-}\mathbf{k}}\right)e^{-\frac{1}{\hbar}\hat{H}_0\tau} = u_{\mathbf{k}}\hat{b}_{\mathbf{k}}(\tau) - v_{\mathbf{k}}\hat{b}_{\text{-}\mathbf{k}}(\tau) \tag{4.14}$$

and

$$\hat{a}_{\mathbf{k}}(\tau)^\dagger = e^{\frac{1}{\hbar}\hat{H}_0\tau}\hat{a}_{\mathbf{k}}e^{-\frac{1}{\hbar}\hat{H}_0\tau} = e^{\frac{1}{\hbar}\hat{H}_0\tau}\left(u_{\mathbf{k}}\hat{b}_{\mathbf{k}} - v_{\mathbf{k}}\hat{b}^\dagger_{\text{-}\mathbf{k}}\right)e^{-\frac{1}{\hbar}\hat{H}_0\tau} = u_{\mathbf{k}}\hat{b}_{\mathbf{k}}(\tau) - v_{\mathbf{k}}\hat{b}_{\text{-}\mathbf{k}}(\tau) \ . \tag{4.15}$$

So, in a sense, including a time-dependence in the Dirac-picture and the Bogoliubov transformation commute, which is very comforting since in the following we can conveniently choose which operation to perform first.

Next, we observe that the Green function depends only on the time-difference of its arguments, which is easily proven by using the trace's cyclical commutativity:

$$G_{\mathbf{k}}(\tau', \tau'') = G_{\mathbf{k}}(\tau' - \tau'') =: G_{\mathbf{k}}(\tau) \tag{4.16}$$

An interesting complication arises in our calculations because of the Bogoliubov transformation. When calculating the trace in the free basis of the $\hat{b}_{\mathbf{k}'s}$, the $\hat{a}_{\mathbf{k}'s}$ are not diagonal anymore. We therefore also have to calculate the $\hat{a} - \hat{a}$ and the $\hat{a}^\dagger - \hat{a}^\dagger$ correlations. At this point one must ask the question whether the ad-hoc prescription of the time-ordering operator acting just as the unity operator at equal times stays valid when using the Bogoliubov transformation. This is indeed the case, which we will later show for $H^{(4)}$ as an example by explicitly calculating the contractions in two possible ways.

4.3 Beyond Bogoliubov

Via the Bogoliubov transformation we succeeded in getting one diagonalized part of the Hamiltonian, which we will denote $\hat{H}_0$, and the remaining terms of third and fourth order in the fluctuations around the ground state, $\hat{H}^3$ and $\hat{H}^4$, which play the role of a perturbation. Up to second order in this perturbation, we have:

$$Z^{(2)} = \mathrm{tr}\left\{ e^{-\beta \hat{H}_0} \left[1 + \int_0^{\hbar\beta} (\hat{H}^3(\tau) + \hat{H}^4(\tau)) d\tau + \int_0^{\hbar\beta} \int_0^{\hbar\beta} \left(\hat{H}^3(\tau_1) + \hat{H}^4(\tau_1) \right) \left(\hat{H}^3(\tau_2) + \hat{H}^4(\tau_2) \right) d\tau_1 d\tau_2 \right] \right\} \tag{4.17}$$

From the standard examples we expect for all expectation values of terms with an uneven number of creation and annihilation operators to vanish. This is also true in our case since an (un-)even number of $\hat{a}$-operators implies an (un-)even number of $\hat{b}$-operators. The expectation value is calculated in the basis of eigenstates to $\hat{H}^{(0)}$, so all terms containing only one power of $\hat{H}^{(3)}$ are zero.

We now encounter a little problem with defining the order of the perturbation, since we actually have combined two: first, the deviations from the condensate ground-state N_0, which we included up to second order. The higher orders then were introduced as a perturbation $\hat{V}$. So, one could, for example, ask the question whether $\hat{H}^{(3)^2}$ or $\hat{H}^{(4)^2}$ should also belong to our second order.

In the Path-Integral formalism the answer is widely known: the order of the loop-expansion corresponds to the order of $\hbar$ (cf. [37]). We will see that the 2-loop-term consists of $\hat{H}^{(4)}$ and $\hat{H}^{(3)^2}$.

4.4 The $\hat{H}^{(4)}$ term

This term (cf. 3.19) is of the form

$$\hat{H}^{(4)} = \frac{1}{2}\frac{U}{N_S}(\frac{-1}{\hbar})\int_0^{\hbar\beta} d\tau \sum_{\mathbf{k},\mathbf{k'},\mathbf{k''},\mathbf{k'''}} \delta_{\mathbf{k}+\mathbf{k'},\mathbf{k''}+\mathbf{k'''}} < \hat{T}(\hat{a}^\dagger_{\mathbf{k}}(\tau)\hat{a}^\dagger_{\mathbf{k'}}(\tau)\hat{a}_{\mathbf{k''}}(\tau)\hat{a}_{\mathbf{k'''}}(\tau)) > \tag{4.18}$$

keeping in mind that all k-sums exclude the zero.

We rewrite this in terms of the $\hat{b}'_{\mathbf{k}}s$ via 3.29 and obtain the expression (without prefactors):

$$< (u_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}} - v^*_{\mathbf{k}}\hat{b}_{\text{-}\mathbf{k}})(u_{\mathbf{k'}}\hat{b}^\dagger_{\mathbf{k'}} - v^*_{\mathbf{k'}}\hat{b}_{\text{-}\mathbf{k'}})(u^*_{\mathbf{k''}}\hat{b}_{\mathbf{k''}} - v_{\mathbf{k''}}\hat{b}^\dagger_{\text{-}\mathbf{k''}})(u^*_{\mathbf{k'''}}\hat{b}_{\mathbf{k'''}} - v_{\mathbf{k'''}}\hat{b}^\dagger_{\text{-}\mathbf{k'''}}) > \tag{4.19}$$

We calculate the trace with the eigenstates of $\hat{H}^0$ which are also eigenstates to all $\hat{n}_{\mathbf{k}}$, therefore only terms with an equal number of creation and annihilation operators contribute, resulting in six terms:

I. $u_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}}u_{\mathbf{k'}}\hat{b}^\dagger_{\mathbf{k'}}u^*_{\mathbf{k''}}\hat{b}_{\mathbf{k''}}u^*_{\mathbf{k'''}}\hat{b}_{\mathbf{k'''}}$

II. $u_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}}v^*_{\mathbf{k'}}\hat{b}_{\text{-}\mathbf{k'}}v_{\mathbf{k''}}\hat{b}^\dagger_{\text{-}\mathbf{k''}}u^*_{\mathbf{k'''}}\hat{b}_{\mathbf{k'''}}$

III. $v^*_{\mathbf{k}}\hat{b}_{\text{-}\mathbf{k}}u_{\mathbf{k'}}\hat{b}^\dagger_{\mathbf{k'}}v_{\mathbf{k''}}\hat{b}^\dagger_{\text{-}\mathbf{k''}}u^*_{\mathbf{k'''}}\hat{b}_{\mathbf{k'''}}$

IV. $u_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}}v^*_{\mathbf{k'}}\hat{b}_{\text{-}\mathbf{k'}}u^*_{\mathbf{k''}}\hat{b}_{\mathbf{k''}}v_{\mathbf{k'''}}\hat{b}^\dagger_{\text{-}\mathbf{k'''}}$

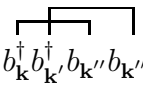
V. $v^*_{\mathbf{k}}\hat{b}_{\text{-}\mathbf{k}}u_{\mathbf{k'}}\hat{b}^\dagger_{\mathbf{k'}}u^*_{\mathbf{k''}}\hat{b}_{\mathbf{k''}}v_{\mathbf{k'''}}\hat{b}^\dagger_{\text{-}\mathbf{k'''}}$

VI. $v^*_{\mathbf{k}}\hat{b}_{\text{-}\mathbf{k}}v^*_{\mathbf{k'}}\hat{b}_{\text{-}\mathbf{k'}}v_{\mathbf{k''}}\hat{b}^\dagger_{\text{-}\mathbf{k''}}v_{\mathbf{k'''}}\hat{b}^\dagger_{\text{-}\mathbf{k'''}}$

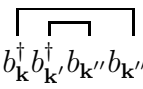
Using Wick's Theorem, there are two possible non-zero complete pairings of each term, we list these 12 here. The two contractions are shown in the table, as well the final results and their δ's.

For brevity only the terms to I and II are listed:

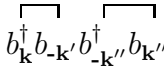
Ia)



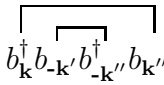
Ib)



IIa)



IIb)



I.a	$u_{\mathbf{k}}u_{\mathbf{k}'}u^*_{\mathbf{k}''}u^*_{\mathbf{k}'''}$	$\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}''}$	$\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}''}$	$\delta_{\mathbf{k},\mathbf{k}''}\delta_{\mathbf{k}',\mathbf{k}'''}$	$= \lvert u_{\mathbf{k}}\rvert^2 \lvert u_{\mathbf{k}'}\rvert^2 \langle\hat{n}_{\mathbf{k}}\rangle\langle\hat{n}_{\mathbf{k}'}\rangle$
I.b		$\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}'''}$	$\hat{b}^\dagger_{\mathbf{k}'}\hat{b}_{\mathbf{k}''}$	$\delta_{\mathbf{k},\mathbf{k}'''}\delta_{\mathbf{k}',\mathbf{k}''}$	$= \lvert u_{\mathbf{k}}\rvert^2 \lvert u_{\mathbf{k}'}\rvert^2 \langle\hat{n}_{\mathbf{k}}\rangle\langle\hat{n}_{\mathbf{k}'}\rangle$
II.a	$u_{\mathbf{k}}v^*_{\mathbf{k}'}v_{\mathbf{k}''}u^*_{\mathbf{k}'''}$	$\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\text{-}\mathbf{k}'}$	$\hat{b}^\dagger_{\text{-}\mathbf{k}''}\hat{b}_{\mathbf{k}'''}$	$\delta_{\mathbf{k},\text{-}\mathbf{k}'}\delta_{\text{-}\mathbf{k}'',\mathbf{k}'''}$	$= u_{\mathbf{k}}v^*_{\mathbf{k}}v_{\mathbf{k}''}u^*_{\mathbf{k}''}\langle\hat{n}_{\mathbf{k}}\rangle\langle\hat{n}_{-\mathbf{k}''}\rangle$
II.b		$\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}'''}$	$\hat{b}_{-\mathbf{k}'}\hat{b}^\dagger_{-\mathbf{k}''}$	$\delta_{\mathbf{k},\mathbf{k}'''}\delta_{-\mathbf{k}',\text{-}\mathbf{k}''}$	$= \lvert u_{\mathbf{k}}\rvert^2 \lvert v_{\mathbf{k}'}\rvert^2 \langle\hat{n}_{\mathbf{k}}\rangle\langle\hat{n}_{-\mathbf{k}'+1}\rangle$
III.a	$v^*_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}''}u_{\mathbf{k}'''}$	$\hat{b}_{-\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}'}$	$\hat{b}^\dagger_{-\mathbf{k}''}\hat{b}_{\mathbf{k}'''}$	$\delta_{-\mathbf{k},\mathbf{k}'}\delta_{-\mathbf{k}'',\mathbf{k}'''}$	$= v^*_{\mathbf{k}'}u_{\mathbf{k}'}v_{\mathbf{k}'''}u^*_{\mathbf{k}'''}\langle\hat{n}_{-\mathbf{k}}+1\rangle\langle\hat{n}_{\mathbf{k}'''}\rangle$
III.b		$\hat{b}_{-\mathbf{k}}\hat{b}^\dagger_{-\mathbf{k}''}$	$\hat{b}^\dagger_{\mathbf{k}'}\hat{b}_{\mathbf{k}'''}$	$\delta_{-\mathbf{k},-\mathbf{k}''}\delta_{\mathbf{k}',\mathbf{k}'''}$	$= \lvert v_{\mathbf{k}}\rvert^2 \lvert u_{\mathbf{k}'}\rvert^2 \langle\hat{n}_{\text{-}\mathbf{k}}+1\rangle\langle\hat{n}_{\mathbf{k}'}\rangle$
IV.a	$u_{\mathbf{k}}v^*_{\mathbf{k}'}u^*_{\mathbf{k}''}v_{\mathbf{k}'''}$	$\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{-\mathbf{k}'}$	$\hat{b}_{\mathbf{k}''}\hat{b}^\dagger_{\text{-}\mathbf{k}'''}$	$\delta_{\mathbf{k},-\mathbf{k}'}\delta_{\mathbf{k}'',-\mathbf{k}'''}$	$= u_{\mathbf{k}}v^*_{\mathbf{k}}v_{\mathbf{k}''}u^*_{\mathbf{k}''}\langle\hat{n}_{\mathbf{k}}\rangle\langle\hat{n}_{\mathbf{k}''}+1\rangle$
IV.b		$\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}''}$	$\hat{b}_{-\mathbf{k}'}\hat{b}^\dagger_{-\mathbf{k}'''}$	$\delta_{\mathbf{k},\mathbf{k}''}\delta_{-\mathbf{k}',-\mathbf{k}'''}$	$= \lvert u_{\mathbf{k}}\rvert^2 \lvert v_{\mathbf{k}'}\rvert^2 \langle\hat{n}_{\mathbf{k}}\rangle\langle\hat{n}_{-\mathbf{k}'}+1\rangle$
V.a	$v^*_{\mathbf{k}}u_{\mathbf{k}'}u^*_{\mathbf{k}''}v_{\mathbf{k}'''}$	$\hat{b}_{-\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}'}$	$\hat{b}_{\mathbf{k}''}\hat{b}^\dagger_{-\mathbf{k}'''}$	$\delta_{-\mathbf{k},\mathbf{k}'}\delta_{\mathbf{k}'',-\mathbf{k}'''}$	$= u_{\mathbf{k}}v^*_{\mathbf{k}}v_{\mathbf{k}''}u^*_{\mathbf{k}''}\langle\hat{n}_{-\mathbf{k}}+1\rangle\langle\hat{n}_{\mathbf{k}''}+1\rangle$
V.b		$\hat{b}_{-\mathbf{k}}\hat{b}^\dagger_{-\mathbf{k}'''}$	$\hat{b}^\dagger_{\mathbf{k}'}\hat{b}_{\mathbf{k}''}$	$\delta_{-\mathbf{k},-\mathbf{k}'''}\delta_{\mathbf{k}',\mathbf{k}''}$	$= \lvert v_{\mathbf{k}}\rvert^2 \lvert u_{\mathbf{k}'}\rvert^2 \langle\hat{n}_{-\mathbf{k}}+1\rangle\langle\hat{n}_{\mathbf{k}'}\rangle$
VI.a	$v^*_{\mathbf{k}}v^*_{\mathbf{k}'}v_{\mathbf{k}''}v_{\mathbf{k}'''}$	$\hat{b}_{-\mathbf{k}}\hat{b}^\dagger_{-\mathbf{k}''}$	$\hat{b}_{-\mathbf{k}'}\hat{b}^\dagger_{-\mathbf{k}'''}$	$\delta_{-\mathbf{k},-\mathbf{k}''}\delta_{-\mathbf{k}',-\mathbf{k}'''}$	$= \lvert v_{\mathbf{k}}\rvert^2 \lvert v_{\mathbf{k}'}\rvert^2 \langle\hat{n}_{-\mathbf{k}}+1\rangle\langle\hat{n}_{-\mathbf{k}'}+1\rangle$
VI.b		$\hat{b}_{-\mathbf{k}}\hat{b}^\dagger_{-\mathbf{k}'''}$	$\hat{b}_{-\mathbf{k}'}\hat{b}^\dagger_{-\mathbf{k}''}$	$\delta_{-\mathbf{k},-\mathbf{k}'''}\delta_{-\mathbf{k}',-\mathbf{k}''}$	$= \lvert v_{\mathbf{k}}\rvert^2 \lvert v_{\mathbf{k}'}\rvert^2 \langle\hat{n}_{-\mathbf{k}}+1\rangle\langle\hat{n}_{-\mathbf{k}'}+1\rangle$

Table 4.1: Terms coming from $H^{(4)}$

As we have seen, a contraction of construction operators at equal times just corresponds to their expectation value. We get for the above examples:

Ia) $\lvert u_{\mathbf{k}}\rvert^2 \lvert u_{\mathbf{k}'}\rvert^2 < n_{\mathbf{k}} >< n_{\mathbf{k}'} > \delta_{\mathbf{k},\mathbf{k}''}\delta_{\mathbf{k}',\mathbf{k}'''}$

Ib) $\lvert u_{\mathbf{k}}\rvert^2 \lvert u_{\mathbf{k}'}\rvert^2 < n_{\mathbf{k}} >< n_{\mathbf{k}'} > \delta_{\mathbf{k},\mathbf{k}'''}\delta_{\mathbf{k}',\mathbf{k}''}$

IIa)$u_{\mathbf{k}}v^*_{\mathbf{k}}v_{\mathbf{k}''}u_{\mathbf{k}'''} < n_{\mathbf{k}} >< n_{\mathbf{k}''} > \delta_{\mathbf{k},\text{-}\mathbf{k}'}\delta_{\text{-}\mathbf{k}'',\mathbf{k}'''}$

IIb)$\lvert u_{\mathbf{k}}\rvert^2 \lvert v_{\mathbf{k}'}\rvert^2 < n_{\mathbf{k}} > (< n_{\mathbf{k}'} > +1)\delta_{\mathbf{k},\mathbf{k}'''}\delta_{\mathbf{k}',\mathbf{k}''}$

It is an important observation that the initial $\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''}$ just acts as the identity operator. That can be seen in 8 of the 12 terms (for example Ia, Ib, IIb) where two δ 's arise from the contractions which relate $\mathbf{k}'s$ from the same side in the initial δ. Take, for example Ia): we have $\delta_{\mathbf{k},\mathbf{k}''}$ and $\delta_{\mathbf{k}',\mathbf{k}'''}$ so our initial δ takes the form $\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}+\mathbf{k}'}$, which is trivially always equal to one. Therefore, we still have two summations. In IIa) as an example for the remaining four terms, we have $\delta_{\mathbf{k},\text{-}\mathbf{k}'}$ and $\delta_{\text{-}\mathbf{k}'',\mathbf{k}'''}$, which implies $\delta_{\mathbf{k}-\mathbf{k},\mathbf{k}''-\mathbf{k}''}$, also always equal to one.

Now we think about how we can use some symmetries to reduce the number of terms we need to calculate. It is clear that $\sum_k \hat{b}_{\mathbf{k}} = \sum_k \hat{b}_{\text{-}\mathbf{k}}$. $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are per definition symmetric. In the same eight terms mentioned above the minus signs appear only pairwise on the $\delta' s$ (or not at all) and since $\delta_{\text{-}\mathbf{k},\text{-}\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'}$, in these terms we can replace **-k** by **k**.

When introducing the Bogoliubov transformation we saw that a number of prefactors u and v are valid solutions to our problem. We had assumed that the phases of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ should be equal. *A posteriori* we can see from our result that this assumption was correct, since in the

$\hat{H}^{(3)}$-term the phase ϕ will cancel out also, as we will soon see.

By renaming the dummy integration variables we can reduce the number of different terms to six. It is to be understood that we have two remaining $\mathbf{k}$-sums, here named $\mathbf{k}$ and $\mathbf{k}'$.

1)$|u_{\mathbf{k}}|^2 |u_{\mathbf{k}'}|^2 \langle n_{\mathbf{k}}\rangle\langle n_{\mathbf{k}'}\rangle$, (these are the terms Ia and Ib)

2)$|v_{\mathbf{k}}|^2 |v_{\mathbf{k}'}|^2 (\langle n_{\mathbf{k}}\rangle + 1)(\langle n_{\mathbf{k}'}\rangle + 1)$ (VIa and VI b)

3)$|u_{\mathbf{k}}|^2 |v_{\mathbf{k}'}|^2 \langle n_{\mathbf{k}}\rangle(\langle n_{\mathbf{k}'}\rangle + 1)$ (IIb, IIIb, IVb, Vb)

4)$u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'}\langle n_{\mathbf{k}}\rangle\langle n_{\mathbf{k}'}\rangle$ (once, this is IIa)

5)$u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'}(\langle n_{\mathbf{k}}+1)\rangle(\langle n_{\mathbf{k}'}\rangle + 1)$ (Va)

6)$u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'}\langle n_{\mathbf{k}}\rangle(\langle n_{\mathbf{k}'}\rangle + 1)$ (IIIa and IVa)

Now that we have gathered all arising terms, we can proceed to sum them up. The time-integral will be trivial, since from eq. (4.7) we see that the time-dependence is expressed by an exponential function, but with different signs for creation and annihilation operators. Since a contraction is always between these two, the time-dependence just cancels out and the integral simply yields the prefactor $\hbar\beta$.

$$\begin{aligned}\hat{H}^{(4)} = \frac{1}{2}\frac{U}{N_S}\sum_{\mathbf{k},\mathbf{k}'}\frac{-1}{\hbar}\hbar\beta\{&[u_{\mathbf{k}}v_{\mathbf{k}}\left(2\langle n_{\mathbf{k}}\rangle + 1\right)u_{\mathbf{k}'}v_{\mathbf{k}'}\left(2\langle n_{\mathbf{k}'}\rangle + 1\right)] \\ &+2\left[u_{\mathbf{k}}^2\langle n_{\mathbf{k}}\rangle + v_{\mathbf{k}}^2\left(\langle n_{\mathbf{k}}\rangle + 1\right)\right]\left[u_{\mathbf{k}'}^2\langle n_{\mathbf{k}'}\rangle + v_{\mathbf{k}'}^2\left(\langle n_{\mathbf{k}'}\rangle + 1\right)\right]\}\end{aligned} \tag{4.20}$$

We will soon see how these terms appear in a diagrammatical depiction.

4.5 The $\hat{H}^{(3)^2}$-term

We had already calculated the form of $H^{(3)}$ in 3.18.

$$\hat{H}^{(3)} = \sqrt{N_0}\frac{U}{N_S}\{\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''}\hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}'}^\dagger\hat{a}_{\mathbf{k}''}\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''} + \hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}'}\hat{a}_{\mathbf{k}''}\delta_{\mathbf{k},\mathbf{k}'+\mathbf{k}''}\} \tag{4.21}$$

In the $\hat{H}^{(3)^2}$-term we therefore get the sum of four different expressions, each consisting of six operators, three each at τ_1 and three at τ_2. For every expression, there are (6-1)!! = 15 possible contractions. Luckily, we will be able to show that only those contracting different times will contribute, that is only 24 contractions total.

As a first step we calculate the a-a correlations, remembering that the time-dependence depends only on the time difference of the operators which we name τ and where no time is given it is assumed to be the operator at time 0: $\hat{a} \equiv \hat{a}(t = 0)$. The time-dependence was calculated in

(4.7):

$$\begin{aligned}\langle\hat{T}\left(\hat{a}^\dagger_{\mathbf{k}}(\tau)\hat{a}^\dagger_{\mathbf{k}'}\right)\rangle =&\langle\hat{T}((u_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}}(\tau)-v^*_{\mathbf{k}}\hat{b}_{\text{-}\mathbf{k}})(u_{\mathbf{k}'}\hat{b}^\dagger_{\mathbf{k}'}(\tau)-v^*_{\mathbf{k}'}\hat{b}_{\text{-}\mathbf{k}'}))\rangle\\ =&-u_{\mathbf{k}}v^*_{\mathbf{k}'}\langle\hat{T}\hat{b}^\dagger_{\mathbf{k}}(\tau)\hat{b}_{\text{-}\mathbf{k}'}\rangle-v^*_{\mathbf{k}}u_{\mathbf{k}'}\langle\hat{T}\hat{b}_{\text{-}\mathbf{k}}(\tau)\hat{b}^\dagger_{\mathbf{k}'}\rangle\\ =&-u_{\mathbf{k}}v^*_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}\left\{e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\left[\Theta(\tau)\langle n_{\mathbf{k}}\rangle+\Theta(-\tau)\langle\hat{n}_{\mathbf{k}}+1\rangle\right]\right.\\ &\left.+e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\left[\Theta(\tau)\langle\hat{n}_{\mathbf{k}}+1\rangle+\Theta(-\tau)\langle\hat{n}_{\mathbf{k}}\rangle\right]\right\}\\ =&-u_{\mathbf{k}}v^*_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}\left\{\Theta(\tau)\left[\langle\hat{n}_{\mathbf{k}}\rangle e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}+\langle\hat{n}_{\mathbf{k}}+1\rangle e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\right]\right.\\ &\left.+\Theta(-\tau)\left[\langle\hat{n}_{\mathbf{k}}+1\rangle e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}+\hat{n}_{\mathbf{k}}e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\right]\right\}\end{aligned}\tag{4.22}$$

Similarly, we get the remaining correlations:

$$\begin{aligned}\langle\hat{T}\left(\hat{a}_{\mathbf{k}}(\tau)\hat{a}_{\mathbf{k}'}\right)\rangle =&-u^*_{\mathbf{k}}v_{\mathbf{k}}\delta_{\mathbf{k},-\mathbf{k}'}\left\{\Theta(\tau)\left[\langle\hat{n}_{\mathbf{k}}+1\rangle e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}+\langle\hat{n}_{\mathbf{k}}\rangle e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\right]\right.\\ &\left.+\Theta(-\tau)\left[\langle\hat{n}_{\mathbf{k}}\rangle e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}+\langle\hat{n}_{\mathbf{k}}+1\rangle e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\right]\right\}\end{aligned}\tag{4.23}$$

$$\begin{aligned}\langle\hat{T}\left(\hat{a}^\dagger_{\mathbf{k}}(\tau)\hat{a}_{\mathbf{k}'}\right)\rangle =&\delta_{\mathbf{k},\mathbf{k}'}\left\{\Theta(\tau)\left[|u_{\mathbf{k}}|^2\langle\hat{n}_{\mathbf{k}}\rangle e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}+|v_{\mathbf{k}}|^2\langle\hat{n}_{\mathbf{k}}+1\rangle e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\right]\right.\\ &\left.+\Theta(-\tau)\left[|u_{\mathbf{k}}|^2\langle\hat{n}_{\mathbf{k}}+1\rangle e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}+|v_{\mathbf{k}}|^2\langle\hat{n}_{\mathbf{k}}\rangle e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\right]\right\}\end{aligned}\tag{4.24}$$

$$\begin{aligned}\langle\hat{T}\left(\hat{a}_{\mathbf{k}}(\tau)\hat{a}^\dagger_{\mathbf{k}'}\right)\rangle =&\delta_{\mathbf{k},\mathbf{k}'}\left\{\Theta(\tau)\left[|u_{\mathbf{k}}|^2\langle\hat{n}_{\mathbf{k}}+1\rangle e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}+|v_{\mathbf{k}}|^2\langle\hat{n}_{\mathbf{k}}\rangle e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\right]\right.\\ &\left.+\Theta(-\tau)\left[|u_{\mathbf{k}}|^2\langle\hat{n}_{\mathbf{k}}\rangle e^{-\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}+|v_{\mathbf{k}}|^2\langle\hat{n}_{\mathbf{k}}+1\rangle e^{\frac{\tau}{\hbar}\hbar\omega_{\mathbf{k}}}\right]\right\}\end{aligned}\tag{4.25}$$

This also completes the proof that the phase for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ indeed cancels out, as we had assumed earlier, so in the following we will again take them to be real numbers.

A comparison shows that the first two terms are actually equal.

Similarly, interchanging τ_1 and τ_2 in one of the last two terms changes the sign of the exponential function and the terms become equal.

Special attention should be paid to the $\delta's$, as we will use them in the following proof to show that all contractions of equal-time-operators vanish.

There are six possibilities for contractions of operators with equal times to appear in the terms (we omit the times and prefactors here):

$$\begin{aligned}\hat{b}^\dagger_{\mathbf{k}_1}\hat{b}^\dagger_{\mathbf{k}_2}\hat{b}_{\mathbf{k}_3} &= ...\delta_{\mathbf{k}_1,-\mathbf{k}_2}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3} = ...\delta_{0,\mathbf{k}_3} = 0\\ \hat{b}^\dagger_{\mathbf{k}_1}\hat{b}^\dagger_{\mathbf{k}_2}\hat{b}_{\mathbf{k}_3} &= ...\delta_{\mathbf{k}_1,\mathbf{k}_3}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3} = ...\delta_{\mathbf{k}_2,0} = 0\\ \hat{b}^\dagger_{\mathbf{k}_1}\hat{b}^\dagger_{\mathbf{k}_2}\hat{b}_{\mathbf{k}_3} &= ...\delta_{\mathbf{k}_1,\mathbf{k}_3}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3} = ...\delta_{\mathbf{k}_2,0} = 0\\ \hat{b}^\dagger_{\mathbf{k}_1}\hat{b}_{\mathbf{k}_2}\hat{b}_{\mathbf{k}_3} &= ...\delta_{\mathbf{k}_2,-\mathbf{k}_3}\delta_{\mathbf{k}_1,\mathbf{k}_2+\mathbf{k}_3} = ...\delta_{\mathbf{k}_1,0} = 0\end{aligned}\tag{4.26}$$

$$\hat{b}^{\dagger}_{\mathbf{k}_1}\hat{b}_{\mathbf{k}_2}\hat{b}_{\mathbf{k}_3} = ...\delta_{\mathbf{k}_1,\mathbf{k}_2}\delta_{\mathbf{k}_1,\mathbf{k}_2+\mathbf{k}_3} = ...\delta_{0,\mathbf{k}_3} = 0$$
$$\hat{b}^{\dagger}_{\mathbf{k}_1}\hat{b}_{\mathbf{k}_2}\hat{b}_{\mathbf{k}_3} = ...\delta_{\mathbf{k}_1,\mathbf{k}_3}\delta_{\mathbf{k}_1,\mathbf{k}_2+\mathbf{k}_3} = ...\delta_{0,\mathbf{k}_2} = 0$$

This leaves us with just six expressions for each of the four terms, 24 altogether. The very first thought of reducing the number of terms is to check whether we can halve the terms by permuting two $\mathbf{k}$'s, since at τ_1 and τ_2 there are always two creation or two annihilation operators. We must not forget the original δ but it is easily seen that halving the terms is possible because one always finds two terms with the same δ. The twelve terms can be reduced even further, but this will be done in the next chapter where it can be visually seen which terms are equal. We will take a little different approach than in the last chapter, since directly inserting the $\hat{b}'_{\mathbf{k}}s$ would lead to a plethora of terms. Instead, we write down the expressions in terms of the $\hat{a}'_{\mathbf{k}}s$, calculate the arising contractions and only then change to the $\hat{b}'_{\mathbf{k}}s$. The second column lists the possible renaming of the variables, one for each of the twelve terms. The others are the contracted operators and the last row shows all $\delta's$ for each term. As before, we observe that one of the original δ's just acts as the unity operator, for example in the first term:
$\delta_{\mathbf{k1,-k4}}\ \delta_{\mathbf{k2,-k5}}\ \delta_{\mathbf{k3,-k6}}\ \delta_{\mathbf{k1+k2,k3}}\ \delta_{\mathbf{k4+k5,k6}} = \delta_{\mathbf{k1,-k4}}\ \delta_{\mathbf{k2,-k5}}\ \delta_{\mathbf{k3,-k6}}\ \delta_{\mathbf{k1+k2,k3}}\ \delta_{\mathbf{-k1-k2,-k3}}$

1.	$\hat{a}_{\mathbf{k4}} \leftrightarrow \hat{a}_{\mathbf{k5}}$	$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}^{\dagger}_{\mathbf{k2}}\hat{a}^{\dagger}_{\mathbf{k5}}$	$\hat{a}_{\mathbf{k3}}\hat{a}_{\mathbf{k6}}$	$\delta_{\mathbf{k1,-k4}}\ \delta_{\mathbf{k2,-k5}}\ \delta_{\mathbf{k3,-k6}}\ \delta_{\mathbf{k1+k2,k3}}$
2.		$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}^{\dagger}_{\mathbf{k2}}\hat{a}_{\mathbf{k6}}$	$\hat{a}_{\mathbf{k3}}\hat{a}^{\dagger}_{\mathbf{k5}}$	$\delta_{\mathbf{k1,-k4}}\ \delta_{\mathbf{k2,k6}}\ \delta_{\mathbf{k3,k5}}\ \delta_{\mathbf{k1+k2,k3}}$
3.		$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}_{\mathbf{k6}}$	$\hat{a}^{\dagger}_{\mathbf{k2}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}_{\mathbf{k3}}\hat{a}^{\dagger}_{\mathbf{k5}}$	$\delta_{\mathbf{k1,k6}}\ \delta_{\mathbf{k2,-k4}}\ \delta_{\mathbf{k3,k5}}\ \delta_{\mathbf{k1+k2,k3}}$
4.	$\hat{a}_{\mathbf{k5}} \leftrightarrow \hat{a}_{\mathbf{k6}}$	$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}^{\dagger}_{\mathbf{k2}}\hat{a}_{\mathbf{k5}}$	$\hat{a}_{\mathbf{k3}}\hat{a}_{\mathbf{k6}}$	$\delta_{\mathbf{k1,-k4}}\ \delta_{\mathbf{k2,k5}}\ \delta_{\mathbf{k3,-k6}}\ \delta_{\mathbf{k1+k2,k3}}$
5.		$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}_{\mathbf{k6}}$	$\hat{a}^{\dagger}_{\mathbf{k2}}\hat{a}_{\mathbf{k5}}$	$\hat{a}_{\mathbf{k3}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\delta_{\mathbf{k1,k6}}\ \delta_{\mathbf{k2,k5}}\ \delta_{\mathbf{k3,k4}}\ \delta_{\mathbf{k1+k2,k3}}$
6.		$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}_{\mathbf{k6}}$	$\hat{a}^{\dagger}_{\mathbf{k2}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}_{\mathbf{k3}}\hat{a}_{\mathbf{k5}}$	$\delta_{\mathbf{k1,k6}}\ \delta_{\mathbf{k2,-k4}}\ \delta_{\mathbf{k3,-k5}}\ \delta_{\mathbf{k1+k2,k3}}$
7.	$\hat{a}_{\mathbf{k4}} \leftrightarrow \hat{a}_{\mathbf{k5}}$	$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}_{\mathbf{k2}}\hat{a}^{\dagger}_{\mathbf{k5}}$	$\hat{a}_{\mathbf{k3}}\hat{a}_{\mathbf{k6}}$	$\delta_{\mathbf{k1,-k4}}\ \delta_{\mathbf{k2,k5}}\ \delta_{\mathbf{k3,-k6}}\ \delta_{\mathbf{k1,k2+k3}}$
8.		$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}^{\dagger}_{\mathbf{4}}$	$\hat{a}_{\mathbf{k2}}\hat{a}_{\mathbf{k6}}$	$\hat{a}_{\mathbf{k3}}\hat{a}^{\dagger}_{\mathbf{k5}}$	$\delta_{\mathbf{k1,-k4}}\ \delta_{\mathbf{k2,-k6}}\ \delta_{\mathbf{k3,k5}}\ \delta_{\mathbf{k1,k2+k3}}$
9.		$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}_{\mathbf{k6}}$	$\hat{a}_{\mathbf{k2}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}_{\mathbf{k3}}\hat{a}^{\dagger}_{\mathbf{k5}}$	$\delta_{\mathbf{k1,k6}}\ \delta_{\mathbf{k2,k4}}\ \delta_{\mathbf{k3,k5}}\ \delta_{\mathbf{k1,k2+k3}}$
10.	$\hat{a}_{\mathbf{k5}} \leftrightarrow \hat{a}_{\mathbf{k6}}$	$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}_{\mathbf{k2}}\hat{a}_{\mathbf{k5}}$	$\hat{a}_{\mathbf{k3}}\hat{a}_{\mathbf{k6}}$	$\delta_{\mathbf{k1,-k4}}\ \delta_{\mathbf{k2,-k5}}\ \delta_{\mathbf{k3,-k6}}\ \delta_{\mathbf{k1,k2+k3}}$
11.		$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}_{\mathbf{6}}$	$\hat{a}_{\mathbf{k2}}\hat{a}_{\mathbf{k5}}$	$\hat{a}_{\mathbf{k3}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\delta_{\mathbf{k1,k6}}\ \delta_{\mathbf{k2,-k5}}\ \delta_{\mathbf{k3,k4}}\ \delta_{\mathbf{k1,k2+k3}}$
12.		$\hat{a}^{\dagger}_{\mathbf{k1}}\hat{a}_{\mathbf{k6}}$	$\hat{a}_{\mathbf{k2}}\hat{a}^{\dagger}_{\mathbf{k4}}$	$\hat{a}_{\mathbf{k3}}\hat{a}_{\mathbf{k5}}$	$\delta_{\mathbf{k1,k6}}\ \delta_{\mathbf{k2,k4}}\ \delta_{\mathbf{k3,-k5}}\ \delta_{\mathbf{k1,k2+k3}}$

One can show that these 12 remaining terms can again be reduced to only four different expressions, using that several contractions are equal, as seen on page 40.By interchanging $\mathbf{k}_1$ and $\mathbf{k}_2$, the second and third and the fourth and sixth expression can be seen to be equal, respectively. Similarly, by replacing $\mathbf{k}_2$ with $\mathbf{k}_3$ in the 7^{th} and 8^{th} as well as in the 11^{th} and 12^{th} term one gets the same expression also. We have to take care if this stays correct for the original $\delta's$, which is indeed the case as can be read off from the above table. The remaining four identifications are listed.

- The fourth and seventh term are equal by changing $\tau_1 \rightleftarrows \tau_2$ as well as $\mathbf{k}_1$ and $\mathbf{k}_3$ in the seventh term.

- The eleventh term becomes equal to the second by interchanging the times and $\{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3\} \to \{\mathbf{k}_3, \mathbf{k}_1, \mathbf{k}_2\}$.
- The first and tenth are obviously equal, considering that $a - a$ and $a^\dagger - a^\dagger$ correlations are equal.
- Finally, the fifth and ninth term are equal by changing the times and substituting $\mathbf{k}_1 \rightleftarrows \mathbf{k}_3$ in the ninth term.

In the next chapter the task will be to express these in terms of the $b'_{\mathbf{k}}s$.

We will now see how the tedious work of identifying equal terms can be approached much more easily. If one were to tackle the next order in the perturbation, it would probably be wise to find a recursive graphical construction within the framework explained in the next section.

4.6 Diagrammatical representation

A very intuitive description of the arising terms is given by drawing the so-called *Feynman-diagrams*, a very powerful tool in quantum field theory . It is often possible to derive all terms in a given order from a few combinatorial prescriptions (cf. for example [38]). We take a step back before employing the Bogoliubov transformation: for the $\hat{H}^{(4)}$-term we had three $\hat{a}$-correlations, namely

$$\hat{a}^\dagger_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}'}\hat{a}_{\mathbf{k}''}\hat{a}_{\mathbf{k}'''} \tag{4.27}$$

$$\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}''}\hat{a}^\dagger_{\mathbf{k}'}\hat{a}_{\mathbf{k}'''} \tag{4.28}$$

$$\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}'''}\hat{a}^\dagger_{\mathbf{k}'}\hat{a}_{\mathbf{k}''} \ . \tag{4.29}$$

After renaming the (dummy integration) variables, the second and third term are equal. A short calculation shows that we get the same twelve terms as in 4.1. Of course, we could have chosen this way of getting all terms also, but the comparison of both calculations serves as further justification of our ad-hoc rule how a contraction at equal times is to be treated.

Feynman graphs represent the terms in perturbation theory as follows: a local interaction (i.e. at equal times, which is obviously not possible when including Relativity, therefore in Quantum Field Theory this looks a bit different) is represented by a dot • and the contractions by lines connecting the different times (or, as in the $\hat{H}^{(4)}$-term, equal times) with arrows indicating which operators to contract. An outgoing line means a particle is created and an incoming line stands for an annihilation of a particle. We adopt the convention that the contraction of two creation operators is denoted by two arrows pointing towards one another, while two arrows pointing away from each other represent the contraction of two annihilation operators (in the usual problems without a Bogoliubov transformation these do not contribute).

The following Feynman rules apply for our problem:

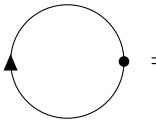
For the correlations at equal times that appear for example in the $\hat{H}^{(4)}$-term we take the limit for the above terms in such a way that $\tau \to 0^+$. Thus it is assured that the correct order of the operators is kept, i.e. in our case *annihilation before creation.*

$$= -u_{\mathbf{k}} v_{\mathbf{k}} \delta_{\mathbf{k},\mathbf{k}'} \left\{ \Theta(\tau) \left[\langle \hat{n}_{\mathbf{k}} \rangle e^{\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} + \langle \hat{n}_{\mathbf{k}} + 1 \rangle e^{-\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} \right] + \Theta(-\tau) \left[\langle \hat{n}_{\mathbf{k}} + 1 \rangle e^{\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} + \hat{n}_{\mathbf{k}} e^{-\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} \right] \right\}$$

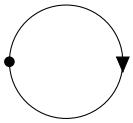
Contracting two creation or two annihilation operators yields the same result

$$= \delta_{\mathbf{k},\mathbf{k}'} \left\{ \Theta(\tau) \left[|u_{\mathbf{k}}|^2 \langle \hat{n}_{\mathbf{k}} + 1 \rangle e^{-\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} + |v_{\mathbf{k}}|^2 \langle \hat{n}_{\mathbf{k}} \rangle e^{\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} \right] + \Theta(-\tau) \left[|u_{\mathbf{k}}|^2 \langle \hat{n}_{\mathbf{k}} \rangle e^{-\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} + |v_{\mathbf{k}}|^2 \langle \hat{n}_{\mathbf{k}} + 1 \rangle e^{\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} \right] \right\}$$

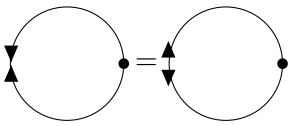
$$= \delta_{\mathbf{k},\mathbf{k}'} \left\{ \Theta(\tau) \left[|u_{\mathbf{k}}|^2 \langle \hat{n}_{\mathbf{k}} \rangle e^{\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} + |v_{\mathbf{k}}|^2 \langle \hat{n}_{\mathbf{k}} + 1 \rangle e^{-\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} \right] + \Theta(-\tau) \left[|u_{\mathbf{k}}|^2 \langle \hat{n}_{\mathbf{k}} + 1 \rangle e^{\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} + |v_{\mathbf{k}}|^2 \langle \hat{n}_{\mathbf{k}} \rangle e^{-\frac{\tau}{\hbar}\epsilon_{\mathbf{k}}} \right] \right\}$$



$$= \delta_{\mathbf{k},\mathbf{k}'} \left\{ u_{\mathbf{k}}^2 \langle n_{\mathbf{k}} + 1 \rangle + v_{\mathbf{k}}^2 \langle n_{\mathbf{k}} \rangle \right\}$$



$$= \delta_{\mathbf{k},\mathbf{k}'} \left\{ u_{\mathbf{k}}^2 \langle n_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \left(\langle n_{\mathbf{k}} \rangle + 1 \right) \right\}$$



$$= -\delta_{\mathbf{k},\mathbf{k}'} \left\{ u_{\mathbf{k}} v_{\mathbf{k}} \left(2 \langle n_{\mathbf{k}} \rangle + 1 \right) \right\}$$

With these rules in mind, we can now list the diagrams that appeared in our calculations, along with their multiplicity:

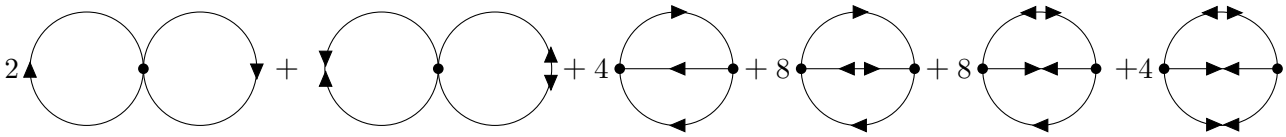


Figure 4.1: Feynman Diagrams for the 2$^{\text{nd}}$ order perturbation

We keep in mind that in the fourth diagram one $\mathbf{k}$ from an $a - a^\dagger$ correlation is the one that is appears on one side of the δ from the Fourier-transformation and is thus equal to the sum of the other two $\mathbf{k}$'s. In the fifth diagram, this is true for one $\mathbf{k}$ from an $a - a$ correlation. For the other two diagrams from the $\hat{H}^{(3)^2}$-term we do not need to keep track of that.

Chapter 5

Calculations with the second order approximation

"*Always try to innovate. If you lose your old fitness, you lose out to Bose-Einstein condensation. I am sure that companies that go under would feel better if they knew that they were victims of Bose-Einstein condensation.*"

Prof. Jennifer Tour Chayes at the MAA 2007 Hedrick Lecture

After having collected all terms in second loop-order, we can in a similar manner as in the preceding chapters, again calculate the Effective Hamiltonian and the Free Energy. From this we can ultimately calculate the particle density that can be checked for a phase transition as well as be used to plot the time-of-flight pictures. In complete analogy to the proceedings in chapter 3 and 4 we first write down the effective potential as

$$V_{\text{eff}} = -\frac{1}{\beta}\ln Z = -\frac{1}{\beta}\ln\left(Z_0\frac{Z}{Z_0}\right) = -\frac{1}{\beta}\ln Z_0 - \frac{1}{\beta}\ln\frac{Z}{Z_0}\ . \tag{5.1}$$

The first term is just $V_{\text{eff}}^{(0)}$, the effective potential for the diagonalized Hamiltonian. The expansion of $\frac{Z}{Z_0}$ is given in eq. 4.5. In short notation without the sums and integrals we thus get (keeping in mind that the perturbation here is $\hat{H}^{(3)} + \hat{H}^{(4)}$:

$$\ln\frac{Z}{Z_0} = \ln\left\{1 - \frac{1}{\hbar}\left(\hat{H}^{(3)} + \hat{H}^{(4)}\right) + \frac{1}{\hbar^2}\left(\hat{H}^{(3)} + \hat{H}^{(4)}\right)^2 + ...\right\} \tag{5.2}$$

We have the Taylor-expansion $\ln(1+x) \approx x - \frac{x^2}{2}$, which we do not calculate here as we have already convinced ourselves that only $\hat{H}^{(4)}$ and $\hat{H}^{(3)^2}$ constitute the second loop order; all remaining terms are either zero or from a higher order.

5.1 The zero-temperature limit

We have already reduced the number of different terms considerably, still there are definitely too many to write them all down or try to go ahead and calculate the Free Energy. Therefore, at this point we already carry out the zero-temperature limit $T \to 0$. Since so far no way of

measuring the temperature of a BEC has been found, we would have taken this limit anyway somewhere along the line.

Let us therefore for now only concentrate on the dependency on T or, equivalently β.

In the $\hat{H}^{(4)}$-term the time-dependence of the operators, as mentioned, cancels out and the one time-integral just gives $\hbar\beta$. This just cancels out with the $-\frac{1}{\beta}$ from the definition of the Effective Potential, so the temperature-dependency is only present in the $\langle n_{\mathbf{k}}\rangle$'s. Since $\lim_{\beta\to\infty}\langle n_{\mathbf{k}}\rangle = \lim_{\beta\to\infty}\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}}} = 0$, only those terms survive that do not include an $\langle n_{\mathbf{k}}\rangle$. From the first diagram (neglecting other prefactors and sums) we thus only have a term with $v_{\mathbf{k}}^2 v_{\mathbf{k}'}^2$ and from the second also only one term with $u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'}$.

The other terms are a little more involved: in eqs. 4.22 ff. we see the time-dependent correlations. In the $\hat{H}^{(3)^2}$-term all arising terms contain three a-correlations, all with τ_1 and τ_2.

We would now like to see correlations in the four Feynman-diagrams expressed via the $b_{\mathbf{k}}$'s. Luckily, by a few considerations we can substantially reduce the number of arising terms. We see that each contraction consists of a term with $\Theta(\tau)$ or a $\Theta(-\tau)$. From the properties of Heaviside-functions it follows that multiplying the same $\Theta's$ is just again the Heaviside-function while multiplying two with a different sign of the argument yields zero. That still leaves quite a lot of terms, so let us now take the zero-temperature limit to simplify these.

At first we shall have a look at the simple $a-a$ correlations and then see how we can translate those results to the actual terms that appear in perturbation theory. We see that the β-dependence manifests itself in one of four different possible combinations:

1. $\int_0^{\hbar\beta}\int_0^{\hbar\beta}\Theta(\tau_1-\tau_2)e^{\hbar\omega_{\mathbf{k}}(\tau_1-\tau_2)}\langle n_{\mathbf{k}}\rangle d\tau_1 d\tau_2$

2. $\int_0^{\hbar\beta}\int_0^{\hbar\beta}\Theta(\tau_1-\tau_2)e^{\hbar\omega_{\mathbf{k}}(\tau_2-\tau_1)}\langle n_{\mathbf{k}}+1\rangle d\tau_1 d\tau_2$

3. $\int_0^{\hbar\beta}\int_0^{\hbar\beta}\Theta(\tau_2-\tau_1)e^{\hbar\omega_{\mathbf{k}}(\tau_1-\tau_2)}\langle n_{\mathbf{k}}+1\rangle d\tau_1 d\tau_2$

4. $\int_0^{\hbar\beta}\int_0^{\hbar\beta}\Theta(\tau_2-\tau_1)e^{\hbar\omega_{\mathbf{k}}(\tau_2-\tau_1)}\langle n_{\mathbf{k}}\rangle d\tau_1 d\tau_2$

First of all, we see that the first and fourth as well as the second and third term are actually the same, so we analyze the two different terms by use of the integrals

$$\int_0^{\hbar\beta}\int_0^{\hbar\beta}\Theta(\tau_1-\tau_2)e^{\omega_{\mathbf{k}}(\tau_1-\tau_2)}d\tau_1 d\tau_2 = \int_0^{\hbar\beta}e^{\omega_{\mathbf{k}}\tau_1}d\tau_2\int_0^{\tau_1}e^{-\omega_{\mathbf{k}}\tau_2}d\tau_2 = \frac{1}{\omega_{\mathbf{k}}}\int_0^{\hbar\beta}e^{\omega_{\mathbf{k}}\tau_1}\left(1-e^{-\omega\tau_1}\right)d\tau_1$$
$$= \frac{1}{\omega_{\mathbf{k}}}\int_0^{\hbar\beta}(e^{\omega_{\mathbf{k}}\tau_1}-1) = -\frac{\hbar\beta}{\omega_{\mathbf{k}}}+\frac{1}{\omega_{\mathbf{k}}^2}\left(e^{\hbar\omega_{\mathbf{k}}\beta}-1\right)$$

and

$$\int_0^{\hbar\beta}\int_0^{\hbar\beta}\Theta(\tau_2-\tau_1)e^{\omega_{\mathbf{k}}(\tau_1-\tau_2)}d\tau_1 d\tau_2 = \frac{\hbar\beta}{\omega_{\mathbf{k}}}+\frac{1}{\omega_{\mathbf{k}}^2}\left(e^{-\hbar\omega_{\mathbf{k}}\beta}-1\right)\ .$$

Realizing that the first term only appears in conjunction with $\langle n_{\mathbf{k}} \rangle$ and the second term with $\langle n_{\mathbf{k}} + 1 \rangle$, we can now calculate the zero-temperature limit:

$$\begin{aligned}\lim_{T\to 0} -\frac{1}{\beta}\left[-\frac{\hbar\beta}{\omega_{\mathbf{k}}} + \frac{1}{\omega_{\mathbf{k}}^2}\left(e^{\hbar\omega_{\mathbf{k}}\beta} - 1\right)\right]\langle n_{\mathbf{k}} \rangle &= \lim_{T\to 0} -\frac{1}{\beta}\left[-\frac{\hbar\beta}{\omega_{\mathbf{k}}} + \frac{1}{\omega_{\mathbf{k}}^2}\left(e^{\hbar\omega_{\mathbf{k}}\beta} - 1\right)\right]\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} \\ &= \lim_{T\to 0} -\frac{1}{\beta}\left[-\frac{\hbar\beta}{\omega_{\mathbf{k}}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} + -\frac{1}{\beta}\frac{1}{\omega_{\mathbf{k}}^2}\right] = 0 \ ,\end{aligned}$$

and for the other term

$$\begin{aligned}&\lim_{T\to 0} -\frac{1}{\beta}\left[\frac{\hbar\beta}{\omega_{\mathbf{k}}} + \frac{1}{\omega_{\mathbf{k}}^2}\left(e^{-\hbar\omega_{\mathbf{k}}\beta} - 1\right)\right]\langle n_{\mathbf{k}} + 1 \rangle \\ &= \lim_{T\to 0} -\frac{1}{\beta}\left[\frac{\hbar\beta}{\omega_{\mathbf{k}}} + \frac{1}{\omega_{\mathbf{k}}^2}\left(e^{-\hbar\omega_{\mathbf{k}}\beta} - 1\right)\right]\frac{e^{\beta\hbar\omega_{\mathbf{k}}}}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} \\ &= \lim_{T\to 0} -\frac{1}{\beta}\left[\frac{\hbar\beta}{\omega_{\mathbf{k}}}\frac{e^{\beta\hbar\omega_{\mathbf{k}}}}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} + \frac{1}{\omega_{\mathbf{k}}^2}\left(\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} - \frac{e^{\beta\hbar\omega_{\mathbf{k}}}}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1}\right)\right] \\ &= -\frac{\hbar}{\omega_{\mathbf{k}}} \ .\end{aligned}$$

We have used that $\langle n_{\mathbf{k}} + 1 \rangle = \frac{e^{\beta\hbar\omega_{\mathbf{k}}}}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1}$ and $\lim_{T\to 0}\langle n_{\mathbf{k}} + 1 \rangle = 1$.

We now look at the terms in $\hat{H}^{(3)^2}$, which are of a similar form but the argument of the exponential in the time-integral is a sum of three $\omega' s$ which is then multiplied with three $n'_{\mathbf{k}} s$. We keep in mind that due to the original δ from the Fourier-transformation, it is $\omega_{\mathbf{k}_3} = \omega_{\mathbf{k}_1 + \mathbf{k}_2}$.

Examining the terms one can first of all conclude that the -1 from the integration can never give any contribution, since either it is multiplied with only $\langle n_{\mathbf{k}} + 1 \rangle$'s which would give a constant but zero with the prefactor $\frac{1}{\beta}$ or there is at least one $\langle n_{\mathbf{k}} \rangle$ involved which goes exponentially to zero when $\beta \to \infty$. The exponential function in the enumerator together with the particle number expectation values is a product of three terms of the form we already examined above. They all tend to zero. Remaining is the first term $\pm\frac{1}{\beta}\frac{\hbar\beta}{\overline{\omega}}$ which is multiplied with the corresponding $n_{\mathbf{k}}$'s, where $\overline{\omega}$ has been defined as $\pm\omega_{\mathbf{k}_1} \pm \omega_{\mathbf{k}_2} \pm \omega_{\mathbf{k}_3}$. Similarly as before, all terms except those only with $\langle n_{\mathbf{k}} + 1 \rangle$'s vanish in our limit. So, the only contribution is of the form

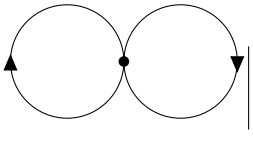
$$-\frac{1}{\beta}\frac{\hbar\beta}{\omega_{\mathbf{k}_1} + \omega_{\mathbf{k}_2} + \omega_{\mathbf{k}_3}} = \frac{-\hbar}{\omega_{\mathbf{k}_1} + \omega_{\mathbf{k}_2} + \omega_{\mathbf{k}_3}} \tag{5.3}$$

This is valid for all Feynman-diagrams, only the prefactors $u_{\mathbf{k}}, v_{\mathbf{k}}$ will of course vary.

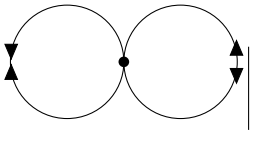
One may ask whether it would be necessary to further examine terms such as $\frac{1}{\omega_{\mathbf{k}_1} - \omega_{\mathbf{k}_2} + \omega_{\mathbf{k}_3}}$ where the denominator could potentially become zero. Luckily, this does not pose a problem: since in these cases the integrand is $e^0 = 1$, the double time-integral will simply result in $(\frac{(\hbar\beta)^2}{2})$. Even with the $-\frac{1}{\beta}$ this expression would seem to diverge, but there is at least one exponential dampening present in the form of an $\langle n_{\mathbf{k}} \rangle$. (Only the case would be problematic when only $n_{\mathbf{k}} + 1$ would be present, but this term, as seen above has the denominator $\omega_{\mathbf{k}_1} + \omega_{\mathbf{k}_2} + \omega_{\mathbf{k}_3}$, so

can never be zero as the energy $\hbar\omega_{\mathbf{k}}$ must always be greater than zero as can be seen from its definition.)

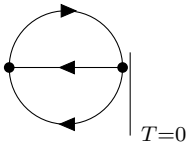
Let us gather all terms for the Effective Potential we now have. For the terms from the second order, this is done by collecting all terms with the same θ (i.e. once for $\theta(\tau_1 - \tau_2)$ and once for $\theta(\tau_2 - \tau_1)$) and for those only the $\langle n_{\mathbf{k}} + 1\rangle$'s and noting their prefactors. We also name the $\mathbf{k}$'s in such a way that $\mathbf{k}'' = \mathbf{k} + \mathbf{k}'$.



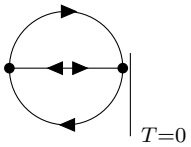
$$= \sum_{\mathbf{k},\mathbf{k}'} v_{\mathbf{k}}^2 v_{\mathbf{k}'}^2$$



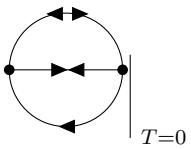
$$= \sum_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}$$



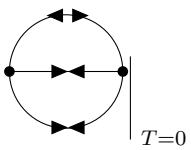
$$= \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''=\mathbf{k}+\mathbf{k}'} \frac{-\hbar}{(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'}+\omega_{\mathbf{k}''})} \left[v_{\mathbf{k}}^2 v_{\mathbf{k}'}^2 u_{\mathbf{k}''}^2 + u_{\mathbf{k}}^2 u_{\mathbf{k}'}^2 v_{\mathbf{k}''}^2\right]$$



$$= \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''=\mathbf{k}+\mathbf{k}'} \frac{-\hbar}{(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'}+\omega_{\mathbf{k}''})} \left[v_{\mathbf{k}}^2 \left(-u_{\mathbf{k}'} v_{\mathbf{k}'}\right) u_{\mathbf{k}''}^2 + u_{\mathbf{k}}^2 \left(-u_{\mathbf{k}'} v_{\mathbf{k}'}\right) v_{\mathbf{k}''}^2\right]$$



$$= \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''=\mathbf{k}+\mathbf{k}'} \frac{-\hbar}{(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'}+\omega_{\mathbf{k}''})} \left[\left(-u_{\mathbf{k}} v_{\mathbf{k}}\right)\left(-u_{\mathbf{k}''} v_{\mathbf{k}''}\right) u_{\mathbf{k}'}^2 + \left(-u_{\mathbf{k}} v_{\mathbf{k}}\right)\left(-u_{\mathbf{k}''} v_{\mathbf{k}''}\right) v_{\mathbf{k}'}^2\right]$$



$$= \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''=\mathbf{k}+\mathbf{k}'} \frac{-\hbar}{(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'}+\omega_{\mathbf{k}''})} 2\left[\left(-u_{\mathbf{k}} v_{\mathbf{k}}\right)\left(-u_{\mathbf{k}'} v_{\mathbf{k}'}\right)\left(-u_{\mathbf{k}''} v_{\mathbf{k}''}\right)\right]$$

Figure 5.1: Feynman Diagrams for the 2nd order perturbation

The prefactors in the Effective Potential are for the first two diagrams (since they come from the $\hat{H}^{(4)}$-term) $\frac{-1}{\hbar}$ and for the others $\frac{1}{2!\hbar^2}$, in addition to their multiplicity. By taking the zero-temperature limit, we have thus reduced the number of terms enough to be able to calculate the particle number density again, this time including the second order perturbation and hope to calculate a phase transition in better agreement with the experimental results.

5.2 The density including the second order perturbation

The Effective Potential up to second order at zero temperature reads:

$$\begin{aligned} V_{\text{eff}} = N_S \left(\frac{1}{2}Un_0^2 - \mu n_0 - Jzn_0\right) + \eta\frac{1}{2}\sum_{\mathbf{k}} \left(\hbar\omega_{\mathbf{k}} - \epsilon_{\mathbf{k}} + Jz + \mu - 2Un_0\right) \\ + \eta^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''=\mathbf{k}+\mathbf{k}'} \Bigg\{ \frac{U}{2N_S}\left(2v_{\mathbf{k}}^2 v_{\mathbf{k}'}^2 + u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}\right) + N_0 \frac{U^2}{2N_S^2} \frac{-1}{\hbar\omega_{\mathbf{k}} + \hbar\omega_{\mathbf{k}'} + \hbar\omega_{\mathbf{k}''}} \\ \Big[4\left(v_{\mathbf{k}}^2 v_{\mathbf{k}'}^2 u_{\mathbf{k}''}^2 + u_{\mathbf{k}}^2 u_{\mathbf{k}'}^2 v_{\mathbf{k}''}^2\right) + 8\left(v_{\mathbf{k}}^2(-u_{\mathbf{k}'}v_{\mathbf{k}'})u_{\mathbf{k}''}^2 + u_{\mathbf{k}}^2(-u_{\mathbf{k}'}v_{\mathbf{k}'})v_{\mathbf{k}''}^2\right) + 8\left((-u_{\mathbf{k}}v_{\mathbf{k}})u_{\mathbf{k}'}^2\,(-u_{\mathbf{k}''}v_{\mathbf{k}''})\right) \\ + (-u_{\mathbf{k}}v_{\mathbf{k}})\,v_{\mathbf{k}'}^2\,(-u_{\mathbf{k}''}v_{\mathbf{k}''})) + 4\left(2(-u_{\mathbf{k}}v_{\mathbf{k}})(-u_{\mathbf{k}'}v_{\mathbf{k}'})(-u_{\mathbf{k}''}v_{\mathbf{k}''})\right)\Big] \Bigg\} \end{aligned} \tag{5.4}$$

We execute the same steps as before: deriving V_{eff} with respect to n_0, setting the result equal to zero and solving and reinserting for n_0. Then, using the particle density equation

$$-\frac{1}{N_S}\frac{\partial V_{\text{eff}}}{\partial \mu} = n \tag{5.5}$$

we eliminate μ and can plot n_0/n over U/J. This time, we hope to get to see a phase transition. We recollect the important expressions as well as their zeroth order denoted by $^{(0)}$ and meaning that the substitution $Un_0 \to Jz + \mu$ has taken place.

$$\epsilon_{\mathbf{k}} = Jz - 2J\sum_{i}^{d}\cos(k_i a) \tag{5.6}$$

$$\hbar\omega_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - Jz - \mu + Un_0)^2 + 2Un_0(\epsilon_{\mathbf{k}} - Jz - \mu + Un_0)} \tag{5.7}$$

$$\hbar\omega_{\mathbf{k}}^{(0)} = \sqrt{{\epsilon_{\mathbf{k}}}^2 + 2\epsilon_{\mathbf{k}}(Jz + \mu)} \tag{5.8}$$

$$\frac{\partial\hbar\omega_{\mathbf{k}}}{\partial n_0} = \frac{U(2\epsilon_{\mathbf{k}} - 2Jz - 2\mu + 3Un_0)}{\hbar\omega_{\mathbf{k}}} \tag{5.9}$$

$$\frac{\partial\hbar\omega_{\mathbf{k}}}{\partial n_0}^{(0)} = \frac{U(2\epsilon_{\mathbf{k}} + Jz + \mu)}{\hbar\omega_{\mathbf{k}}^{(0)}} \tag{5.10}$$

$$v_{\mathbf{k}}^2 + 1 = u_{\mathbf{k}}^2 = \frac{1}{2}\left(\frac{\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0}{\hbar\omega_{\mathbf{k}}} + 1\right) \tag{5.11}$$

$$u_{\mathbf{k}}^{2\,(0)} = \frac{1}{2}\left(\frac{\epsilon_{\mathbf{k}} + Jz + \mu}{\hbar\omega_{\mathbf{k}}^{(0)}} + 1\right) \tag{5.12}$$

When deriving with respect to n_0, we will need $\frac{\partial v_{\mathbf{k}}^2}{\partial n_0}$, which is obviously the same as $\frac{\partial u_{\mathbf{k}}^2}{\partial n_0}$:

$$\frac{\partial v_{\mathbf{k}}^2}{\partial n_0} = \frac{1}{2}\frac{2U\hbar\omega_{\mathbf{k}} - (\epsilon_{\mathbf{k}} - Jz - \mu + 2Un_0)\frac{\partial \hbar\omega_{\mathbf{k}}}{\partial n_0}}{(\hbar\omega_{\mathbf{k}})^2} \tag{5.13}$$

$$\frac{\partial v_{\mathbf{k}}^2}{\partial n_0}^{(0)} = \frac{1}{2}\frac{2U\hbar\omega_{\mathbf{k}}^{(0)} - (\epsilon_{\mathbf{k}} + Jz + \mu)U\frac{2\epsilon_{\mathbf{k}}+Jz+\mu}{\hbar\omega_{\mathbf{k}}}}{(\hbar\omega_{\mathbf{k}})^{(0)^2}} \tag{5.14}$$

The expression $u_{\mathbf{k}}v_{\mathbf{k}}$ can be simplified:

$$\sqrt{\frac{1}{2}\left(\frac{\epsilon_k - Jz - \mu + 2Un_0}{\hbar\omega_{\mathbf{k}}} + 1\right)}\sqrt{\frac{1}{2}\left(\frac{\epsilon_k - Jz - \mu + 2Un_0}{\hbar\omega_{\mathbf{k}}} - 1\right)} = \sqrt{\frac{1}{4}\frac{U^2{n_0}^2}{\hbar\omega\mathbf{k}^2}} = \frac{1}{2}\frac{Un_0}{\hbar\omega_{\mathbf{k}}}\ , \tag{5.15}$$

where we have used the third binomial formula as well as (5.7), and the fact that U,n_0 and $\hbar\omega_{\mathbf{k}}$ are not negative so we do not need to include a modulus when taking the square root.

$$\frac{\partial u_{\mathbf{k}}v_{\mathbf{k}}}{\partial n_0} = \frac{1}{2}\frac{U\hbar\omega_{\mathbf{k}} - Un_0\frac{\partial \hbar\omega_{\mathbf{k}}}{\partial n_0}}{\hbar\omega_{\mathbf{k}}^2} \tag{5.16}$$

$$\frac{\partial u_{\mathbf{k}}v_{\mathbf{k}}}{\partial n_0}^{(0)} = \frac{1}{2}\frac{U\hbar\omega_{\mathbf{k}}^{(0)} - U(Jz+\mu)(2\epsilon_{\mathbf{k}} + Jz + \mu)}{\hbar\omega_{\mathbf{k}}^{(0)^2}} \tag{5.17}$$

The now following procedures are very complex and we will not write down each one in detail. The steps are:

- Deriving the Effective Potential including the second order with respect to n_0.
- Solving for n_0. We get n_0 in zeroth and first order, which are of course the same terms as in chapter 3 and a new second order,${n_0}^{(2)}$.
- Inserting n_0 while disregarding orders higher than two. The n_0's which are originally in zeroth order thus get replaced by the whole expression when we solved for n_0. In second order we just replace n_0 by its zeroth order approximation, i.e. $n_0 = \frac{Jz+\mu}{U}$, just like before.

  Any n_0 appearing in first order has to be replaced by an approximation up to first order, which is

  $$ {n_0}^{(0)} + \eta {n_0}^{(1)} = \frac{Jz+\mu}{U} - \eta\sum_{\mathbf{k}}\frac{(2\epsilon_{\mathbf{k}} + Jz + \mu)}{\hbar\omega_{\mathbf{k}}^{(0)}} - 1 \tag{5.18}$$

  A little complication arises here because n_0 appears in first order in a square root in $\hbar\omega_{\mathbf{k}}$. Here it is necessary to perform a Taylor-expansion of the square root to get the correct expressions up to second order (see below).
- After thus having calculated the grand-canonical potential, we differentiate with respect to μ to get the particle density n.

- Solving this equation for the chemical potential and again reinserting, we can eliminate μ.

- By setting $n = 1$ (one could also choose another density) we can proceed to plot the equation

$$n - n_0 = f(n, U/J) \tag{5.19}$$

and hope for a solution, meaning that $n_0 \to 0$ for a particular value of the experimental parameters U/J which could of course be compared to the experiment.

Unfortunately, after having done all these things, we encountered a surprising problem: in the terms appear *infrared divergencies*, obviously a problem when we turn from sums to integrals which run over the zero. This problem was also encountered in [39] when calculating the second order perturbation theory via the formulism of path integrals.

This means we will have to be content to prove the existence of these divergencies and thereby show that the method of reinserting unfortunately is not feasible. For brevity, we will omit in the following calculations the contribution from the $H^{(3)^2}$-term. It can easily be seen that those omitted terms cannot cancel out the divergencies we write down now, because the rest. So, if we encounter divergencies in the rest, the whole Hamiltonian has to have them.

$$\begin{aligned} V_{\text{eff}} = N_S \left(\frac{1}{2} U n_0^2 - \mu n_0 - J z n_0 \right) + \eta \frac{1}{2} \sum_{\mathbf{k}} \left(\hbar\omega_{\mathbf{k}} - \epsilon_{\mathbf{k}} + Jz + \mu - 2Un_0 \right) \\ + \eta^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''=\mathbf{k}+\mathbf{k}'} \frac{U}{2N_S} \left(2 v_{\mathbf{k}}^2 v_{\mathbf{k}'}^2 + u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \right) \end{aligned} \tag{5.20}$$

n_0 has to be inserted basically in five different places: in the first one it needs to be squared, so we get

$$\left({n_0}^{(0)} + \eta {n_0}^{(1)} + \eta^2 {n_0}^{(2)} \right)^2 = {n_0^{(0)}}^2 + 2\eta {n_0}^{(0)} {n_0}^{(1)} + \eta^2 {n_0^{(1)}}^2 + 2\eta^2 {n_0}^{(0)} {n_0}^{(2)} + O(\eta^3) \; . \tag{5.21}$$

Depending on the place of the n_0, the zeroth, first, or second order approximation has to be inserted. We have

$$\begin{aligned} {n_0}^{(2)} &= -\frac{1}{2} \sum_{\mathbf{k}} \frac{\partial \hbar\omega_{\mathbf{k}}}{\partial n_0}^{(1)} - \frac{1}{2} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} 2 \left(\frac{\partial {v_{\mathbf{k}}}^2}{\partial n_0} {v_{\mathbf{k}'}}^2 + \frac{\partial {v_{\mathbf{k}'}}^2}{\partial n_0} {v_{\mathbf{k}}}^2 \right) + \frac{\partial u_{\mathbf{k}} v_{\mathbf{k}}}{\partial n_0} u_{\mathbf{k}'} v_{\mathbf{k}'} + \frac{\partial u_{\mathbf{k}'} v_{\mathbf{k}'}}{\partial n_0} u_{\mathbf{k}} v_{\mathbf{k}} \\ &= -\frac{1}{2} \sum_{\mathbf{k}} \frac{\partial \hbar\omega_{\mathbf{k}}}{\partial n_0}^{(1)} - \sum_{\mathbf{k}} \sum_{\mathbf{k}'} 2 \frac{\partial {v_{\mathbf{k}}}^2}{\partial n_0} {v_{\mathbf{k}'}}^2 + \frac{\partial u_{\mathbf{k}} v_{\mathbf{k}}}{\partial n_0} u_{\mathbf{k}'} v_{\mathbf{k}'} \; , \end{aligned} \tag{5.22}$$

where we have used that $U n_0(0) = Jz + \mu$.

The square root appearing in the $\hbar\omega_{\mathbf{k}}$ in first order has to be expanded up to first order, yielding

$$\begin{aligned}
&\sqrt{(\epsilon_{\mathbf{k}} + \eta {n_0}^{(1)})^2 + 2U({n_0}^{(0)} + \eta {n_0}^{(1)})(\epsilon_{\mathbf{k}} + \eta U {n_0}^{(1)})} \\
&= \sqrt{{\epsilon_{\mathbf{k}}}^2 + 2\epsilon_{\mathbf{k}} U {n_0}^{(0)}} + \eta \frac{2\epsilon_{\mathbf{k}} {n_0}^{(1)} U + {n_0}^{(0)} {n_0}^{(1)} U^2}{\sqrt{{\epsilon_{\mathbf{k}}}^2 + 2\epsilon_{\mathbf{k}} U {n_0}^{(0)}}} \\
&= \hbar {\omega_{\mathbf{k}}}^{(0)} + \eta \frac{2\epsilon_{\mathbf{k}} {n_0}^{(1)} U + {n_0}^{(0)} {n_0}^{(1)} U^2}{\hbar {\omega_{\mathbf{k}}}^{(0)}} \ .
\end{aligned} \tag{5.23}$$

Similarly, we perform an expansion of $\frac{\partial \hbar\omega_{\mathbf{k}}}{\partial n_0}$:

$$\frac{\partial \hbar {\omega_{\mathbf{k}}}^{(1)}}{\partial n_0} = U^2 \left(\frac{2\epsilon_{\mathbf{k}'} + U n_0}{\widetilde{\hbar 2\omega_{\mathbf{k}'}{}^{(0)}}} - 1\right) \frac{\epsilon_{\mathbf{k}} - U n_0}{\widetilde{\hbar \omega_{\mathbf{k}}{}^{(0)}}^3} \tag{5.24}$$

One should take care that the sum which appears in ${n_0}^{(1)}$ needs to run over a index different from $\mathbf{k}$.

With that, we can write down the grand-canonical potential. We limit ourselves to the second order, the zeroth and first remain the same as in the earlier chapters, of course.

$$\Omega^{(2)} = \frac{1}{2} U {n_0}^{(1)^2} + \frac{1}{2} \sum_{\mathbf{k}} [\hbar {\omega_{\mathbf{k}}}^{(1)} - 2U {n_0}^{(1)}] + \frac{U}{2} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} 2 {v_{\mathbf{k}}^2}^{(0)} {u_{\mathbf{k}'}^2}^{(0)} + u_{\mathbf{k}} {v_{\mathbf{k}}}^{(0)} u_{\mathbf{k}'} {v_{\mathbf{k}'}}^{(0)} \tag{5.25}$$

Interestingly, ${n_0}^{(2)}$ cancels out in Ω, which is very convenient since that means we will not need the derivatives of $H^{(4)}$.

In the next step, we take the derivatives with respect to the chemical potential in order to solve for the particle density. When reinserting, we use a tilde,"˜", to denote the result, so as not to create a confusion with "(0)".

$$\frac{\partial \hbar {\omega_{\mathbf{k}}}^{(0)}}{\partial \mu} = \frac{\epsilon_{\mathbf{k}}}{\hbar {\omega_{\mathbf{k}}}^{(0)}} \tag{5.26}$$

$$\widetilde{\hbar \omega_{\mathbf{k}}{}^{(0)}} = \sqrt{\epsilon \mathbf{k}^2 + 2\epsilon_{\mathbf{k}} U n} \tag{5.27}$$

$$\frac{\partial \widetilde{u_{\mathbf{k}} v_{\mathbf{k}}{}^{(0)}}}{\partial \mu} = \frac{1}{2} \frac{U}{\widetilde{\hbar \omega_{\mathbf{k}}{}^{(0)}}} \left(1 - \frac{U n}{\epsilon_{\mathbf{k}}^2 + 2\epsilon_{\mathbf{k}} U n}\right) \tag{5.28}$$

$$\frac{\partial \widetilde{{v_{\mathbf{k}}}^{2(0)}}}{\partial \mu} = \frac{1}{\widetilde{2\hbar \omega_{\mathbf{k}}{}^{(0)}}} \left(1 - \frac{{\epsilon_{\mathbf{k}}}^2 + \epsilon_{\mathbf{k}} U n}{\epsilon_{\mathbf{k}}^2 + 2\epsilon_{\mathbf{k}} U n}\right) \tag{5.29}$$

$$\frac{\partial \widetilde{\hbar {\omega_{\mathbf{k}}}^{(1)}}}{\partial \mu} = -U \frac{\epsilon_{\mathbf{k}'} (2\epsilon_{\mathbf{k}} + U n)(-\epsilon_{\mathbf{k}'} + U n)}{2\hbar \omega_{\mathbf{k}} \hbar {\omega_{\mathbf{k}'}}^3} - U \frac{\epsilon_{\mathbf{k}} (2\epsilon_{\mathbf{k}} + U n)(1 - \frac{2\epsilon_{\mathbf{k}'} + U n}{2\hbar \omega_{\mathbf{k}}})}{\hbar {\omega_{\mathbf{k}}}^3} + U \frac{1 - \frac{2\epsilon_{\mathbf{k}'} + U n}{\hbar \omega_{\mathbf{k}'}}}{\hbar \omega_{\mathbf{k}}} \tag{5.30}$$

We will now examine the behavior for small k, i.e. the infrared domain.

We begin with $\epsilon_{\mathbf{k}}$, which was basically $1-\cos(k)$, which, as we remarked earlier, results in the k^2-behavior of $\epsilon_{\mathbf{k}}$ for small k.

For $\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}$ we can therefore observe a linear dependency on k for small k:

$$\sqrt{\epsilon_{\mathbf{k}}}\sqrt{\epsilon_{\mathbf{k}}+Un} \sim \sqrt{k^2}\sqrt{k^2+\text{const.}} \sim k \tag{5.31}$$

$$\widetilde{n_0{}^{(1)}} \sim \frac{\epsilon_{\mathbf{k}}+2Un}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}} - 1 \sim k + \frac{1}{k} + \text{const.} \sim \frac{1}{k} \tag{5.32}$$

$$\frac{\widetilde{\partial n_0{}^{(1)}}}{\partial\mu} \sim \frac{1}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}} \frac{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}}+2Un)}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}} \sim k^3 + k + \frac{1}{k} + \text{const.} \sim \frac{1}{k} \tag{5.33}$$

$$\widetilde{u_{\mathbf{k}}v_{\mathbf{k}}{}^{(0)}} \sim \frac{Un}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}} \sim \frac{1}{k} \tag{5.34}$$

$$\frac{\widetilde{\partial u_{\mathbf{k}}v_{\mathbf{k}}{}^{(0)}}}{\partial\mu} \sim \frac{1}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}}(1 - \frac{Un}{\epsilon_{\mathbf{k}}{}^2+2Un}) \sim \frac{1}{k}(1-\frac{1}{k^4+1}) \sim \frac{1}{k} \tag{5.35}$$

$$\widetilde{v_{\mathbf{k}}{}^{2(0)}} \sim \frac{\epsilon_{\mathbf{k}}+Un}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}} - 1 \sim \frac{k^2+\text{const.}}{k} + \text{const.} \sim \frac{1}{k} \tag{5.36}$$

$$\frac{\widetilde{\partial v_{\mathbf{k}}{}^{2(0)}}}{\partial\mu} \sim \frac{1}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}}(1 - \frac{\epsilon_{\mathbf{k}}{}^2+\epsilon_{\mathbf{k}}Un}{\epsilon_{\mathbf{k}}^2+2\epsilon_{\mathbf{k}}Un}) \sim \frac{1}{k}(\text{const.} - \frac{k^4+k^2}{k^4+k^2}) \sim \frac{1}{k} \tag{5.37}$$

And, finally

$$\begin{aligned}\frac{\widetilde{\partial\hbar\omega_{\mathbf{k}}{}^{(1)}}}{\partial\mu} &= \frac{\epsilon_{\mathbf{k}'}(2\epsilon_{\mathbf{k}}+Un)(-\epsilon_{\mathbf{k}'}+Un)}{2\hbar\omega_{\mathbf{k}}\hbar\omega_{\mathbf{k}'}{}^3} - U\frac{\epsilon_{\mathbf{k}}(2\epsilon_{\mathbf{k}}+Un)(1-\frac{2\epsilon_{\mathbf{k}'}+Un}{2\hbar\omega_{\mathbf{k}}})}{\hbar\omega_{\mathbf{k}}{}^3} + U\frac{1-\frac{2\epsilon_{\mathbf{k}'}+Un}{\hbar\omega_{\mathbf{k}'}}}{\hbar\omega_{\mathbf{k}}} \\ &\sim \frac{k'^2(k^2+\text{const.})(k'^2+\text{const.})}{kk'^3} - \frac{k(k^2+\text{const.})(1-\frac{k'+\text{const.}}{k})}{k^3} + \frac{1-\frac{k'^2+\text{const.}}{k'}}{k} \\ &\sim \frac{1}{kk'} - \frac{1}{kk'} + \frac{1}{kk'} \sim \frac{1}{kk'}\ .\end{aligned} \tag{5.38}$$

Looking back at 5.25, we see that k and k', respectively, diverge at most linearly. This does not present a problem, since when integrating and switching to spherical coordinates, we get from the Jacobian a k^2 (or k'^2), so the integrals possess a finite value.

So far, the calculated terms do not give any divergencies. Problems arise only when taking the derivatives $\frac{\partial v_{\mathbf{k}}{}^2}{\partial n_0}$ and $\frac{\partial v_{\mathbf{k}}u_{\mathbf{k}}}{\partial n_0}$, which we will show now.

We have the needed derivatives already calculated, see 5.17, 5.14 and 5.24.

Eliminating μ (here we simply need to insert the lowest order) yields

$$\widetilde{\frac{\partial u_{\mathbf{k}} v_{\mathbf{k}}{}^{(0)}}{\partial n_0}} = \frac{1}{2}\left(\frac{U}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}} - \frac{U^2 n(2\epsilon_{\mathbf{k}} + Un)}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}^3}\right) \tag{5.39}$$

$$\widetilde{\frac{\partial v_{\mathbf{k}}{}^{(0)}{}^2}{\partial n_0}} = \frac{1}{2}\left(\frac{2U}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}} - \frac{(\epsilon_{\mathbf{k}} + Un)U(2\epsilon_{\mathbf{k}} + Un)}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}^3}\right) \tag{5.40}$$

and

$$\widetilde{\frac{\partial \hbar\omega_{\mathbf{k}}{}^{(1)}}{\partial n_0}} = U^2\left(\frac{2\epsilon_{\mathbf{k}'} + Un}{\widetilde{2\hbar\omega_{\mathbf{k}'}{}^{(0)}}} - 1\right)\frac{\epsilon_{\mathbf{k}} - Un^2}{\widetilde{\hbar\omega_{\mathbf{k}}{}^{(0)}}^3} \ . \tag{5.41}$$

We have the product of two $v_{\mathbf{k}}{}^2$'s and two $u_{\mathbf{k}}v_{\mathbf{k}}$'s so when deriving and renaming we get twice the product where one part has been derived. We also include all the prefactors from **??**, resulting in the three terms:

$$-\frac{1}{2}22{v_{\mathbf{k}}}^2\frac{\partial {v_{\mathbf{k}'}}^2}{\partial n_0} = -2\frac{1}{2}\left(\frac{\epsilon_{\mathbf{k}} + Un}{\hbar\omega_{\mathbf{k}}} - 1\right)\frac{1}{2}\left[\frac{2U}{\hbar\omega_{\mathbf{k}'}} - \frac{(\epsilon_{\mathbf{k}'} + Un)U(2\epsilon_{\mathbf{k}'} + Un)}{{\hbar\omega_{\mathbf{k}'}}^3}\right] \tag{5.42}$$

$$-\frac{1}{2}2u_{\mathbf{k}}v_{\mathbf{k}}\frac{\partial u_{\mathbf{k}'}v_{\mathbf{k}'}}{\partial n_0} = -\frac{Un}{2\hbar\omega_{\mathbf{k}}}\frac{1}{2}\left[\frac{U}{\hbar\omega_{\mathbf{k}'}} - \frac{U^2 n(2\epsilon_{\mathbf{k}'} + Un)}{{\hbar\omega_{\mathbf{k}'}}^3}\right] \tag{5.43}$$

$$-\frac{1}{2U}\frac{\partial \hbar\omega_{\mathbf{k}}{}^{(1)}}{\partial n_0} = -\frac{-Un_{\mathbf{k}'}{}^{(1)}(\epsilon_{\mathbf{k}} - Un)^2}{{\hbar\omega_{\mathbf{k}}}^3} \tag{5.44}$$

From these three equations we extract the "problematic" terms, i.e. those which diverge with a power greater than two. This only happens where the third power of $\hbar\omega$ appears in the denominator.

$$\begin{gathered}\frac{1}{2}\left(\frac{\epsilon_{\mathbf{k}} + Un}{\hbar\omega_{\mathbf{k}}} - 1\right)\frac{-U^3n^2}{{\hbar\omega_{\mathbf{k}'}}^3} \\ \frac{1}{4}\frac{Un}{\hbar\omega_{\mathbf{k}}}\frac{U^3n^2}{{\hbar\omega_{\mathbf{k}'}}^3} \\ \frac{1}{2}\frac{U^3n^2}{{\hbar\omega_{\mathbf{k}}}^3}\left(\frac{-2\epsilon_{\mathbf{k}'} - Un}{2\hbar\omega_{\mathbf{k}'}} + 1\right)\end{gathered} \tag{5.45}$$

where the last factor in the third equation is $n_{\mathbf{k}'}{}^{(1)}$.

Although the terms look very similar (when swapping the variables in the third equation), they unfortunately do not quite cancel each other out, we get stuck with

$$\frac{U^4n^2}{2\hbar\omega_{\mathbf{k}}{\hbar\omega_{\mathbf{k}'}}^3} \tag{5.46}$$

so we see that the term is divergent, at least in one variable.

With that, we have shown that our original ansatz unfortunately cannot lead to a useful approximation in second order. One possible solution could be to just cancel the divergent term, viewing it as "unphysical". We decided not to do that.

5.3 Can Popov help us?

Maybe the variational ansatz $\mu \to M + \eta\Delta$ can help us once again, as it did before.

Unfortunately, no. Inserting the relation above in Ω cf. 3.64 yields for the lowest order:

$$-\frac{N_S}{2U}(Jz+\mu)^2 \to -\frac{N_S}{2U}(Jz+M+\eta\Delta)^2 \tag{5.47}$$

Consequently, deriving yields:

$$\frac{\partial(Jz+M+\eta\Delta)^2}{\partial M} = 2(Jz+M+\eta\Delta) \tag{5.48}$$

With the elimination of Δ via $\Delta = \frac{\mu-M}{M}$ we see that M does not appear anymore. Therefore, we are unable to solve for M and reinsert.

The situation was different when we only included the first order, because then we actually discarded a term in the quadratic μ. VPT thus will not help us here, we have to concede at this point that we will not be able to get a result for the second order.

Chapter 6

Calculations without reinserting

"*I wish to God these calculations had been executed by steam.*"
Charles Babbage

6.1 Why we cannot see a phase transition

We now show that the condition $\frac{\partial V_{\text{eff}}}{\partial n_0}$ for n_0 does not have a solution for $n_0 = 0$ when reinserting. (Since both equations have to be satisfied for a solution, our whole system of equations cannot have a solution.)

When deriving and going to $n_0 \to 0$ we encounter the problem, for example in $\hbar\omega_{\mathbf{k}}$, that we have to take the root of a square which results in the modulus if negative values are possible:

$$\sqrt{(\epsilon_{\mathbf{k}} - Jz - \mu)^2} = |\epsilon_{\mathbf{k}} - Jz - \mu| \tag{6.1}$$

Taking all the derivatives, then taking the limit of a vanishing condensate density yields

expression	expression taken at $n_0 = 0$	$\lvert\epsilon_{\mathbf{k}} - Jz - \mu\rvert > 0$	$\lvert\epsilon_{\mathbf{k}} - Jz - \mu\rvert < 0$
$\hbar\omega_{\mathbf{k}}$	$\lvert\epsilon_{\mathbf{k}} - Jz - \mu\rvert$	$\epsilon_{\mathbf{k}} - Jz - \mu$	$-(\epsilon_{\mathbf{k}} - Jz - \mu)$
$\frac{\partial\hbar\omega_{\mathbf{k}}}{\partial n_0}$	$2U\frac{\epsilon_{\mathbf{k}}-Jz-\mu}{\lvert\epsilon_{\mathbf{k}}-Jz-\mu\rvert}$	$2U$	$-2U$
${u_{\mathbf{k}}}^2$	$\frac{1}{2}(\frac{\epsilon_{\mathbf{k}}-Jz-\mu}{\lvert\epsilon_{\mathbf{k}}-Jz-\mu\rvert}+1)$	1	0
${v_{\mathbf{k}}}^2$	$\frac{1}{2}(\frac{\epsilon_{\mathbf{k}}-Jz-\mu}{\lvert\epsilon_{\mathbf{k}}-Jz-\mu\rvert}-1)$	0	-1
$\frac{\partial {u_{\mathbf{k}}}^2}{\partial n_0} = \frac{\partial {v_{\mathbf{k}}}^2}{\partial n_0}$	$\frac{1}{2}(\frac{2U}{\lvert\epsilon_{\mathbf{k}}-Jz-\mu\rvert} - \frac{\epsilon_{\mathbf{k}}-Jz-\mu}{\lvert\epsilon_{\mathbf{k}}-Jz-\mu\rvert^2}2U\frac{\epsilon_{\mathbf{k}}-Jz-\mu}{\lvert\epsilon_{\mathbf{k}}-Jz-\mu\rvert})$	0	0
$u_{\mathbf{k}}v_{\mathbf{k}}$	0	0	0
$\frac{\partial u_{\mathbf{k}}v_{\mathbf{k}}}{\partial n_0}$	$\frac{U}{2\lvert\epsilon_{\mathbf{k}}-Jz-\mu\rvert}$	$\frac{U}{2\epsilon_{\mathbf{k}}-Jz-\mu}$	$\frac{-U}{2\epsilon_{\mathbf{k}}-Jz-\mu}$

So, we see that any term that includes as a factor $u_{\mathbf{k}}v_{\mathbf{k}}$ or $\frac{\partial {u_{\mathbf{k}}}^2}{\partial n_0}$, (or $\frac{\partial {v_{\mathbf{k}}}^2}{\partial n_0}$) goes to zero when n_0 goes to zero.

Thus we see that the derivative of $H^{(4)}$ becomes zero for $n_0 \to 0$.

The ${H^{(3)}}^2$-term is a little bit more involved: since it is multiplied with n_0, the derivative is of the form $(...) + n_0 \frac{\partial(...)}{\partial n_0}$. The second part is zero, what about the first?

It consists of a product of $\frac{1}{\hbar\omega_{\mathbf{k}}+\hbar\omega_{\mathbf{k}'}+\hbar\omega_{\mathbf{k}''}}$and 7 terms, divided in 4 subgroups. These groups are (without prefactors):

I. $v_{\mathbf{k}}^2 v_{\mathbf{k}'}^2 u_{\mathbf{k}''}^2 + u_{\mathbf{k}}^2 u_{\mathbf{k}'}^2 v_{\mathbf{k}''}^2$
II. $v_{\mathbf{k}}^2(-u_{\mathbf{k}'}v_{\mathbf{k}'})u_{\mathbf{k}''}^2 + u_{\mathbf{k}}^2(-u_{\mathbf{k}'}v_{\mathbf{k}'})v_{\mathbf{k}''}^2$
III. $(-u_{\mathbf{k}}v_{\mathbf{k}})u_{\mathbf{k}'}^2(-u_{\mathbf{k}''}v_{\mathbf{k}''}) + (-u_{\mathbf{k}}v_{\mathbf{k}})v_{\mathbf{k}'}^2(-u_{\mathbf{k}''}v_{\mathbf{k}''})$
IV. $(-u_{\mathbf{k}}v_{\mathbf{k}})(-u_{\mathbf{k}'}v_{\mathbf{k}'})(-u_{\mathbf{k}''}v_{\mathbf{k}''})$

Let us first look at the terms which are derived: in I, each term in the derivative has to include either $\frac{\partial v_{\mathbf{k}}^2}{\partial n_0}$ or $\frac{\partial u_{\mathbf{k}}^2}{\partial n_0}$ which means, as was just proved, that they are all zero.
In II, we have either again the derivatives as in I that make it go to zero, but we also have the part where only the $u_{\mathbf{k}}v_{\mathbf{k}}$ gets derived. But, we have the product of a $u_{\mathbf{k}}^2$ with a $v_{\mathbf{k}'}^2$ which is again zero, but we have to proof this.

A case distinction for the moduli for three $\mathbf{k}'s$ would suggest 8 different possibilities, but actually there are only 6: since $\mathbf{k}'' = \mathbf{k} + \mathbf{k}'$, the sign of $\mathbf{k}$ is already determined when the signs of $\mathbf{k}$ and $\mathbf{k}'$ are equal. From the $v_{\mathbf{k}}^2(-u_{\mathbf{k}'}v_{\mathbf{k}'})u_{\mathbf{k}''}^2$ term only those parts of the integration remain where $\mathbf{k} < 0$ and $\mathbf{k}'' > 0$. That is only one: $\mathbf{k} < 0, \mathbf{k}' > 0, \mathbf{k}'' > 0$.
From the $u_{\mathbf{k}}^2(-u_{\mathbf{k}'}v_{\mathbf{k}'})v_{\mathbf{k}''}^2$ term, likewise only one is nonzero, namely the one for which $\mathbf{k} > 0, \mathbf{k}' < 0, \mathbf{k}'' < 0$ is valid.

In the limit $n_0 \to 0$ we thus have for II: $-1 * \frac{U}{2(\epsilon_{\mathbf{k}'}-Jz-\mu)} * 1 + 1 * \frac{-U}{2(\epsilon_{\mathbf{k}'}-Jz-\mu)} * (-1) = 0$.

In III and IV, at least one $u_{\mathbf{k}}v_{\mathbf{k}}$ does not get derived, so all contributions are zero.

Now to the part, where these terms are not derived (but $\frac{1}{\hbar\omega_{\mathbf{k}}+\hbar\omega_{\mathbf{k}'}+\hbar\omega_{\mathbf{k}''}}$ is):

in I, the requirement for both terms to be nonzero is for $\mathbf{k}$ and $\mathbf{k}'$ to have the same sign, but for $\mathbf{k}''$ to have the other sign. As we mentioned above, this is impossible due to the definition of $\mathbf{k}''$.

In II, III and IV, at least one $u_{\mathbf{k}}v_{\mathbf{k}}$ in each term results in zero for all of them.

We have thus shown that the second order cannot give any new results compared to the first order approximation. Therefore, we will try another way that avoids the reinserting.

6.2 Numerical calculations

As we have seen, the method of reinserting and then taking the limit $n_0 \to 0$ the $\mathbf{k}$-integrals results in IR-divergencies. Therefore, we take a step back and this time do not reinsert but rather solve the system of implicit equations

$$\frac{\partial V_{\text{eff}}}{\partial n_0} = 0 \tag{6.2}$$

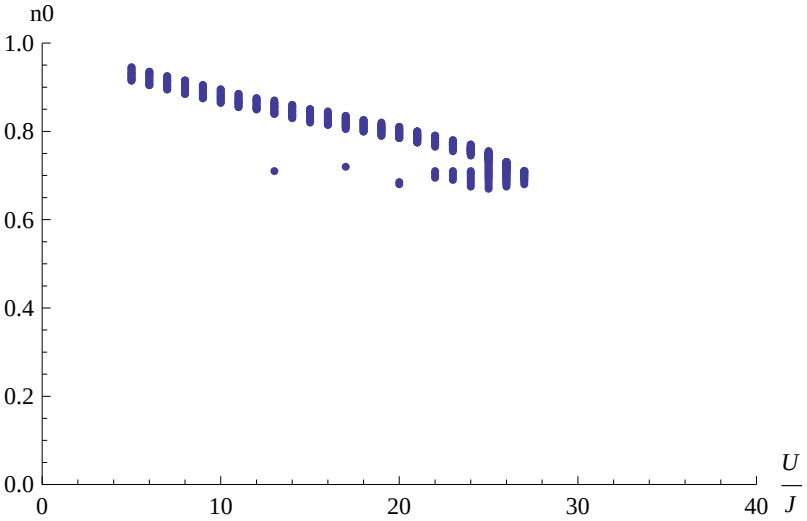


Figure 6.1: Numerical calculations without reinserting for the first order.

$$\frac{-1}{N_S}\frac{\partial V_{\text{eff}}}{\partial \mu} = n \tag{6.3}$$

simultaneously. This has the advantage that we do not add a further error which occurs when omitting higher terms in the resubstitutions, but the disadvantage that we now have to deal with a system of two coupled implicit equations instead of one. This will be solved by a numerical program written in C which is included in the appendix.

The needed derivatives are extremely complicated, namely the derivative of ${H^{(3)}}^2$. Therefore, we will not write down a step-by-step calculation as this would be very tiresome for us and the reader. The result can be found in the appendix. It has been calculated symbolically by using *Mathematica*.

The program works as follows: it first looks for solutions to one equation (of course, one has to allow for an error since numerically, the equation will never be *exactly* zero.). These solutions are inserted in the second equation, and if they solve that equation too, we save the result and plot it.

Of course, we get more solutions than there are in reality, since they all fall within the error interval. Still, one can see the expected behavior, n_0 starting at 1 for $U/J = 0$ (for a vanishing lattice, all particles are in the superfluid state) and then decreasing for higher values of U/J. At $U/J = 26$, however, no further solutions are found at all. This is very close to the expected value of 29, but should not be interpreted as such. The value of n_0 is clearly still very much too large to suggest the transition to the MI state.

For the second order, we also see the qualitatively expected behavior, furthermore the condensate density decreases faster than in the first order, as it should be. Unfortunately, again no phase transition takes place.

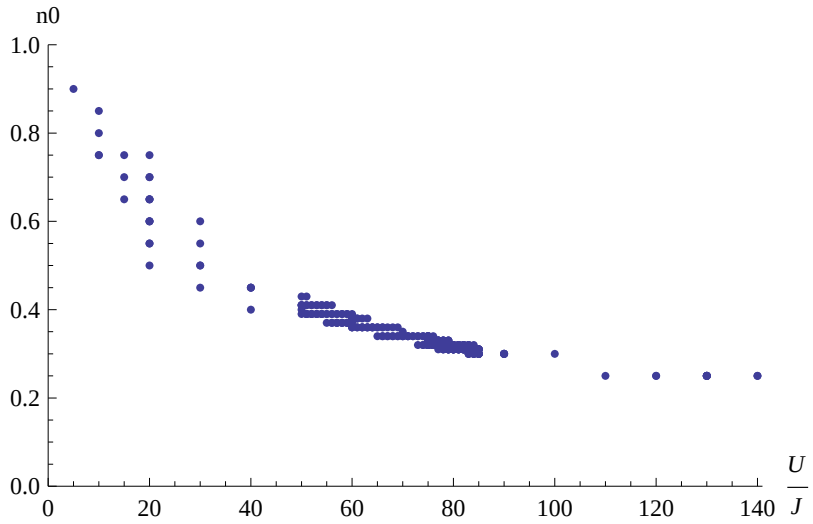


Figure 6.2: Numerical calculations without reinserting for the first and second order.

Chapter 7

Summary and Outlook

"*Study the past, if you would divine the future.*"
Confucius

In this thesis we tried to find the critical value for U/J that takes a BEC in an optical lattice from the superfluid to the Mott-insulator state, which should be revealed as the point where the condensate density goes to zero.

The Bogoliubov transformation was introduced in **chapter 3** in order to describe the BEC in the superfluid state as basically the (classical) ground state plus a small correction. When we were not able to identify a phase transition, we turned to Variational Perturbation theory which was successful in the way that we now had a critical value although its value was much larger than other calculations predicted.

Hoping to refine this result, in **chapter 4** we developed a diagrammatical representation for the second order perturbation, of which we took the zero-temperature limit in **chapter 5** in order to see whether now a phase transition would arise. Unfortunately, this did not happen as we encountered infrared divergencies and we also showed that VPT would not help us this time.

In **chapter 6** we gave a proof that reinserting can never lead to a new solution for one of the two equations. The problem with the divergencies appeared when we reinserted the equations into themselves in order to sort for the orders in the perturbations. Therefore, we took a step back and solved both equations numerically as they originally were. We saw that including the second order in the numerical calculations was indeed an improvement in the way that the condensate density decreases faster than in first order. But unfortunately, in both plots, n_0 still did not reach zero for some U/J.

At this point, we must conclude that including the second order perturbation did not give the result we hoped for. It is questionable whether including even higher orders would lead to a successful outcome. The mathematical effort needed would also increase dramatically, a numerical calculation as we have done will probably not be feasible for the next few years due to the limts of computing power .

With the method of treating the interactions only approximately it seems not possible to get "enough" interaction in order to reach the MI state. Other models should be explored which, for example, treat the interactions exactly but approximate the kinetic energy.

Appendix

"*Computers are useless. They can only give you answers.*"
Pablo Picasso

We used Mathematica to symbolically derive the Effective Potential with respect to n_0 and μ. The second order contributions to each are inserted in the functions f2 and g2, respectively. This is the result as well as the file f.h used later when numerically integrating in C. The naming of the variables and functions should be self-explanatory, expparam standing for U/J, density for n_0 and chempot for μ. We set the density per site as $n = 1$.

```
#define Power(x,y) pow (x,y)

DBL ukvk(DBL fhomega)
 {
  return (0.5*expparam*density/fhomega);
 }

DBL uksquare(DBL fek, DBL fhomega)
 {
 return (0.5*(( fek-6-chempot+2*expparam*density)/fhomega+1));
 }

DBL vksquare(DBL fek, DBL fhomega)
 {
 return (0.5*(( fek-6-chempot+2*expparam*density)/fhomega-1));
 }

DBL f2()
 {
 return (expparam*(-(density*Power(expparam,2)*(-2*chempot + 3*
     density*expparam + 2*fek2))/
       (2.*Power(fhomega2,3)) + expparam/(2.*fhomega2))*
     fukvk1 + 2*expparam*(-(expparam*(-chempot + 2*density*expparam +
         fek2)*
          (-2*chempot + 3*density*expparam + 2*fek2))/(2.*Power(
             fhomega2,3)) +
       expparam/fhomega2)*fvksquare1
```

```
-(density*Power(expparam,2)*(4*(-(expparam*(-chempot + 2*density*
    expparam + fek12)*
              (-2*chempot + 3*density*expparam + 2*fek12))/
            (2.*Power(fhomega12,3)) +
           expparam/fhomega12)*fuksquare1*
         fuksquare2 + 8*(-(density*Power(expparam,2)*
              (-2*chempot + 3*density*expparam + 2*fek12))/
            (2.*Power(fhomega12,3)) +
           expparam/(2.*fhomega12))*fuksquare2*
         fukvk1 - 8*(-(expparam*(-chempot + 2*density*expparam +
            fek12)*
              (-2*chempot + 3*density*expparam + 2*fek12))/
            (2.*Power(fhomega12,3)) +
           expparam/fhomega12)*fuksquare1*
         fukvk2 - 8*(-(expparam*(-chempot + 2*density*expparam +
            fek1)*
              (-2*chempot + 3*density*expparam + 2*fek1))/(2.*
                 Power(fhomega1,3)) +
           expparam/fhomega1)*fuksquare12*
         fukvk2 - 8*(-(density*Power(expparam,2)*
              (-2*chempot + 3*density*expparam + 2*fek12))/
            (2.*Power(fhomega12,3)) +
           expparam/(2.*fhomega12))*fukvk1*
         fukvk2 + 8*(-(density*Power(expparam,2)*
              (-2*chempot + 3*density*expparam + 2*fek1))/(2.*
                 Power(fhomega1,3)) +
           expparam/(2.*fhomega1))*fuksquare2*
         fukvk12 -
        8*(-(density*Power(expparam,2)*(-2*chempot + 3*density*
           expparam + 2*fek2))/
            (2.*Power(fhomega2,3)) + expparam/(2.*fhomega2))*
         fukvk1*fukvk12 +
        16*(-(expparam*(-chempot + 2*density*expparam + fek2)*(-2*
           chempot + 3*density*expparam + 2*fek2))/
            (2.*Power(fhomega2,3)) + expparam/fhomega2)*
         fukvk1*fukvk12 -
        8*(-(density*Power(expparam,2)*(-2*chempot + 3*density*
           expparam + 2*fek1))/
            (2.*Power(fhomega1,3)) + expparam/(2.*fhomega1))*
         fukvk2*fukvk12 -
        8*(-(density*Power(expparam,2)*(-2*chempot + 3*density*
           expparam + 2*fek2))/
            (2.*Power(fhomega2,3)) + expparam/(2.*fhomega2))*
         fuksquare12*fvksquare1 +
        4*(-(expparam*(-chempot + 2*density*expparam + fek2)*(-2*
           chempot + 3*density*expparam + 2*fek2))/
            (2.*Power(fhomega2,3)) + expparam/fhomega2)*
```

```
        fuksquare12*fvksquare1 -
       8*(-(expparam*(-chempot + 2*density*expparam + fek12)*
             (-2*chempot + 3*density*expparam + 2*fek12))/
         (2.*Power(fhomega12,3)) +
        expparam/fhomega12)*fukvk2*
       fvksquare1 + 4*(-(expparam*(-chempot + 2*density*expparam
         + fek1)*
             (-2*chempot + 3*density*expparam + 2*fek1))/(2.*
               Power(fhomega1,3)) +
        expparam/fhomega1)*fuksquare12*
       fvksquare2 + 8*(-(density*Power(expparam,2)*
             (-2*chempot + 3*density*expparam + 2*fek12))/
         (2.*Power(fhomega12,3)) +
        expparam/(2.*fhomega12))*fukvk1*
       fvksquare2 + 8*(-(density*Power(expparam,2)*
             (-2*chempot + 3*density*expparam + 2*fek1))/(2.*
               Power(fhomega1,3)) +
        expparam/(2.*fhomega1))*fukvk12*
       fvksquare2 + 4*(-(expparam*
             (-chempot + 2*density*expparam + fek12)*
             (-2*chempot + 3*density*expparam + 2*fek12))/
         (2.*Power(fhomega12,3)) +
        expparam/fhomega12)*fvksquare1*
       fvksquare2 - 8*(-(density*Power(expparam,2)*
             (-2*chempot + 3*density*expparam + 2*fek2))/(2.*
               Power(fhomega2,3)) +
        expparam/(2.*fhomega2))*fuksquare1*
       fvksquare12 +
       4*(-(expparam*(-chempot + 2*density*expparam + fek2)*(-2*
         chempot + 3*density*expparam + 2*fek2))/
          (2.*Power(fhomega2,3)) + expparam/fhomega2)*
       fuksquare1*fvksquare12 +
       4*(-(expparam*(-chempot + 2*density*expparam + fek1)*(-2*
         chempot + 3*density*expparam + 2*fek1))/
          (2.*Power(fhomega1,3)) + expparam/fhomega1)*
       fuksquare2*fvksquare12 -
       8*(-(expparam*(-chempot + 2*density*expparam + fek1)*(-2*
         chempot + 3*density*expparam + 2*fek1))/
          (2.*Power(fhomega1,3)) + expparam/fhomega1)*
       fukvk2*fvksquare12))/
  (2.*(fhomega1 + fhomega2 +
      fhomega12)) +
 (density*Power(expparam,2)*((expparam*(-2*chempot + 3*density*
     expparam + 2*fek1))/
      fhomega1 + (expparam*(-2*chempot + 3*density*expparam + 2*
         fek2))/
      fhomega2 + (expparam*(-2*chempot + 3*density*expparam + 2*
```

```
            fek12))/
          fhomega12)*
       (8*fuksquare2*fukvk1*
          fukvk12 -
         8*fukvk1*fukvk2*
          fukvk12 -
         8*fuksquare12*fukvk2*
          fvksquare1 + 8*fukvk1*
          fukvk12*fvksquare2 +
         4*fuksquare12*fvksquare1*
          fvksquare2 + 4*fuksquare1*fuksquare2*
          fvksquare12 -
         8*fuksquare1*fukvk2*
          fvksquare12))/
    (2.*Power(fhomega1 + fhomega2 +
         fhomega12,2)) -
   (Power(expparam,2)*(8*fuksquare2*fukvk1*
          fukvk12 -
         8*fukvk1*fukvk2*
          fukvk12 -
         8*fuksquare12*fukvk2*
          fvksquare1 + 8*fukvk1*
          fukvk12*fvksquare2 +
         4*fuksquare12*fvksquare1*
          fvksquare2 + 4*fuksquare1*fuksquare2*
          fvksquare12 -
         8*fuksquare1*fukvk2*
          fvksquare12))/
    (2.*(fhomega1 + fhomega2 +
         fhomega12)));
 }


DBL g2()
 {
 return ((density*Power(expparam,2)*(-chempot + 2*density*expparam +
      fek2)*fukvk1)/
    (2.*Power(fhomega2,3)) +
   2*expparam*(Power(-chempot + 2*density*expparam + fek2,2)/(2.*
       Power(fhomega2,3)) -
       1/(2.*fhomega2))*fvksquare1
 +
 (density*Power(expparam,2)*(4*(Power(-chempot + 2*density*expparam
    + fek12,2)/
             (2.*Power(fhomega12,3)) -
            1/(2.*fhomega12))*fuksquare1*
          fuksquare2 + (4*density*expparam*
```

```
    (-chempot + 2*density*expparam + fek12)*fuksquare2*
    fukvk1)/Power(fhomega12,3) -
8*(Power(-chempot + 2*density*expparam + fek12,2)/
     (2.*Power(fhomega12,3)) -
    1/(2.*fhomega12))*fuksquare1*
 fukvk2 - 8*(Power(-chempot + 2*density*expparam + fek1,2)/
     (2.*Power(fhomega1,3)) - 1/(2.*fhomega1))*
 fuksquare12*fukvk2 -
(4*density*expparam*(-chempot + 2*density*expparam + fek12)*
    fukvk1*
    fukvk2)/Power(fhomega12,3) +
(4*density*expparam*(-chempot + 2*density*expparam + fek1)*
    fuksquare2*
    fukvk12)/Power(fhomega1,3) +
16*(Power(-chempot + 2*density*expparam + fek2,2)/(2.*Power(
    fhomega2,3)) -
    1/(2.*fhomega2))*fukvk1*
 fukvk12 -
(4*density*expparam*(-chempot + 2*density*expparam + fek2)*
    fukvk1*
    fukvk12)/Power(fhomega2,3) -
(4*density*expparam*(-chempot + 2*density*expparam + fek1)*
    fukvk2*
    fukvk12)/Power(fhomega1,3) +
4*(Power(-chempot + 2*density*expparam + fek2,2)/(2.*Power(
    fhomega2,3)) -
    1/(2.*fhomega2))*fuksquare12*
 fvksquare1 - (4*density*expparam*(-chempot + 2*density*
     expparam + fek2)*
    fuksquare12*fvksquare1)/
 Power(fhomega2,3) -
8*(Power(-chempot + 2*density*expparam + fek12,2)/
     (2.*Power(fhomega12,3)) -
    1/(2.*fhomega12))*fukvk2*
 fvksquare1 + 4*(Power(-chempot + 2*density*expparam + fek1
     ,2)/
     (2.*Power(fhomega1,3)) - 1/(2.*fhomega1))*
 fuksquare12*fvksquare2 +
(4*density*expparam*(-chempot + 2*density*expparam + fek12)*
    fukvk1*
    fvksquare2)/Power(fhomega12,3) +
(4*density*expparam*(-chempot + 2*density*expparam + fek1)*
    fukvk12*
    fvksquare2)/Power(fhomega1,3) +
4*(Power(-chempot + 2*density*expparam + fek12,2)/
     (2.*Power(fhomega12,3)) -
    1/(2.*fhomega12))*fvksquare1*
```

```
          fvksquare2 + 4*(Power(-chempot + 2*density*expparam + fek2
              ,2)/
             (2.*Power(fhomega2,3)) - 1/(2.*fhomega2))*
          fuksquare1*fvksquare12 -
         (4*density*expparam*(-chempot + 2*density*expparam + fek2)*
            fuksquare1*
            fvksquare12)/Power(fhomega2,3) +
         4*(Power(-chempot + 2*density*expparam + fek1,2)/(2.*Power(
            fhomega1,3)) -
            1/(2.*fhomega1))*fuksquare2*
          fvksquare12 -
         8*(Power(-chempot + 2*density*expparam + fek1,2)/(2.*Power(
            fhomega1,3)) -
            1/(2.*fhomega1))*fukvk2*
          fvksquare12))/
     (2.*(fhomega1 + fhomega2 +
         fhomega12)) -
    (density*Power(expparam,2)*(-((-chempot + 2*density*expparam +
       fek1)/fhomega1) -
         (-chempot + 2*density*expparam + fek2)/fhomega2 -
         (-chempot + 2*density*expparam + fek12)/fhomega12)
        *(8*fuksquare2*fukvk1*
          fukvk12 -
         8*fukvk1*fukvk2*
          fukvk12 -
         8*fuksquare12*fukvk2*
          fvksquare1 + 8*fukvk1*
          fukvk12*fvksquare2 +
         4*fuksquare12*fvksquare1*
          fvksquare2 + 4*fuksquare1*fuksquare2*
          fvksquare12 -
         8*fuksquare1*fukvk2*
          fvksquare12))/
     (2.*Power(fhomega1 + fhomega2 +
         fhomega12,2)));
}
```

This is the program used for the simultaneous solving of two coupled implicit equations. It is written in the C programming language.

```
#include <stdio.h>
#include <math.h>

typedef int             INT;
typedef double          DBL;
#define pi 3.14159
#define n 1         // one particle per site
```

```
#define NEQ 7   // number of intervals per dimension, 13 for the
    first order

DBL expparam, density, chempot;  // U/J, n_0, chemical potential
DBL _eq[NEQ+1][NEQ+1][NEQ+1];   // all possible values for eq are
    evulated beforehand to save computing time
DBL fek1, fek2, fek12, fhomega1, fhomega2, fhomega12, fukvk1, fukvk2
    , fukvk12, fuksquare1, fuksquare2, fuksquare12, fvksquare1,
    fvksquare2, fvksquare12;

DBL eq (DBL q1, DBL q2, DBL q3)
 {
 return (-2.0 * cos (2.0 * pi * q1) -2.0 * cos (2.0 * pi * q2) -2.0
    * cos (2.0 * pi * q3));
 }

DBL homega (DBL feq)
 {
 return (sqrt (pow (feq - chempot + expparam * density, 2) + 2.0 *
    expparam * density * (feq - chempot + expparam * density)));
 }

#include "f.h" // the second order terms

DBL f (INT n1, INT n2, INT n3)          // integrand for the first
    order of the
 {
 DBL r, feq = _eq[n1][n2][n3];
 DBL fhomega = homega (feq);

 r = (2.0 * feq - 2.0 * chempot + 3.0 * expparam * density) / (2.0 *
     fhomega) - 1.0;
// printf ("%f %f %f %f\n", n1, n2, n3, r);     This is for testing
    purposes.
 return (r);
 }

DBL g (INT n1, INT n2, INT n3)          // integrand for the first
    order of the
 {
 DBL r, feq = _eq[n1][n2][n3];
 DBL fhomega = homega (feq);

 r = (feq - chempot + 2.0 * expparam * density) / fhomega - 1.0;
// printf ("%f %f %f %f\n", n1, n2, n3, r);
 return (r);
```

```
 }

DBL numitg (DBL f())     // numerical integral for a function with
    three variables, e.g. for the first order
 {
 DBL dq, z0, z1, z2, z3, z4, z5, z6, z7, max, min, u = 0.0, o = 0.0;
 INT n1, n2, n3;


 dq = 1.0 / NEQ;    // step lenght

 for (n1 = 0; n1 < NEQ; ++n1)
  for (n2 = 0; n2 < NEQ; ++n2)
   for (n3 = 0; n3 < NEQ; ++n3)
    {
    z0 = f (n1,     n2,     n3);
    z1 = f (n1,     n2,     n3 + 1);
    z2 = f (n1,     n2 + 1, n3);
    z3 = f (n1,     n2 + 1, n3 + 1);
    z4 = f (n1 + 1, n2,     n3);
    z5 = f (n1 + 1, n2,     n3 + 1);
    z6 = f (n1 + 1, n2 + 1, n3);
    z7 = f (n1 + 1, n2 + 1, n3 + 1);

    max = z0; min = z0;
    if (z1 > max) max = z1; if (z1 < min) min = z1;
    if (z2 > max) max = z2; if (z2 < min) min = z2;
    if (z3 > max) max = z3; if (z3 < min) min = z3;
    if (z4 > max) max = z4; if (z4 < min) min = z4;
    if (z5 > max) max = z5; if (z5 < min) min = z5;
    if (z6 > max) max = z6; if (z6 < min) min = z6;
    if (z7 > max) max = z7; if (z7 < min) min = z7;

    u += min; o += max;
    }
 return ((u + o) * dq * dq * dq / 2.0);      // Mittelwert von Ober-
     und Untersumme
 }

DBL numitg6 (DBL f())  //numerical integral for a function with six
    variables, e.g. for the second order
 {
 DBL dq = 1.0 / NEQ, z, max, min, u = 0.0, o = 0.0;
 INT n1x, n1y, n1z, n2x, n2y, n2z;
 INT k1x, k1y, k1z, k2x, k2y, k2z;

 for (n1x = 0; n1x < NEQ; ++n1x)
```

```
  for (n1y = 0; n1y < NEQ; ++n1y)
   for (n1z = 0; n1z < NEQ; ++n1z)
    for (n2x = 0; n2x < NEQ; ++n2x)
     for (n2y = 0; n2y < NEQ; ++n2y)
      for (n2z = 0; n2z < NEQ; ++n2z)
       {
       if (n1x + n2x >= NEQ) continue;  // wegen k3 = k1 + k2
       if (n1y + n2y >= NEQ) continue;
       if (n1z + n2z >= NEQ) continue;
       max = -999.9; min = 999.9;
       for (k1x = n1x; k1x <= n1x + 1; ++k1x)
        for (k1y = n1y; k1y <= n1y + 1; ++k1y)
         for (k1z = n1z; k1z <= n1z + 1; ++k1z)
          for (k2x = n2x; k2x <= n2x + 1; ++k2x)
           for (k2y = n2y; k2y <= n2y + 1; ++k2y)
            for (k2z = n2z; k2z <= n2z + 1; ++k2z)
             {
             //here, all possible function values are calculated
                before f is called

             fek1 = _eq[k1x][k1y][k1z];
             fek2 = _eq[k2x][k2y][k2z];
             fek12 = _eq[k1x+k2x][k1y+k2y][k1z+k2z];
             fhomega1 = homega (fek1);
             fhomega2 = homega (fek2);
             fhomega12 = homega (fek12);
             fukvk1 = ukvk (fhomega1);
             fukvk2 = ukvk (fhomega2);
             fukvk12 = ukvk (fhomega12);
             fuksquare1 = uksquare (fek1, fhomega1);
             fuksquare2 = uksquare (fek2, fhomega2);
             fuksquare12 = uksquare (fek12, fhomega12);
             fvksquare1 = vksquare (fek1, fhomega1);
             fvksquare2 = vksquare (fek2, fhomega2);
             fvksquare12 = vksquare (fek12, fhomega12);
             z = f ();
             if (z > max) max = z; if (z < min) min = z;
             }
       u += min; o += max;
       }

 return ((u + o) * pow (dq, 6) / 2.0);
 }

DBL impf ()          // the complete implicit function for the
   derivation with respect to n_0
 {
```

```
 DBL r;

 r = -6.0 - chempot + expparam * density + expparam * numitg (f) +
    numitg6 (f2);  //for calculating only up to first order, delete
    + numitg6(f2)
 return (r);
 }

DBL impg ()     // the complete implicit function for the particle
   density
 {
 DBL r;

 r = -n + density + 0.5 * numitg (g) + numitg6(g2);    //for
    calculating only up to first order, delete + numitg6(g2)
 return (r);
 }


calceq ()   // here, all the values for eq are calculated and saved
 {
 INT n1, n2, n3;

 for (n1 = 0; n1 <= NEQ; ++n1)
  for (n2 = 0; n2 <= NEQ; ++n2)
   for (n3 = 0; n3 <= NEQ; ++n3)
    _eq[n1][n2][n3] = eq ((DBL) n1 / NEQ - 0.5, (DBL) n2 / NEQ -
       0.5, (DBL) n3 / NEQ - 0.5);
 }




#define EPSF 0.5  // the allowed error interval in which we taka
   solutions as zero
#define EPSG 0.3

main (INT argc, STR argv[])     // when executing, it is necessary
   to specify the output file, e.g. .... > out.txt
 {
 DBL rf, rg;

 calceq ();

 printf ("expparam  density  chempot     rf        rg\n");
 fprintf (stderr, "expparam  density  chempot     rf        rg\n");
 for (expparam = 75.00; expparam <= 140.0; expparam += 1.000)
```

```
    // the chosen range for our variables
  {
  for (density = 0.20; density <= 0.95; density += 0.01)
   {
   for (chempot = 6.0; chempot <= 20.0; chempot += 0.1)
    {
    fprintf (stderr, "%f %f %f\r", expparam, density, chempot);
       fflush (stderr);
    rg = impg ();
    if (rg >= -EPSG && rg <= EPSG)            // only if g is within
       its error intervall,there can be a solution
     {
     rf = impf ();
     if (rf >= -EPSF && rf <= EPSF)  // only if both functions are
        within their error intervall, we assume a solution
      {
      printf ("%f %f %f %f %f\n", expparam, density, chempot, rf, rg
         ); fflush (stdout); //output monitor
      fprintf (stderr, "%f %f %f %f %f\n", expparam, density,
         chempot, rf, rg); fflush (stderr);   //output file
      }
     }
    }
   }
  }
}
```

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"*The secret to creativity is knowing how to hide your sources.* "

Albert Einstein

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"*The one exclusive sign of a thorough knowledge is the power of teaching.*"
Aristotle

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"*My pen is at the bottom of a page,*
Which being finished, here the story ends;
'Tis to be wish'd it had been sooner done,
But stories somehow lengthen when begun."
Lord Byron

Erklärung

Hiermit versichere ich, dass ich die vorliegende Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe, dass alle Stellen der Arbeit, die wörtlich oder sinngemäß aus anderen Quellen übernommen wurden, als solche kenntlich gemacht sind und dass die Arbeit in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegt wurde.

Berlin, den 30.05.2012 Pascal Mattern