# Fluctuational Effects in Interacting Bosonic Systems

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# **Thesis Abstract**

This thesis consists of two projects which are seemingly disconnected, yet closely related. The first part explores the effects of Bose-Einstein condensation at temperatures close to, but slightly above, criticality. Following a general introduction into bosonic condensation we justify why a phenomenological theory, similar to the Ginzburg-Landau theory for fermions, holds for weakly interacting Bose gases. From this theory we predict the divergence of certain observables, in particular the quasi-magnetic susceptibility, and discuss the effects of a trapping potential.

The divergence of the magnetic susceptibility motivates the introduction of an original scheme in order to measure it, published in *Phys. Rev. A 93, 041602(R)*. The scheme uses modulated laser fields to create well-controlled gradients of artificial magnetic fields. In addition we discuss how rotational schemes might be helpful in detecting different quantum phases by exploiting different signatures in their moments of inertia.

The second part investigates binary mixtures in one dimension. We show that in certain limits such systems behave like two simply coupled Luttinger liquids, which effectively describe polaronic modes. We study and calculate explicitly how an impurity immersed in the one dimensional system creates two depletion clouds and a phase drop in each of the liquids. After arguing that these clouds and phase drops necessitate a coupling of the impurity to the low-lying excitation modes of the Luttinger liquids, we derive the edge-state singularities of the bosonic and fermionic dynamical structure factors which depend on the coupling between the liquids.

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This thesis is dedicated to my parents and my grandfather.

# **Publications**

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### Chapter 1

# Overview

Condensation of quantum particles is hardly a new concept. Already in 1925, after having been inspired by Bose's ideas [1] about the importance of quantum statistical physics and its deviation from classical statistical physics, Einstein predicted the possibility of the condensation of matter below a critical temperature [2].

Though a simple and very elegant concept, direct experimental verification of bosonic condensation remained elusive for almost seventy years. However, the concept of bosonic condensation has been used with varying degrees of success to explain interesting experimental facts. Superconductivity, which has been observed only fourteen years earlier by Kamerlingh Onnes in pure mercury at a temperature of 4.2 K, seemed to share some of the properties expected in a Bose-Einstein-Condensate (BEC), for instance the low but finite critical temperature. Though Fritz London [3] tried to explain superconductivity as well as the recently discovered superfluidity of helium-4 [4, 5] in terms of BECs, doubts about the exact nature of these condensates remained. Conventional superconductivity was later explained with an alternative microscopic theory in which electrons of opposite spin couple to form states that can be interpreted as composite bosons in 1957 [6]. Superfluid helium-4 on the other hand shows some characteristics that were not expected from Einstein's theory, such as the fact that only a fraction of particles show superfluid behaviour, even at absolute zero.

The final experimental verification came only in 1995 when Bose-Einstein-Condensation in cold gases was achieved and tell-take BEC signatures were found [7, 8]. Finally scientists have the means to clearly distinguish bosonic and fermionic superfluidity, which opens up a whole new field of investigation, as properties that are

found in superconducting fermionic systems, for instance magnetic flux quantisation [9], can be observed in purely bosonic condensates as well [10].

A large and interesting class of such fermionic phenomena are fluctuational effects, where superconducting signatures can be observed slightly above the critical temperature as well as significant fluctuational corrections to condensates below the critical temperature. The first estimation of such effects were done by Ginzburg [11] and he deemed them unlikely ever to be observed. However shortly afterwards, in 1967, Glover found strange signatures in the resistivity of amorphous bismuth films [12]. Very quickly it was realized that the fluctuational contributions that according to Ginzburg were supposed to be small could become quite considerable in size if the geometry of the system changes, for instance in thin wires, or the systems themselves are disordered [13, 14, 15]. These new theories fit the experiments very well.

The next logical step was to ask the question, whether or not such behaviour persists in bosonic systems and how it can be addressed experimentally. Not only was this motivated by pure academic curiosity, but recent experimental innovations allow for a careful examination of close-to-criticality behaviour [16]. This is where this thesis starts. In chapter 2 we describe a general framework to describe weakly interacting bosonic systems in equilibrium and some aspects of out-of-equilibrium behaviour. We proceed in chapter 3 to apply this framework to the question of close-to-criticality fluctuations. We show that they exist and that their magnitude should be larger than in conventional superconducting systems. Also we show that the trap that holds the cold atoms is instrumental in determining the actual properties of the fluctuational observables and therefore cannot be neglected. Further we establish an equivalence between bosonic and fermionic fluctuational effects by exploiting the BCS-BEC crossover. However, we were unaware that such a connection has been made before us [17]. We still went a little further and considered how trap rotations can be used to explicitly find fluctuational observables. We constructed a scheme that creates gradients in artificial magnetic fields using space-dependent angular momentum imprintment. Such schemes can also be used for purposes other than the detection of fluctuational properties. We also suggest how rotational schemes might be used to find other, even more elusive transitions, such as the superfluid-Bose glass transition. Possibly helpful in characterizing the different phases will be the quantum version of Steiner's theorem in classical mechanics, which we derived at the end of chapter 3.

The study of the relationship between bosons and fermions did not always proceed along the lines of con-

densates though. It turns out that in the system where no bosonic condensation is possible, namely in one dimension, spin-free fermions and interacting bosons are practically identical, at least at low energies. The first half of this insight came first from Tomanaga [18] and later independently from Luttinger [19]. They found that the excitations of interacting fermions can be mapped onto non-interacting phononic excitations. This also means that in one dimension, even interacting fermionic systems can be solved exactly. At about the same time Lieb and Liniger showed that also interacting one-dimensional Bose systems can be solved using a Bethe-like ansatz [20]. In the limit of very strong repulsive bosons, their solution mimicked the non-interacting fermion physics. It still took a couple of years until these two ideas were formally combined by Haldane into the framework of Luttinger liquids [21]. In the same article he also argued that the low energy boson theory and the low energy fermion theory obey the same universal action.

This formal equivalence of the two systems, as well as their similar mathematical make-up, invites the study of their mixtures in one dimension. It was soon found that there exist regions in parameter space where such mixtures are stable [22] and can be described as mixtures of polaronic modes [23]. This motivated us to study effects where remnants of the somewhat contrary nature of bosons and fermions persist even in one dimension, the edge-state singularities [24, 25]. In chapter four we first rederive the effective Hamiltonian of the mixture. Because we want to study some higher-energy effects, it becomes necessary to study the mobile impurities that are created with higher energies than the polaronic modes that couple with them. Because these impurities are coupled to two Luttinger liquids, their thermodynamic characteristics are slightly altered, which we calculate explicitly. Afterwards we show that under fairly general conditions the intrinsic differences between the bosonic and fermionic nature leads to a suppression of the edge-state singularities, for fermionically as well as bosonically excited systems. Quite generally the most stable (long-range) modes of the respective unperturbed Luttinger liquids couple to unstable modes in the opposite liquid if interactions are turned on. We then draw parallels to the X-ray absorption edge singularity in transition metals that help build a more intuitive understanding of these effects.

### Chapter 2

# An Introduction to Bose-Einstein Condensation

### 2.1 Bosonic fields

This thesis focusses on properties of bosons close to or in the condensed phase. We think it is in order to give a general introduction to bosonic condensation for weakly interacting dilute bosonic gases.

There are many different ways of defining Bose condensation, whether it is via a macroscopic occupation of a state or long range coherences [2, 26, 27]. We focus first on the field theoretic description by Popov [28] and others [29, 30, 31, 32, 26, 33, 34] that leads up to the conventional properties. Only after having identified the bosonic condensation as a significant effect, we will reverse the direction and start from an operator picture that leads us, via the introduction of coherent states, to the original bosonic field representation and closes the circle.

In this description the many-particle system, here a dilute interacting gas of bosonic particles with integer spin [35, 36], is described by complex fields  $\psi(\mathbf{x}, \tau)$  in imaginary time  $\tau$  that exist on some spatial support  $\mathbf{x} \in V \subset \mathbb{R}^d$  in *d*-dimensional space, which for the most part of the thesis will be three-dimensional. The imaginary time  $0 \le \tau \le \frac{1}{T} = \beta$  is used to describe the effects of temperature. This of course means that For now we are only interested in the uniform three-dimensional system, so we specify the gas to be in a cube of volume  $V = L^3$ . Under periodic boundary conditions, which in the thermodynamic limit and the systems we study does not affect the bulk properties of the gas, the fields are described in terms of their Fourier coefficients  $a(\mathbf{k}, \omega)$ ,  $a^*(\mathbf{k}, \omega)$ 

$$\Psi(\mathbf{x},\tau) = \frac{1}{\sqrt{\beta L^3}} \sum_{\mathbf{k},\omega} e^{i(\omega\tau + \mathbf{k}x)} a(\mathbf{k},\omega)$$

$$\bar{\Psi}(\mathbf{x},\tau) = \frac{1}{\sqrt{\beta L^3}} \sum_{\mathbf{k},\omega} e^{-i(\omega\tau + \mathbf{k}x)} a^*(\mathbf{k},\omega).$$
(2.1)

The arguments of the Fourier coefficients are quantized as  $\omega_n = 2\pi nT$  and  $k_{i,n} = 2\pi n/L$ , where i = x, y, z and the *n* are integers. The quantization of the imaginary time in such a way follows from the bosonic requirement that  $\psi(\mathbf{x}, \tau) = \psi(\mathbf{x}, \tau + \beta)$ . The thermal action that contains an (imaginary) time evolution is introduced as

$$S = \int_{0}^{\beta} d\tau \int d\mathbf{x} \bar{\psi}(\mathbf{x}, \tau) \partial_{\tau} \psi(\mathbf{x}, \tau) - \int_{0}^{\beta} H(\tau) d\tau.$$
(2.2)

The functional *H* is the integral over the Hamiltonian density. For the system we wish to describe, it contains the kinetic energy, a term that controls the number of particles via the chemical potential  $\mu$ , and a pair interaction potential  $u(\mathbf{x})$ , which describes a general instantaneous interaction between two particles

$$H = \int d\mathbf{x} \left( \frac{1}{2m} \nabla \bar{\psi}(\mathbf{x}, \tau) \nabla \psi(\mathbf{x}, \tau) - \mu \bar{\psi}(\mathbf{x}, \tau) \psi(\mathbf{x}, \tau) \right)$$
  
+ 
$$\int d\mathbf{x} d\mathbf{y} u(\mathbf{x} - \mathbf{y}) \bar{\psi}(\mathbf{x}, \tau) \bar{\psi}(\mathbf{y}, \tau) \psi(\mathbf{y}, \tau) \psi(\mathbf{x}, \tau).$$
(2.3)

This action can be partially diagonalized by transforming the interaction potential, alongside the operators, into Fourier space

$$u(\mathbf{x}) = \frac{1}{L^3} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{x}} \tilde{u}(\mathbf{k}).$$

Then the action becomes a sum of two terms,  $S = S_0 + S_1$ , the first of which is

$$S_0 = \sum_{\omega_n, \mathbf{k}} \left( i\omega_n - \frac{\mathbf{k}^2}{2m} + \mu \right) a^*(\mathbf{k}, \omega_n) a(\mathbf{k}, \omega_n)$$

and diagonal; the second one is a momentum conserving term

$$S_{1} = -\frac{T}{4V} \sum_{\mathbf{k}_{1} + \mathbf{k}_{2} = \mathbf{k}_{3} + \mathbf{k}_{4}} \left[ \tilde{u} \left( \mathbf{k}_{1} - \mathbf{k}_{3} \right) + \tilde{u} \left( \mathbf{k}_{1} - \mathbf{k}_{4} \right) \right] a^{*} \left( \mathbf{k}_{1} \right) a^{*} \left( \mathbf{k}_{2} \right) a \left( \mathbf{k}_{4} \right) a \left( \mathbf{k}_{3} \right)$$

To make physical predictions, one has to find quantities that are directly related to physical observables, like densities of states or absorbtion properties. In our case this will be the one-particle Green's functions [28]

$$G(\mathbf{x}, au; \mathbf{x}', au') = -\langle \psi(\mathbf{x}, au) \overline{\psi}(\mathbf{x}', au') 
angle.$$

The average  $\langle \dots \rangle$  is the functional average weighted by the exponential of the action

$$\left\langle \psi(\mathbf{x},\tau)\,\bar{\psi}\left(\mathbf{x}',\tau'\right)\right\rangle = rac{\int\mathrm{e}^{S}\psi(\mathbf{x},\tau)\,\bar{\psi}\left(\mathbf{x}',\tau'\right)D\bar{\psi}D\psi}{\int\mathrm{e}^{S}D\bar{\psi}D\psi},$$

where  $D\psi D\bar{\psi}$  is the functional integration measure. Of course, the integration measure can instead be taken over the Fourier coefficients (they are technically coherent state representations). Because of Plancherel's theorem we have that  $D\psi D\bar{\psi} = \prod_p da^*(p) da(p)$ , where p is a composite variable containing **k** and  $\omega$ .

Technically one has to introduce cutoffs,  $\mathbf{k}_0$ ,  $\omega_0$ , as the physical system is naturally bound by a lower length scale. The particle motion can not happen on a subatomic scale, however we do not need to specify the exact cutoff length other than by saying it is some large number. Because the Green's function is defined for a nondriven, uniform system, we can deduce that it is translation-invariant  $G(\mathbf{x}, \tau; \mathbf{x}', \tau') = G(\mathbf{x} + \mathbf{R}, \tau + \tau_0; \mathbf{x}' + \mathbf{R}, \tau' + \tau_0)$ . This of course implies that the Fourier basis as defined above is a good basis as well and that the Green's function itself can best be described by its Fourier transform

$$G_0(p) = -\langle a(p)a^*(p) \rangle$$
  
=  $-\frac{\int \left[e^{S(p)}\prod_p da^*(p)da(p)\right]a(p)a^*(p)}{\int \left[e^{S(p)}\prod_p da^*(p)da(p)\right]}$ 

We note that  $\left[e^{S(p)}\prod_{p} da^{*}(p) da(p)\right]$  is the measure, by which each instance p is weighted.

It is quite instructive to find the behaviour of the free theory, where  $u(\mathbf{k}) = 0$ . To do this we calculate the generating functional  $Z_0(\eta, \eta^*)$  of the free theory, from which we infer the correlator  $G_0(p)$ . At this point we need Gaussian integrals, of which a short summary can be found in the appendix 5.1.

The full generator after integration is thus given by

$$Z_0\left([\eta,\eta^*]\right) = \exp\left[-\sum_p \eta^*(p)\left(i\omega - \frac{\mathbf{k}^2}{2m} + \mu\right)^{-1}\eta(p)\right].$$

Using that gives

$$G_o(p,p') = -\frac{\partial^2}{\partial \eta(p)\partial \eta^*(p')} Z_0\left([\eta(p),\eta^*(p)]\right) = \delta_{p,p'} \frac{1}{\left(i\omega_n - \frac{\mathbf{k}^2}{2m} + \mu\right)}.$$

Taking higher derivatives allows us to get all higher moments of the theory

$$\left\langle \prod_{i=1}^{n} a(p_i) \prod_{j=1}^{n'} a^*(p_j) \right\rangle_0 = \frac{\partial^{n+n'}}{\prod_{i=1}^{n} \partial \eta(p_i) \prod_{j=1}^{n'} \partial \eta^*(p_j)} Z_0\left( [\eta(p), \eta^*(p)] \right).$$

The result is the famous Wick's theorem, which states that for a quadratic theory the higher moment average is just the sum over all possible decompositions of the set  $[p_{i,j}]$  into pairs  $\langle a(p)a^*(p)\rangle$ . In order for the average not to vanish, n = n'. As a simple example one can take the four point average

$$\langle a(p_1)a(p_2)a^*(p_3)a^*(p_4)\rangle_0 = \langle a(p_1)a^*(p_3)\rangle_0 \langle a(p_2)a^*(p_4)\rangle_0 + \langle a(p_1)a^*(p_4)\rangle_0 \langle a(p_2)a^*(p_3)\rangle_0 \langle a(p_2)a^*(p_3)\rangle_0 \langle a(p_2)a^*(p_4)\rangle_0 + \langle a(p_1)a^*(p_4)\rangle_0 \langle a(p_2)a^*(p_4)\rangle_0 + \langle a(p_1)a^*(p_2)\rangle_0 + \langle a(p_1)a^*(p_2)\rangle_0 + \langle a(p_1)a^*(p_2)\rangle_0 + \langle a(p_1)a^*(p_2)\rangle_0 + \langle$$

We want to see how the particle density and the occupations of the individual  $\mathbf{k}$  modes depend on tempera-

ture. Using again the property of translation invariance, we have that for the total particle number N

$$N = \left\langle \int d\mathbf{x} \bar{\psi}(\mathbf{x}, \tau) \psi(\mathbf{x}, \tau) \right\rangle = L^3 \lim_{\mathbf{x} \to \mathbf{x}', \tau \to \tau'} \left\langle \psi(\mathbf{x}, \tau) \bar{\psi}(\mathbf{x}', \tau') \right\rangle.$$

We can express the average by the free Green's functions

$$\langle \psi(\mathbf{x},\tau) \,\overline{\psi}(\mathbf{x}',\tau') \rangle = -\frac{1}{\beta L^3} \sum_{\mathbf{k},\omega} \left( i\omega - \frac{\mathbf{k}^2}{2m} + \mu \right)^{-1} \mathrm{e}^{i\omega(\tau-\tau')+i\mathbf{k}(\mathbf{x}-\mathbf{x}')}.$$

In order to obtain the correct average, one has to demand that  $\tau' < \tau$ , which can be interpreted as that the particle density is first created and then annihilated. So we introduce the infinitesimal  $\varepsilon$ , such that  $\tau' + \varepsilon = \tau$ , which we later let go to zero. Evaluating the single particle Green's function at  $\mathbf{x} = \mathbf{x}'$  we can perform the summation over the Matsubara frequencies. A short summary of the technique is found in the appendix. Applying the case of a single pole, we find

$$\frac{1}{\beta}\sum_{\omega_n}\frac{\mathrm{e}^{i\omega\varepsilon}}{i\omega_n-\frac{\mathbf{k}^2}{2m}+\mu}=\frac{\mathrm{e}^{\varepsilon\left(\frac{\mathbf{k}^2}{2m}-\mu\right)}}{\mathrm{e}^{\beta\left(\frac{\mathbf{k}^2}{2m}-\mu\right)}-1}\to_{\varepsilon\to0}\frac{1}{\mathrm{e}^{\beta\left(\frac{\mathbf{k}^2}{2m}-\mu\right)}-1}$$

Or, for the total particle number,

$$N = \sum_{\mathbf{k}} n_{\mathbf{k}} = \sum_{\mathbf{k}} \frac{1}{\mathrm{e}^{\beta(e(\mathbf{k}) - \mu)} - 1},$$

where  $e(\mathbf{k}) = |\mathbf{k}|^2 / 2m$  is the free particle energy dispersion relation.

Retracing the calculation it is clear that the exact relation between energy e and  $\mathbf{k}$  did not matter. For any bosonic system that can be diagonalized for some states  $\{\lambda\}$ , one finds that the density of particles in the state  $\lambda$  is

$$n_{\lambda} = \frac{1}{\mathrm{e}^{\beta(\varepsilon_{\lambda}-\mu)}-1},$$

and the total particle number to be

$$N=\sum_{\lambda}n_{\lambda}.$$

The function  $n_{\lambda}$  is the Bose function and it is responsible for a whole plethora of interesting properties starting with condensation.

### 2.2 Bose condensation

Now that we know how the particles occupy the energy eigenstates in thermodynamic equilibrium, it is worthwhile to study those occupations a little further. The denominator in the Bose function

$$f_B = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}-1}$$

can in principle become arbitrarily small due to the -1. This should be compared to the Fermi distribution

$$f_F = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}+1},$$

where the occupation is limited to a number between 0 and 1.

In order to avoid an ill defined Bose function, the chemical potential  $\mu$  must be smaller than the smallest energy  $\varepsilon_0$ . However one can see that the Bose nature allows for multiple occupations of the lowest energy state, in fact, favors it for low temperatures. A natural question to ask is whether the occupation of a single or a few states can be so large compared to the others, that the physical behaviour is dominated by one state, or a small set of neighboring states.

To answer this, let us isolate that single state and observe how its occupancy compares with the rest of the particles. We assume a system with a finite number of particles. However, all states besides the ground state are supposed to be continuously distributed. Rather than looking at a specific system, we characterize a system by the way its density of states  $\rho(\varepsilon)$  changes when the energy is varied. We define the energetic dimension  $d_{\varepsilon}$  as

$$\rho\left(\varepsilon\right)\sim\varepsilon^{d_{\varepsilon}-1}.$$

It should be noted, that the energetic dimension does not have to be integer. In fact, it allows us to compare harmonically trapped systems (generally integer  $d_{\varepsilon}$ ) and uniform systems (generally  $d_{\varepsilon}$  is a multiple of  $\frac{1}{2}$ ) and their combinations in the same picture. The prefactor can be determined by a specific case and generalized.

Take the three-dimensional harmonic oscillator with

$$\varepsilon_n = \hbar \omega_0 \left[ (n_x + n_y + n_z) + 3/2 \right].$$

The number of states Z(E) with an energy less than E can be found as

$$Z(E) = \frac{1}{(\hbar\omega_0)^3} \int_0^E dE_x \int_0^{E-E_x} dE_y \int_0^{E-E_x-E_y} dE_z = \frac{E^3}{6(\hbar\omega_0)^3}$$

(It follows from the quantization of the spectrum that a state essentially occupies the volume  $(\hbar\omega_0)^3$ ).

This generalizes for higher dimensions (real ones) to

$$Z(E) = \frac{E^d}{d! \left(\hbar \omega_0\right)^d}.$$

For the density of states this gives

$$\rho(E) = \frac{dZ(E)}{dE} = \frac{E^{d-1}}{(d-1)! (\hbar \omega_0)^d}.$$

Note that even in the uniform case, one can find the equivalent of the oscillator strength  $(\hbar \omega_0 = 2\pi \hbar^2 / m L_{x,y,z}^2)$ . If the system consists of *k* different frequencies  $\omega_i$ , then  $\omega_0$  will be the geometric mean of the constituent frequencies,  $\omega_0 = (\prod \omega_i)^{1/k}$ . On the other hand the (d-1)! can be extended to the Gamma function  $\Gamma(d_{\varepsilon}-1)$ , which is also defined for non-integer arguments (it is only non-defined for negative integers)

$$\Gamma(z) = \int_0^\infty x^{z-1} \mathrm{e}^{-x} dx.$$

Let us decompose the total number of particles into the ground state number of particles  $N_0$  and the thermal component  $N_{th}$ 

$$N = N_0 + N_{th}$$

Given a particle number, we have to ask how many particles fit in the thermal states. If all do, then the ground

state occupation will necessarily be small. If however a significant fraction of particles were forced into the ground state because the number of particles in the thermal states was bounded, condensation would occur. The chemical potential would in that case be close to the ground state energy. The number of thermal particles can be calculated as (energies are measured from the ground state)

$$N_{th} = \int_0^\infty \rho(\varepsilon) f_B(\varepsilon) d\varepsilon = \frac{1}{d_{\varepsilon}! (\hbar \omega_0)^{d_{\varepsilon}}} \int_0^\infty \frac{\varepsilon^{d_{\varepsilon}-1}}{e^{\beta \varepsilon} - 1} d\varepsilon = \left(\frac{T}{\hbar \omega_0}\right)^{d_{\varepsilon}} \operatorname{Li}_{d_{\varepsilon}}(1).$$

The function

$$\operatorname{Li}_{d_{\varepsilon}}(z) = \frac{1}{\Gamma(d_{\varepsilon})} \int_{0}^{\infty} \frac{t^{d_{\varepsilon}-1}}{\mathrm{e}^{t}/z - 1} dt$$

is the polylogarithm. The overall behaviour is interesting, as it tells us that the number of particles at a given temperature in the thermal states can be limited for different values of  $d_{\varepsilon}$ . This in turn means that if the total particle number is larger than the number  $\left(\frac{T}{\hbar\omega_0}\right)^{d\varepsilon}$  Li<sub> $d_{\varepsilon}$ </sub>(1), any excess particles occupy the ground state. On the same basis, if the temperature is lowered until the number of occupied states is much smaller than the total particle number, condensation into the ground state occurs. Generally one speaks of a macroscopic occupation if in the thermodynamic limit a finite fraction of the particles occupy that state. The resultant condensate is the so called Bose-Einstein condensate (BEC). The critical point at which this happens is when  $N = N_{th}$  which gives a useful criterion for the critical temperature

$$T_c = \hbar \omega_0 \frac{N^{1/d_{\varepsilon}}}{\left(\mathrm{Li}_{d_{\varepsilon}}(1)\right)^{1/d_{\varepsilon}}}.$$

The function  $\operatorname{Li}_{d_{\varepsilon}}(1)$  equals  $\zeta(d_{\varepsilon})$ , the Riemann-Zeta function  $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$ . The equation fully highlights the impact of the bosonic statistics. Because the number of particles can be very large, the critical temperature can be several orders of magnitude larger than the defining energy scale  $\hbar\omega_0$ , which would be the order of the temperature were condensation-like effects were to occur in a Boltzmann gas. Another way of looking at Bose condensation is to use the de Broglie relation to see the typical wave-length a particle has at temperature *T* 

$$\lambda_B = \left(\frac{2\pi\hbar^2}{mT}\right)^{1/2}$$



Figure 2.1: The inverse polylog  $\text{Li}_x^{-1}(1)$ . It shows that for  $d_{\varepsilon} = 1$ , the critical temperature vanishes.

and compare it to the interparticle distance  $n^{1/d}$ . If they are of the same order, then, so the heuristic explanation goes, the particles cannot be distinguished from each other and form one coherent unit. For a harmonic trap this applies for the de-Broglie wavelength at the center of the trap and inversion for  $T_c$  indeed returns the same scaling. Such condensates have been observed experimentally [7, 8].

Because  $\text{Li}_1(1) = \infty$ , this equations tells us that the critical temperature for  $d_{\varepsilon} = 1$  is zero (see figure 2.1).

This means that a one dimensional harmonically trapped gas or a two dimensional uniform Bose gas could not truly condense at finite temperature and resembles the Wagner-Mermin theorem [37, 38], which states that no continuous symmetry can be spontaneously broken in a uniform system at finite temperature for  $d \le 2$ because long-range fluctuations that can destroy such an order do not cost much energy. At this point it has to be mentioned that lower dimensional phase transitions can still happen, just that they do not exhibit a phase that has a true long range order. In two dimensions these transitions are called Berezinskii-Kosterlitz-Thouless (BKT) transitions [39, 40], where the correlation length switches from polynomial to exponential fall-off at a finite temperature and which have been predicted and observed in a range of systems, such as Josephson junction arrays and granular superconducting systems [41, 42, 43, 44, 45].

We can estimate the number of condensed particles close to the transition. We find that

$$N_c = N - N_{\rm th} = N \left[ 1 - \left( \frac{T}{T_c} \right)^{d_{\varepsilon}} \right], \qquad (2.4)$$

where we used that by substitution for  $T < T_c$ ,  $N_{\rm th} = N \left(T/T_c\right)^{d_{\rm E}}$ .

Here we want to point out that a macroscopic number of particles is in one particular state, so it seems

sensible that they share the same phase. It is this observation of many particles sharing all properties of that state, including the wave function of that state, that characterizes the Bose condensate. Though the wave function itself is not observable, it clearly leads to observable effects, most importantly that it has a phase, whose change over spatial distance costs distortion energy (phase stiffness) that is responsible for many of the phenomena associated with superfluidity.

### 2.3 Second quantization

We started first with a complex field in an action and derived the bosonic occupation statistics. Here we want to go the reverse way and start with an operator formalism that leads to the same occupation statistics and introduce the idea of coherent states. This is useful as it exemplifies the connection between particle number and phase, which is crucial in understanding condensed systems. We want to introduce the famous Bose-Hubbard model and discuss why also this case can be described in the complex field representation provided earlier. In the next section we return to the non-lattice case and describe some of the superfluid properties of bosonic condensates. The ideas in this section follow some of the standard references [46, 47, 26, 45].

One starts with a single lattice site with no further internal structure in which a boson may sit. Such a site can be occupied by any number of non-interacting bosons, including zero bosons. The Hilbert space of that single site is thus spanned by the orthonormal set

$$\left|0
ight
angle,\left|1
ight
angle,\left|2
ight
angle\ldots$$

which extend to infinity. To transition from one state to another one which differs only by one boson, we can define the bosonic creation and annihilation operators  $\hat{a}^{\dagger}$  and  $\hat{a}$  such that

$$\begin{split} \hat{a}^{\dagger} \left| n \right\rangle &= \sqrt{n+1} \left| n+1 \right\rangle, \\ \hat{a} \left| n \right\rangle &= \sqrt{n} \left| n-1 \right\rangle. \end{split}$$

One can clearly see that  $\hat{a}^{\dagger}$  and  $\hat{a}$  do not commute

$$\begin{split} \left[\hat{a}, \hat{a}^{\dagger}\right] \left|n\right\rangle &= \hat{a} \hat{a}^{\dagger} \left|n\right\rangle - \hat{a}^{\dagger} \hat{a} \left|n\right\rangle \\ &= \sqrt{n+1} \hat{a} \left|n+1\right\rangle - \sqrt{n} \hat{a}^{\dagger} \left|n-1\right\rangle \\ &= \left(n+1\right) \left|n\right\rangle - n \left|n\right\rangle = \left|n\right\rangle, \end{split}$$

which means  $[\hat{a}, \hat{a}^{\dagger}] = 1$ . If we extend the number of lattice sites, then the creation/annihilation operators only do not commute on the same site, i.e.

$$[\hat{a}_i, \hat{a}_j] = \begin{bmatrix} \hat{a}_i^{\dagger}, \hat{a}_j^{\dagger} \end{bmatrix} = 0, \quad \begin{bmatrix} \hat{a}_i, \hat{a}_j^{\dagger} \end{bmatrix} = \delta_{ij}.$$

During the extension we also expanded the orthonormal basis of our Hilbert space to include all states with integer number of bosons on each site

$$|\{n_i\}\rangle\equiv\prod_i|n_i\rangle.$$

It is common to call the "empty" state  $|0,0,...\rangle$  the vacuum  $|vac\rangle$ . To obtain a state with arbitrary occupation, we can apply the appropriate number of creation operators to the vaccum

$$|\{n_i\}\rangle = \left(\prod_i \frac{\left(\hat{a}_i^{\dagger}\right)^{n_i}}{\sqrt{n_i!}}\right) |\text{vac}\rangle.$$

A useful operator to determine the number of particles on said lattice site *i* is  $\hat{n}_i \equiv \hat{a}_i^{\dagger} \hat{a}_i$  since

$$\hat{n} |n_i\rangle = n_i |n_i\rangle$$
.

So far we considered only states with a well-defined number of particles, so-called Fock states. However, because these states are part of a Hilbert space, superpositions of Fock-states are allowed physical states. Since we look at material systems in which the number of particles,  $N = \sum_i n_i$ , is generally conserved, we need to take into account a reservoir (as we implicitly did above to define the chemical potential  $\mu$ ), or we have to couple different sites so that the overall number of bosons is conserved while the number of bosons on each site may

be allowed to fluctuate.

The simplest case considers two coupled sites, i = 1, 2, about which N particles are distributed. Since the number of particles is conserved, we can label the Fock states by the difference in their occupation  $n_1 = N/2 + \Delta N$  and  $n_2 = N/2 - \Delta N$ , where for even N,  $\Delta N$  can take the values -N/2, -N/2 + 1, ..., N/2 - 1, N/2and the Fock state simply becomes

$$\left|\Delta N\right\rangle \equiv \frac{\left(\hat{a}_{1}^{\dagger}\right)^{N/2+\Delta N} \left(\hat{a}_{2}^{\dagger}\right)^{N/2-\Delta N}}{\sqrt{\left(N/2+\Delta N\right)! \left(N/2-\Delta N\right)!}} \left|\operatorname{vac}\right\rangle.$$

To better describe such a state, it is convenient to define the operator that measures the difference in occupation between both sites

$$\hat{\Delta N} = \hat{n}_1 - \hat{n}_2 = \hat{a_1}^{\dagger} \hat{a}_1 - \hat{a_2}^{\dagger} \hat{a}_2,$$

for which the difference state is an eigenstate

$$\Delta \hat{N} |\Delta N\rangle = \Delta N |\Delta N\rangle.$$

Whereas in this state really all particle numbers are well defined, one can imagine the opposite case, where each particle itself is in a superposition of both lattice sites, respectively with probability  $p_1$  and  $p_2 = 1 - p_1$ , and an additional phase difference  $\Delta \theta$ , so the total state is

$$|\Delta\theta, p_1, p_2
angle = rac{\left(\sqrt{p_1}\mathrm{e}^{i\Delta\theta/2}\hat{a}_1^{\dagger} + \sqrt{p_2}\mathrm{e}^{-i\Delta\theta/2}\hat{a}_2^{\dagger}
ight)^N}{\sqrt{N!}} |\mathrm{vac}
angle.$$

Since the Fock basis is complete, the state  $|\Delta\theta\rangle$  can be expanded in said basis

$$\left|\Delta\theta\right\rangle = \sum_{\Delta N} \frac{p_1^{(N-\Delta N)/4} p_2^{(N+\Delta N)/4}}{\sqrt{(N/2+\Delta N)! (N/2-\Delta N)!}} e^{i\frac{\Delta N}{2}\Delta\phi} \left|\Delta N\right\rangle.$$

This state is called a relative phase eigenstate, as each particle has a relative phase difference. The occurrence of the term  $e^{i\frac{\Delta N}{2}\Delta\phi}$  already hints at that the states with well defined phase difference are complementary to the states with well defined difference in particle numbers. This is not quite exact, as *N* and therefore the sum

is finite. However when the number of particles is large,  $N \gg 1$ , then it becomes possible to define a phase difference operator [48]

$$\hat{\Delta \theta} \equiv -i \arg \left[ \frac{\hat{a}_1^{\dagger} \hat{a}_2}{\sqrt{(N/2 + \Delta N)! (N/2 - \Delta N)!}} \right],$$

which in the limit of large N approximately satisfies a Heisenberg relation as typical for conjugate variables

$$\left[\hat{\Delta N}, \hat{\Delta \theta}\right] = -2i.$$

This has important consequences. Because the commutator is bounded, but the amplitude of the many-particle wave function can become macroscopic  $\sim \sqrt{N}$ , quantum effects which are of the order of the commutator are negligible with respect the mean field effects as  $N^{-1/2}$ , which justifies the commonly used approximation of replacing the quantum state by a purely classical field [49, 50].

The Fock states can be decomposed into a superposition of states  $|\Delta\theta, p_1 = p_2 = 1/2\rangle$ . However, instead of describing the states in terms of phase differences, it is very convenient to define states with a well defined phase on site *i* and average occupation  $Np_i \rightarrow N_i$ , so called coherent states or Glauber states  $|\theta_i, N_i\rangle$  [51, 52, 53]. The definition of  $\langle \theta_1, \theta_2 | \hat{\Delta\theta} | \theta_1, \theta_2 \rangle = (\theta_1 - \theta_2)$  suggests that the coherent state should be an eigenstate of the annihilation operator

$$\hat{a}|\theta,N\rangle = \sqrt{N} \mathrm{e}^{i\theta}|\theta,N\rangle$$

and hence that

$$\langle \theta, N | \hat{a}^{\dagger} = \sqrt{N} \mathrm{e}^{-i\theta} \langle \theta, N |.$$

To find the representation in terms of the single site Fock states, we use

$$\langle n-1|\hat{a}|\theta,N\rangle = \sqrt{n} \langle n|\theta\rangle = \sqrt{N} \mathrm{e}^{i\theta} \langle n-1|\theta,N\rangle.$$

This can be solved iteratively and after normalization one finds

$$\begin{aligned} |\theta, N\rangle &= e^{-N/2} \sum_{n=0}^{\infty} \frac{\left(\sqrt{N}e^{i\theta}\right)^n}{\sqrt{n!}} |n\rangle \\ &= e^{-N/2} \left( \sum_n \frac{\left(\sqrt{N}e^{i\theta}\hat{a}^{\dagger}\right)^n}{n!} \right) |vac\rangle \\ &= e^{-N/2} e^{\sqrt{N}e^{i\theta}\hat{a}^{\dagger}} |vac\rangle \,. \end{aligned}$$
(2.5)

Clearly the number of particles is not well defined. Instead, the probability to find n particles is Poisson distributed like

$$P_n = \frac{N^n}{n!} \mathrm{e}^{-N}.$$

For the Poisson distribution we do know that the mean equals the variance, i.e. there is always a spread in the number of particles on the site

$$\langle n \rangle = \langle n^2 \rangle - \langle n \rangle^2 = N.$$

The states  $|\theta, N\rangle$  are not orthonormal to each other. Instead

$$|\langle \boldsymbol{\theta}_1, N_1 | \boldsymbol{\theta}_2, N_2 \rangle|^2 = \mathrm{e}^{-\left|\sqrt{N_1}\mathrm{e}^{i\boldsymbol{\theta}_1} - \sqrt{N_2}\mathrm{e}^{i\boldsymbol{\theta}_2}\right|^2}$$

and the identity can be decomposed as

$$I = \frac{1}{\pi} \int d\left(\operatorname{Re}\psi\right) d\left(\operatorname{Im}\psi\right) \left|\psi\right\rangle \left\langle\psi\right|,\tag{2.6}$$

where  $\psi = \sqrt{N}e^{i\theta}$ , a precursor of the complex Bose field (2.1) but which also hints at the condensate field  $\Phi$  which will occur when the Hamiltonian is at a minimum for a coherent state (or set of coherent states, after all we usually have many sites and a global phase shift leaves the Hamiltonian invariant).

To complete the circle back to the field representation, we introduce a Hamiltonian to the system. A popular

#### CHAPTER 2. AN INTRODUCTION TO BOSE-EINSTEIN CONDENSATION

choice with many practical applications is the Bose-Hubbard Hamiltonian

$$\hat{H}_{HB} = -J \sum_{\langle ij \rangle} \left( \hat{a}_i^{\dagger} \hat{a}_j + \hat{a}_j^{\dagger} \hat{a}_i \right) - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i \left( \hat{n}_i - 1 \right).$$

$$(2.7)$$

Clearly this Hamiltonian conserves total particle number  $N = \sum_i n_i$  since  $\hat{N} = \sum_i \hat{n}_i$  commutes with the Hamiltonian  $[\hat{N}, \hat{H}_{HB}] = 0$ . Each of the terms in the Hamiltonian has an interpretation. The first term destroys a particle on one site and creates another one on a neighboring site. It is hence a hopping term which leads to a delocalization of particles. The second term controls the particle number via an external reservoir that fixes the chemical potential  $\mu$ , whereas the last term which acts on a single site only represents all onsite pairwise interaction of a particle on site *i* with the  $n_i - 1$  other particles on the same site.

To as before see the thermodynamics of the system, we have to start with the partition function

$$Z = \mathrm{Tre}^{-\beta \hat{H}}$$

In order to find an appropriate description in terms of complex fields, it is useful to introduce a time slicing that equates the finite temperature *T* to an evolution in imaginary time  $\tau$  from  $\tau = 0$  to  $\tau = \beta$ . The safe procedure is to start with a discrete slicing which then is extended to the infinite case in a well defined limiting procedure. We define the limit

$$Z = \operatorname{Tr}\left[\lim_{N \to \infty} \prod_{i=1}^{N} \mathrm{e}^{-\Delta \tau_{i} \hat{H}}\right].$$

with  $|\Delta \tau_i| = \beta/N$ . Next we connect the slices of time by inserting the identity (2.6) written as

$$I=\frac{1}{\pi}\int d\psi_{\tau_i}|\psi_{\tau_i}\rangle\langle\psi_{\tau_i}|$$

at each intersection. Because the time slices are small, we can approximate the overlap between neighboring

times as

$$\begin{split} \left\langle \psi_{\tau_i} | \mathrm{e}^{-\Delta \tau \hat{H}} | \psi_{\tau_i + \Delta \tau} \right\rangle &\approx \left\langle \psi_{\tau_i} | 1 - \Delta \tau \hat{H} | \psi_{\tau_i + \Delta \tau} \right\rangle \\ &\approx 1 - \Delta \tau \left\langle \psi_{\tau_i} | \frac{d}{d \tau_i} | \psi_{\tau_i} \right\rangle - \Delta \tau \left\langle \psi_{\tau_i} | \hat{H} | \psi_{\tau_i} \right\rangle \\ &\approx \exp \left[ -\Delta \tau \left\langle \psi_{\tau_i} | \frac{d}{d \tau_i} | \psi_{\tau_i} \right\rangle - \Delta \tau H \left( \psi, \psi^* \right) \right], \end{split}$$

where in the last approximation we used that within the Hamiltonian all instances of creation and annihilation operators are replaced by the fields due to the defining property of the coherent states (this is also the reason why we usually insist on normal ordering of the Hamiltonian). The trace operation itself can be understood as an integral over the states

$$\mathrm{Tr}X = \frac{1}{\pi} \int d\psi \langle \psi_{\tau=0} | X | \psi_{\tau=0} \rangle$$

As the trace connects the last time slice at  $\tau = \beta = 1/T$ , we automatically obtain the bosonic condition  $\psi(0) = \psi(\beta)$ , which in our first formulation was taken as an axiom via the selection of Matsubara frequencies. There remains a subtlety that neighboring slices can have arbitrarily different values, but a more careful analysis shows that it is usually well behaved [54, 55] and one can use the naive substitution of the operators  $\hat{\psi}, \hat{\psi}^{\dagger}$  with the fields  $\psi, \psi^*$ 

$$\left\langle \psi_{\tau} | \frac{d}{d\tau} | \psi_{\tau} \right\rangle = \mathrm{e}^{-|\psi_{\tau}|^2} \left\langle \mathrm{vac} | \mathrm{e}^{\psi_{\tau}^* \hat{a}} | \frac{d}{d\tau} \mathrm{e}^{\psi_{\tau} \hat{a}^{\dagger}} | \mathrm{vac} \right\rangle = \psi_{\tau}^* \frac{d}{d\tau} \psi_{\tau}.$$

If we now take the limit of the time slicing  $\Delta \tau \rightarrow 0$  and denote by  $D\psi = \lim \prod_i d\psi_{\tau_i}$  we obtain the functional integral representation with the action given in (2.2)

$$Z = \int_{\psi_0 = \psi_\beta} D\psi_\tau \mathrm{e}^{-\int_0^\beta d\tau \left[\psi^* \frac{d}{d\tau} \psi + H(\psi^*, \psi)\right]}.$$

To describe the full Bose-Hubbard model one has to extend the field integration over all lattice sites i

$$Z = \int \prod_i D\psi_i \mathrm{e}^{-S\left[\left\{\psi_i, \psi_i^*\right\}\right]}.$$

It is also fascinating to see how the Bose-Hubbard model can have similarities to the continuous model when the lattice spacing is taken to the limit of a continuous distribution and under the assumption that contributions other than  $\psi_{i+e_x} \approx \psi_i + \Delta x \mathbf{e}_x \nabla \psi_i$  are strongly suppressed, such that in an expansion to second order a term of the form of the kinetic energy in the continuous model appears. In cases where higher orders can be neglected, this means that also lattice models can be often described in terms of continuous models with local interactions. This is generally true when the single particle states extend beyond many lattice sites, as is common at second order phase transitions where the coherence length diverges.

### 2.4 **Properties of Bose-Einstein condensates**

We want to present a small selection of a wide range of phenomena that accompany Bose gases. The contents of this section are based on the expositions of Pethick/Smith [34], Stringari/Pitaevskii [50] and Griffin/Nikuni/Zaremba (ZNG) [31, 56]. In particular we focus on dilute gases with short range s-wave interactions such that  $u(\mathbf{x} - \mathbf{y}) \rightarrow g = 4\pi a\hbar^2/m \delta(\mathbf{x} - \mathbf{y})$ , where *a* is the scattering length which can be tuned in many cold atom situations.

In fact, to obtain a systematic expansion, let us start with the underlying quantum field operators that set the effective fields in equation (2.1). One can alternatively start directly with the fields and a decomposition into slow and fast moving components and finding the saddle-point approximation of the action (see [28]), however this decomposition is not exact and a rather inconvenient way of obtaining a set of effective equations that allows the determination of the defining properties of dilute Bose gases. Another alternative is to start from the coherent state picture and use a Hubbard-Stratonovich transformation to find the appropriate mean-field theory. As we are also interested in the behaviour of the thermal component, the approach we choose is most convenient.

In the quantum field operator approach, the condensate wave function is simply defined as the part of the operator that is not vanishing under a simple average (reflects a broken symmetry), whereas the operator that does vanish is considered thermal. This reflects the fact that the condensate is a coherent state without a well defined particle number, as the particle number of the ground state is only an order of magnitude estimation, but with a well defined phase and the quantum corrections of that field are small. We revert to a real time description,

as we are interested in the dynamic properties of the condensate and assume all thermal information is in the states themselves. A large part of the discussion will be for the T = 0 case, as there the condensate properties are at their purest and the thermal component is negligible.

We start by writing the Hamiltonian (2.3) in the form

$$\hat{H} = \int d\mathbf{x} \hat{\psi}^{\dagger} \left( -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right) \hat{\psi} + \int d\mathbf{x} d\mathbf{y} g \delta(\mathbf{x} - \mathbf{y}) \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}^{\dagger}(\mathbf{y}) \hat{\psi}(\mathbf{y}) \hat{\psi}(\mathbf{x}),$$

where we suppressed the real time index *t* and added the trapping potential  $V(\mathbf{x})$ . In addition we limit ourselves to the case g > 0, i.e. the repulsive case, as there are stability issues with the attractive case ([57, 58]).

The dynamics of the field operator are described by the Heisenberg equation of motion

$$i\hbar \partial_t \hat{\psi}(\mathbf{x},t) = -\left[\hat{H}, \hat{\psi}(\mathbf{x})\right]$$
$$= \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{x})\right] \hat{\psi}(\mathbf{x},t) + g \hat{\psi}^{\dagger}(\mathbf{x},t) \hat{\psi}(\mathbf{x},t) \hat{\psi}(\mathbf{x},t).$$
(2.8)

In case of a broken symmetry, a macroscopically occupied coherent state occurs and, similar to the coherent state representation,

$$\langle \hat{\boldsymbol{\psi}}(\mathbf{x},t) \rangle = \boldsymbol{\Phi}(\mathbf{x},t).$$

This calls for the following decomposition

$$\hat{\boldsymbol{\psi}}(\mathbf{x},t) = \boldsymbol{\Phi}\hat{\boldsymbol{l}} + \hat{\boldsymbol{\phi}},$$

where  $\hat{I}$  is the identity operator and  $\hat{\phi}$  the part of quantum operator for which

$$\left\langle \hat{\phi} \right\rangle = 0.$$
 (2.9)

If we average over equation (2.8) we obtain an equation of motion in terms of the condensate field  $\Phi$  and the different averages of the moments of the quantum operator  $\hat{\phi}$ . This is convenient, as we returned to a picture

with no explicit operators, yet the operator nature can be taken into account in the averaging procedure. In addition it is a good starting point to discuss possible approximations. The averaging procedure of (2.8) yields

$$i\hbar\partial_t \Phi = \left[ -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{x}) \right] \Phi(\mathbf{x}, z)$$
$$+ g \left\langle \hat{\psi}^{\dagger} \hat{\psi} \hat{\psi} \right\rangle(\mathbf{x}, t).$$

The remaining operator can be decomposed even further

$$\hat{\psi}^{\dagger}\hat{\psi}\hat{\psi} = |\Phi|^2 \Phi + 2 |\Phi|^2 \hat{\phi} + \Phi^2 \hat{\phi}^{\dagger} + \Phi^* \hat{\phi} \hat{\phi} + 2\Phi \hat{\phi}^{\dagger} \hat{\phi} + \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi}.$$

Averaging using 2.9 gives

$$\langle \hat{\psi}^{\dagger} \hat{\psi} \hat{\psi} \rangle = n_c \Phi + n_a \Phi^* + 2n \Phi + \langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \rangle,$$

where

$$n_{c}(\mathbf{x},t) = |\Phi(\mathbf{x},t)|^{2}, \text{ is the condensate density;}$$
$$n_{a}(\mathbf{x},t) = \langle \hat{\phi} \hat{\phi} (\mathbf{x},t) \rangle, \text{ is the anomalous density;}$$
$$n(\mathbf{x},t) = \langle \hat{\phi}^{\dagger} \hat{\phi} (\mathbf{x},t) \rangle, \text{ is the thermal density.}$$

So far, no approximations have been made, except for the nature of the two particle interaction. The final form of the equation of motion is

$$i\hbar\partial_t \Phi(\mathbf{x},t) = \left[ -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{x}) + gn_c(\mathbf{x},t) + 2gn(\mathbf{x},t) \right] \Phi(\mathbf{x},t) + gn_a(\mathbf{x},t) \Phi^*(\mathbf{x},t) + g\left\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \right\rangle(\mathbf{x},t).$$
(2.10)

(Note how the non-condensate density acts twice as strong as the condensate density, another statistical property.)

The simplest approximation is for the case when nearly all particles are in the condensate and the density is low enough  $(na^3 \ll 1)$  such that depletion is not an issue. The resulting equation is called the Gross-Pitaevskii

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(GP) equation

$$i\hbar\partial_t \Phi(\mathbf{x},t) = \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{x}) + gn_c(\mathbf{x},t)\right] \Phi(\mathbf{x},t), \qquad (2.11)$$

and has the form of a mean field equation. Because of  $n_c = |\Phi|^2$  one could view the GP equation as a non-linear Schrödinger equation.

Other common approximations are:

- Hartree-Fock-Bogoliubov (HFB): All terms are kept except the  $\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \rangle$  term. All other densities have to be calculated self-consistently and need additional equations of motions.
- Dynamic Popov approximation: Involves setting  $\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \rangle$  and  $n_a$  to zero.
- Static Popov approximation: Assumes that the thermal component  $n(\mathbf{x},t) \rightarrow n(\mathbf{x})$  is time-independent.

For the time being we want to focus on the GP equation as the "purest" of the condensate equations, but we need the latter approximations to understand the behaviour close to the transition, where the thermal components cannot be neglected.

As we introduced the amplitude-phase representation earlier, we can use it in the GP equation as

$$\Phi = \sqrt{n_c(\mathbf{x},t)} e^{-i\theta(\mathbf{x},t)}.$$
(2.12)

To obtain an interpretation of this energy in equilibrium, we consider an alternative derivation of the GP equation under the assumption that all atoms are in the stationary condensate state such that  $n_c(\mathbf{x},t) = n_c(\mathbf{x})$ , yet are subject to a particle reservoir. Then the Hamiltonian (2.3) can be written as an energy functional,

$$E\left(\Phi\right) = \int d\mathbf{x} \left[\frac{\hbar^2}{2m} \left|\nabla\Phi\right|^2 + V\left(\mathbf{x}\right) \left|\Phi\right|^2 + \frac{g}{2} \left|\Phi\right|^4\right],$$

which, according to thermodynamics, should be minimized in equilibrium under the constraint that the average particle number  $N_c = \int d\mathbf{x} |\Phi|^2$  is given. To do so, one introduces the Lagrange multiplier  $\mu$  to minimize the functional  $E - \mu N$  under variations of  $\Phi^*$ . The equation for  $\delta E - \mu \delta N$  in terms of variations in  $\Phi^*$  gives

$$-\frac{\hbar^2}{2m}\nabla^2 \Phi + V(\mathbf{x})\Phi + g|\Phi|^2\Phi = \mu\Phi, \qquad (2.13)$$

the time-independent GP equation, however with the right hand side described by the thermodynamic chemical potential. Applying the stationary solution (2.12) where  $n_c(\mathbf{x},t) \rightarrow n_c(\mathbf{x})$  gives

$$\mu \Phi = i\hbar \partial_t \Phi = \hbar \dot{\theta} \Phi$$
  

$$\rightarrow \dot{\theta} = \frac{\mu}{\hbar}, \qquad (2.14)$$

which is the famous Josephson equation that relates the phase dynamics of a condensate to its chemical potential [59].

To understand better the condensate specific properties, let us consider the uniform case of (2.13). From the bulk part of the equation we can see that

$$\mu = g \left| \Phi \right|^2 = g n_c. \tag{2.15}$$

To see some behaviour specific to the condensate, let us introduce a box with infinitely high potential walls. Far away from the walls the condensate density should be "flat" and the value of the condensate density  $|\Phi_0|^2$  correspond to the potential given above, i.e.  $|\Phi_0|^2 = \mu/g$ . On the other hand close to the wall, the condensate must vanish. If *L* is the position of the box wall, then  $|\Phi(L)|^2 = 0$ . From the GP equation (2.13)

$$\frac{\hbar^2}{2m} \frac{d^2 \Phi(x)}{dx^2} = -g \left( |\Phi_0|^2 - |\Phi(x)|^2 \right) \Phi(x)$$

we can infer the condensate behaviour close to the wall. It is easy to verify by substitution that the ansatz

$$\Phi(x) = \Phi_0 \tanh\left(\frac{L-x}{\xi}\right)$$

solves this equation, where  $\xi$  is given by the characteristic length scale of the problem

$$\xi = \frac{\hbar}{\sqrt{mn_c g}}.$$

This scale is usually called the healing length, because it describes how far away from an impurity, in this case the wall, the condensate looks like an unperturbed condensate. The healing length is in most experiments usually much smaller than the trap dimensions.

#### CHAPTER 2. AN INTRODUCTION TO BOSE-EINSTEIN CONDENSATION

When the interaction constant is written in terms of the scattering length, it follows that

$$\xi \sim rac{1}{\sqrt{n_c a}} \sim r_s \sqrt{rac{r_s}{a}},$$

where  $r_s$  is the average distance between particles. The ratio  $r_s/a$  is the dimensionless quantity determining the behaviour of the gas and measures its diluteness. A more common way of writing is indeed the dimensionless gas parameter  $(na^3)$ , which will appear more often throughout the thesis.

In order to understand the superfluid properties of the BEC, we have to calculate its excitation spectrum. To do so we take the time-dependent GP equation (2.11) and add a small perturbation  $\delta \Phi$ ,  $\delta \Phi^*$  to the stationary solution  $\Phi$ . The resultant equations describing the perturbations are

$$i\hbar\partial_t \delta\Phi = -\frac{\hbar^2}{2m} \nabla^2 \delta\Phi + V\delta\Phi + 2g |\Phi|^2 \delta\Phi + g\Phi^2 \delta\Phi^*$$
  
$$-i\hbar\partial_t \Phi^* = -\frac{\hbar^2}{2m} \nabla^2 \delta\Phi^* + V\delta\Phi^* + 2g |\Phi|^2 \delta\Phi^* + g\Phi^{*2}\delta\Phi.$$
(2.16)

From an earlier discussion, see eq. (2.14), we remember that the condensate phase evolves in the stationary case with the chemical potential. So we set the overall phase to be zero at t = 0 and choose the uniform wave function

$$\Phi(\mathbf{x},t) = \sqrt{n_c} \mathrm{e}^{-i\mu t/\hbar}.$$

For the perturbation  $\delta\Phi$  we take an ansatz of the form

$$\delta \Phi = \mathrm{e}^{-i\mu t/\hbar} \left[ u(\mathbf{x}) \,\mathrm{e}^{-i\omega t} - v^*(\mathbf{x}) \,\mathrm{e}^{i\omega t} \right].$$

Here we separated already the fast condensate dynamics  $\sim \mu/\hbar$  out and left only the slow dynamics with frequency  $\omega$ . The superposition of the two frequencies  $\pm \omega$  is necessary, as in equation (2.16) both components,  $\Phi$  and  $\Phi^*$  are coupled. The relative phase of *u* and *v*<sup>\*</sup> is chosen so that after the analysis, *u* and *v* can be chosen both to be positive.

Along the same lines of reasoning as above, we can choose  $u(\mathbf{x})$  and  $v(\mathbf{x})$  to be represented in momentum form, as the problem is for  $V(\mathbf{x}) = 0$  translational invariant. The normalized ansatz for a particular component

is

$$u(\mathbf{x}) = u_q \frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{L^{3/2}}, \quad v(\mathbf{x}) = v_q \frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{L^{3/2}}$$

In that basis the perturbation eq. (2.16) becomes

$$\begin{pmatrix} \left(\frac{\hbar^2 q^2}{2m} + n_c g - \hbar \omega\right) & -n_c g \\ -n_c g & \left(\frac{\hbar^2 q^2}{2m} + n_c g + \hbar \omega\right) \end{pmatrix} \begin{pmatrix} u_q \\ v_q \end{pmatrix} = 0$$

In order for this equation system to support non-trivial solutions  $(u_q, v_q \neq 0)$  the determinant of the matrix has to vanish. This leads to the condition

$$\hbar\omega = \pm \left| \boldsymbol{\varepsilon}_{q} \right| = \pm \sqrt{\left(\frac{\hbar^{2}q^{2}}{2m} + n_{c}g\right)^{2} - (n_{c}g)^{2}} = \pm \sqrt{\boldsymbol{\varepsilon}_{q}^{0}\left(\boldsymbol{\varepsilon}_{q}^{0} + 2n_{c}g\right)},\tag{2.17}$$

where  $\varepsilon_q^0$  is the free particle excitation spectrum  $\hbar^2 q^2/2m$ . One can see that for large momenta,  $\hbar \omega \sim \varepsilon_q^0 + n_c g$ , so a highly excited particle behaves like a free, massive particle that feels a mean field potential by the surrounding condensate. If however the excitation carries little momentum, then

$$\hbar\omega\sim\sqrt{\frac{n_cg}{m}}\hbar q=c\hbar q$$

This is a dispersion of a sound wave that moves with speed of sound  $c = \sqrt{n_c g/m}$ . This indicates that the excitations are collective in nature, rather than of single particle character as for the highly excited particles. It is indeed this linear low energy spectrum that is responsible for much of the superfluid behaviour of the cloud of particles. If one estimates the wave-length of the particles for which the cross-over from collective to free particle behaviour occurs, one finds the healing length  $\xi = \hbar/\sqrt{mn_cg} = \hbar/mc$ . This is hardly surprising, as this is the only length scale governing the many-particle problem, and it is quite intuitive that a perturbation smaller than the healing length behaves like a pointlike impurity, whereas a larger perturbation necessitates a large modulation. This separation into small and large length scale behaviour will be especially useful when discussing the influence of a one-dimensional condensate mixture on an impurity.

To complete our picture we want to study the excitations. Choosing the positive solution  $\hbar \omega > 0$  one finds
that

$$v_q = \frac{n_c g}{\hbar \omega + \varepsilon_q^0 + n_c g} u_q.$$

This shows that the  $v_q$  component is strictly smaller than the  $u_q$  (any overall phase can be multiplied out in equation (2.16), therefore allowing for  $u_q$  and  $v_q$  to be real quantities). The normalization of the state suggests that  $u_q \rightarrow 1$  for large momenta q. As both  $u_q$  and  $v_q$  grow with low momenta, a normalization that is independent of momenta can be hypothesized to be

$$\left|u_q\right|^2 - \left|v_q\right|^2 = 1,$$

which can be verified and is convenient in a microscopic picture, where the positive and negative frequency components are described as coupled bosonic particles. This normalization keeps their commutation relation normalized. The solutions becomes then

$$u_q^2 = \frac{1}{2} \left( \frac{\varepsilon_q^0 + n_c g}{\sqrt{\varepsilon_q^0 \left(\varepsilon_q^0 + 2n_c g\right)}} + 1 \right), \quad v_q^2 = \frac{1}{2} \left( \frac{\varepsilon_q^0 + n_c g}{\sqrt{\varepsilon_q^0 \left(\varepsilon_q^0 + 2n_c g\right)}} - 1 \right),$$

which confirms the limiting behaviour as described previously. The solution just presented goes back to Bogoliubov [60]. Additionally, in the non-uniform system there exist collective excitations of the whole condensate.

Knowing that the system has a linear dispersion, at least for the lowest lying excitations, we can apply it to the question of how an impurity dissipates energy and momentum. The basic insight here is that both, energy and momentum, must be conserved, so there must be a transfer of both quantities into the surrounding liquid. The liquid must create excitations to accommodate them. Following an argument first proposed by Landau [61], we derive a kinematic condition for the possibility of momentum transfer.

Let us take the picture of an impurity moving with velocity  $\mathbf{v}$  in a large but finite liquid (at rest) of N particles, each with mass m. From standard mechanics we know how the energy of a system with energy E, mass M and momentum  $\mathbf{q}$  changes when observed in a frame moving with velocity  $\mathbf{v}$  relative to the original frame,

$$E(\mathbf{v}) = E - \mathbf{q} \cdot \mathbf{v} + \frac{1}{2}M|\mathbf{v}|^2.$$

We look at the energy of the liquid in the frame in which the obstacle is motionless. Because we start from

the frame in which the liquid carries no momentum,  $\mathbf{q} = 0$ , and the mass of the liquid is M = Nm, its energy becomes

$$E\left(\mathbf{v}\right)=E_{0}+\frac{1}{2}Nm\left|\mathbf{v}\right|^{2},$$

where  $E_0$  is the ground state energy. The moving liquid has to be compared to a state with an excitation with momentum **p** and energy  $\varepsilon_p$  moving relative to a motionless impurity. Said energy is

$$E_{\mathrm{ex}} = E_0 + \varepsilon_p - \mathbf{p} \cdot \mathbf{v} + \frac{1}{2} Nm \left| \mathbf{v} \right|^2.$$

The difference in both energies,  $\varepsilon_p - \mathbf{p} \cdot \mathbf{v}$  is the necessary energy that allows the excitation to happen (at least in principle, there could still be a kinetic suppression that makes this a very slow process). This energy cannot come from the impurity though, as it stands still in that picture and we assume there is no internal energy carrying structure that could be disexcited. Thus only at a velocity *v* where

$$v = \frac{\varepsilon_p}{p},$$

can the liquid create excitations. Keeping in mind that the impurity can give off momentum in small units, then the necessary condition of non-dissipation is that

$$v < v_c = \min_p \left(\frac{\varepsilon_p}{p}\right),$$

namely that not a single excitation is possible to absorb momentum of the impurity. The velocity  $v_c$  is called the *Landau critical velocity*. To illustrate the concept, let us look at a free gas. Here  $\varepsilon_q = \frac{q^2}{2m}$  and  $v_c = \min_q q/2m = 0$ , meaning that there exists an arbitrarily small velocity at which the momentum can be absorbed.

In contrast for the low energy excitations of the GP equation, see eq. (2.17), we have that

$$v_c = \min_q \left(\frac{\varepsilon_q}{\hbar q}\right) = \min_q \frac{1}{\sqrt{2m}} \sqrt{\frac{\hbar^2 q^2}{2m}} + 2n_c g = \sqrt{\frac{n_c g}{m}} = c.$$

This means that any excitation moving below the speed of sound c (in a uniform system) is forbidden from

dissipating energy. Along the same line one can say that the condensate moving below that speed will stay excitationless, unless external energy is pumped into the system or due to trapping other excitations for the liquid become available. That effect is what is commonly called superfluidity.

Apart from being dissipationless, the superfluid flow described by the GP equation is still different from ordinary fluid flow, as described by the Euler equation. To see this, we have to first identify what the superfluid velocity  $\mathbf{v}_s$  is. If we multiply the GP equation (2.11) by  $\Phi^*(\mathbf{x},t)$  and its conjugate with  $\Phi(\mathbf{x},t)$  and subtract them from each other, we find that

$$\frac{\partial |\Phi|^2}{\partial t} + \nabla \cdot \left[ \frac{\hbar}{2mi} \left( \Phi^* \nabla \Phi - \Phi \nabla \Phi^* \right) \right] = 0.$$

This has the form of a continuity equation

$$\frac{\partial n}{\partial t} + \nabla \cdot j = 0,$$

which is further supported by the quantum mechanical interpretation of  $\Phi$  being a classical wave function such that the condensate density is  $n_c(\mathbf{x},t) = |\Phi(\mathbf{x},t)|^2$ . Given that the particle flow **j** is the product of particle density and superfluid velocity, then the local velocity is

$$\mathbf{v}_{s}=-i\frac{\hbar}{2m}\frac{\left(\Phi^{*}\nabla\Phi-\Phi\nabla\Phi^{*}\right)}{\left|\Phi\right|^{2}}.$$

If we rewrite the condensate wavefunction in terms of amplitude and phase field, eq. (2.12), then

$$\mathbf{v}_{s}(\mathbf{x},t)=\frac{\hbar}{m}\nabla\boldsymbol{\theta}\left(\mathbf{x},t\right).$$

This is a very special flow, as  $\theta(\mathbf{x}, t)$  is a scalar phase variable. Gradient flows, i.e. flow profiles that follow a gradient of a scalar term are just a small subset of all possible flows. It immediately follows that their vorticity

$$abla imes \mathbf{v}_s = \frac{\hbar}{m} \nabla \times \nabla \boldsymbol{\theta} = 0,$$

i.e. the fluid is irrotational. From classical hydrodynamics, for example the laminar flow around a rotating body, it is well known that such a flow can still carry a non-zero circulation  $\Gamma = \oint \mathbf{v}_s \cdot d\mathbf{x} \neq 0$ , but, that there must be

regions inside the contour in which the fluid is ill-defined, which could be an impurity or simply a "hole" in the liquid. Here however it comes into play that  $\theta$  is a phase variable, meaning that it is at each point well defined up to a multiple of  $2\pi$ . This means that the phase gradient over a contour can only span phase differences  $n2\pi$ , which means for the circulation that

$$\oint \mathbf{v}_s \cdot d\mathbf{x} = \frac{\hbar}{m} \oint \nabla \theta \cdot d\mathbf{x} = \frac{2\pi\hbar}{m} n = \frac{\hbar}{m} n.$$

This shows that the circulation is quantized in a bosonic superfluid as was first predicted by Onsager [62]. A flow that is irrotational and carries circulation in a two-dimensional plane centered around the z-axis has a velocity profile

$$v_s = n \frac{\hbar}{m\rho},$$

where  $\rho$  is the distance from the *z*-axis. One sees that such a flow is ill-defined at the origin and the condensate density must vanish there to avoid a divergence of the energy. Such a structure is called a vortex and one of the most astonishing observations regarding Bose Einstein Condensates [10]. Most notably, each particle participating in the vortex carries the same amount of angular momentum around the axis ( $\hbar n$ ). So rather than increasing momentum slowly when rotating a condensate of *N* particles, momentum is added in multiples of  $\hbar Nm$ . This also explains why a weakly rotated condensate will remain motionless unless a critical frequency  $\omega_c$ is applied ([63]) to create one vortex. The vortices themselves are interesting quantum objects that for example can form lattices with different quantum phases on top of that [64, 65].

This concludes our technical overview of Bose Einstein condensation and superfluidity close to T = 0. There are many interesting phenomena we left out, e.g. the second sound [66] or collective excitations of a trap [67], which are not part of the analysis that follows. In the next chapter we are going to focus on higher temperatures, where  $n_c$  is small and the thermal components are important.

## **Chapter 3**

# **Bosonic fluctuations close to criticality**

## **3.1** General bosonic fluctuations close to criticality

In the previous chapter we looked at properties of a pure single condensate at very low temperatures. In this chapter we want to investigate how bosonic gases behave as the critical point is approached from below and especially what happens just above it.

Close to criticality the non-condensate particles  $\hat{\phi}$  are important and motivated from (2.10) it becomes clear that we have to understand how they evolve in time, especially how the averages  $n_a$  and  $\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \rangle$  behave. The equation of motion for the field can be obtained by subtracting from the exact operator equation (2.8) the equation for the condensate field (2.10) to obtain

$$\begin{split} i\hbar \frac{\partial \hat{\phi}}{\partial t} &= \left( -\frac{\hbar^2 \nabla^2}{2m} + V + 2g \left[ n_c + n \right] \right) \hat{\phi} - 2gn \hat{\phi} + g \Phi^2 \hat{\phi^\dagger} \\ &+ g \Phi^* \left( \hat{\phi} \hat{\phi} - n_a \right) + 2g \Phi \left( \hat{\phi^\dagger} \hat{\phi} - n \right) + g \left( \hat{\phi^\dagger} \hat{\phi} \hat{\phi} - \langle \hat{\phi^\dagger} \hat{\phi} \hat{\phi} \rangle \right), \end{split}$$

as is described in [56]. The technique to find approximate solutions to this equation was first introduced by Kirkpatrick and Dorfman [68].

Instead of describing the evolution of the operators directly, we investigate the unitary operators  $\hat{U}$  that are responsible for the time evolution of  $\hat{\phi}$ 

$$\hat{\boldsymbol{\phi}}(\mathbf{x},t) = \hat{U}(t,t_0)^{\dagger} \,\hat{\boldsymbol{\phi}}(\mathbf{x},t_0) \,\hat{U}(t,t_0) \,.$$

Since at  $t = t_0$  the original operators have to be recovered, it is natural to demand  $\hat{U}(t,t) = \hat{1}$ .

The equation of motion for the unitary operator can be found by inserting the definition into the Heisenberg equation

$$i\hbar\frac{d\hat{U}(t,t_0)}{dt} = \left(\hat{H}_0 + \hat{H}_{nc}\right)\hat{U}(t,t_0).$$

The Hamiltonian  $H_0$  is the term that drives the principal time evolution that conserves the number of particles (Hartree-Fock term)

$$H_0 = \int d\mathbf{x} \,\hat{\phi}^{\dagger} \left[ -\frac{\hbar^2}{2m} \nabla^2 + V + 2g\left(n_c + n\right) \right] \hat{\phi}.$$

The operator  $\hat{H}_{nc}$  is the sum of four contributions,

$$egin{aligned} \hat{H}_{nc} &= \sum_{i=1}^4 \hat{H}_i, \ \hat{H}_1 &= \int d\mathbf{x} \left[ -g \left( 2n \Phi + n_a \Phi^* + \left\langle \hat{\phi}^\dagger \hat{\phi} \hat{\phi} \right\rangle 
ight) \hat{\phi}^\dagger + \mathrm{h.c.} 
ight], \ \hat{H}_2 &= rac{g}{2} \int d\mathbf{x} \left[ \Phi^2 \hat{\phi}^\dagger \hat{\phi}^\dagger + \mathrm{h.c.} 
ight], \ \hat{H}_3 &= g \int d\mathbf{x} \left[ \Phi^* \hat{\phi}^\dagger \hat{\phi} \hat{\phi} + \mathrm{h.c.} 
ight], \ \hat{H}_4 &= rac{g}{2} \int d\mathbf{x} \left[ \hat{\phi}^\dagger \hat{\phi}^\dagger \hat{\phi} \hat{\phi} - 4n \hat{\phi}^\dagger \hat{\phi} 
ight], \end{aligned}$$

labeled by how many thermal fields are involved in the interaction; the first three do not conserve the number of thermal particles (and hence the number of condensate particles).

There is a certain liberty in choosing the specific decomposition. Here we deliberately chose  $\hat{H}_0$  to be the Hartree-Fock approximation, as it makes the resulting Boltzmann picture clearer. It also has to be kept in mind that there is an implicit time dependence in all of these operators.

To capture all correlations and the fact that the problem contains classical statistics, it is convenient to use a density operator description of the thermal gas. In this description the average of an observable  $\hat{O}(t)$  of the system is the trace of the original observable multiplied by the time evolved density matrix  $\hat{\rho}(t)$ 

$$\left\langle \hat{O}(t) \right\rangle = \operatorname{Tr}\left[\hat{\rho}\left(t\right)\hat{O}\left(t_{0}\right)\right] = \operatorname{Tr}\left[\hat{U}\left(t,t_{0}\right)\hat{\rho}\left(t_{0}\right)\hat{U}^{\dagger}\left(t,t_{0}\right)\hat{O}\left(t_{0}\right)\right].$$
(3.1)

One has to remember that the time evolution of the density operator is in the reverse order from the time evolution of ordinary operators. As the definition suggests, the density operator also evolves in time as dictated by the Hamiltonian

$$i\hbarrac{d\hat{
ho}(t)}{dt}=\left[\hat{H}_0(t)+\hat{H}_{nc}(t),\hat{
ho}(t)
ight].$$

Integration gives the formal solution  $(t \rightarrow \hbar t$ , subsequently  $\hbar \equiv 1$ )

$$\hat{\rho}(t) = \hat{U}_{0}(t,t_{0})\hat{\rho}(t_{0})\hat{U}_{0}^{\dagger}(t,t_{0}) + i\int_{t_{0}}^{t} dt'\hat{U}(t,t') \left[\hat{H}_{nc},\hat{\rho}(t')\right]\hat{U}_{0}(t,t'),$$

which has to be solved self-consistently, as  $\hat{\rho}(t)$  also appears under the integral sign. The unitary evolution,

$$\hat{U}_0(t,t_0) = T e^{-i \int_{t_0}^t dt' \hat{H}_0(t')},$$

describes the evolution under the Hartree-Fock term only. For small times the density matrix has not evolved that far and in the integrand it can be replaced by the unperturbed matrix  $\hat{\rho}(t_0)$ 

$$\hat{\rho}(t) \simeq \hat{U}_0(t,t_0)\hat{\rho}(t_0)\hat{U}_0^{\dagger}(t,t_0) + i \int_{t_0}^t dt' \hat{U}(t,t') \left[\hat{H}_{nc}, \hat{U}_0(t,t_0)\hat{\rho}(t_0)\hat{U}_0^{\dagger}(t,t_0)\right] \hat{U}_0(t,t').$$
(3.2)

In principle the iteration can be continued to arbitrary order. However, we are interested in a Markov-like description, i.e. the system dynamics only depends on its current state which is assumed to be in quasi-equilibrium, that allows us to determine the behaviour of the condensate. Given an initial state at time  $t_0$  the first order approximation is good enough for our purposes.

Indeed one can approximate the short-time evolution of any observable, by inserting the approximation (3.2)

into (3.1) to find

$$\langle \hat{O}(t) \rangle = \text{Tr} \hat{\rho}(t_0) \left\{ \hat{O}_0(t) - i \int_{t_0}^t dt' \hat{U}_0^{\dagger}(t,t') \left[ \hat{U}_0^{\dagger}(t,t') \hat{O}(t_0) \hat{U}_0(t,t'), \hat{H}_{nc}(t') \right] \hat{U}_0(t',t_0) \right\}$$

$$(3.3)$$

This is essentially the Kubo formula, where  $\hat{O}_0(t) \equiv \hat{U}_0^{\dagger}(t,t_0)\hat{O}(t_0)\hat{U}_0(t,t_0)$  is the ordinarily evolved observable.

Usually a more convenient way of describing the state of the thermal component other than the density matrix is the Wigner operator and its average, the (Wigner) distribution function. The Wigner operator is defined as (for instance in [69])

$$\hat{f}(\mathbf{k},\mathbf{x},t) \equiv \int d\mathbf{x}' \,\mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}'} \hat{\phi}^{\dagger}\left(\mathbf{x}+\mathbf{x}'/2,t\right) \hat{\phi}\left(\mathbf{x}-\mathbf{x}'/2,t\right).$$

The Wigner distribution function is then defined as

$$f(\mathbf{k}, \mathbf{x}, t) = \operatorname{Tr} \boldsymbol{\rho}(t) \hat{f}(\mathbf{k}, \mathbf{x}, t_0).$$

Though it is only a quasi-probability function, meaning that it is normalized but can be negative, it is still very helpful to get an intuition. The regions in space where it is indeed negative are small, similar to the size of quantization in phase space. On the other hand it is the quantum generalization of the classical distribution function  $f(\mathbf{p}, \mathbf{x}, t)$  which expresses the likelihood of finding a particle with momentum  $\mathbf{p}$  at position  $\mathbf{x}$  and time t is. Classically, such a distribution follows the Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}},$$

where the left hand side describes the evolution of the distribution function via evolution of the space variable as dictated by momentum and the evolution of the momenta by the application of an external force **F**, whereas the right hand side, the complicated part, describes how collisions change the distribution. It is this part that is model dependent. To get closer to the classical formulation, let us restore the  $\hbar$  so that the quantum mechanical momentum coincides with the classical momentum  $\mathbf{p} = \hbar \mathbf{k}$ . One can find a similar equation for the Wigner distribution. By quantum mechanics we have that

$$\frac{\partial f}{\partial t} = \frac{1}{i\hbar} \operatorname{Tr} \boldsymbol{\rho} \left( t \right) \left[ \hat{f} \left( \hbar \mathbf{k}, \mathbf{x}, t_0 \right), \hat{H}_0(t) + \hat{H}_{nc}(t) \right],$$
(3.4)

which is equivalent with

$$\frac{\partial f}{\partial t} + \frac{i}{\hbar} \operatorname{Tr} \rho \left( t \right) \left[ \hat{f} \left( \hbar \mathbf{k}, \mathbf{x}, t_0 \right), \hat{H}_0(t) \right] = \frac{1}{i\hbar} \operatorname{Tr} \rho \left( t \right) \left[ \hat{f} \left( \hbar \mathbf{k}, \mathbf{x}, t_0 \right), \hat{H}_{nc}(t) \right] 
\frac{\partial f}{\partial t} + \frac{\hbar \mathbf{k}}{m} \cdot \nabla f - \frac{\partial U_{HF}}{\partial \mathbf{x}} \cdot \frac{\partial f}{\partial \hbar \mathbf{k}} = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}.$$
(3.5)

The role of the external potential is taken by the effective Hartree-Fock potential

$$U_{HF}(\mathbf{x},t) = V(\mathbf{x}) + 2g[n_c(\mathbf{x},t) + n(\mathbf{x},t)].$$

We return now to the exact equation of motion for the condensate field (2.10)

$$i\hbar\partial_t \Phi(\mathbf{x},t) = \left[ -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{x}) + gn_c(\mathbf{x},t) + 2gn(\mathbf{x},t) \right] \Phi(\mathbf{x},t) + gn_a(\mathbf{x},t) \Phi^*(\mathbf{x},t) + g\left\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \right\rangle(\mathbf{x},t).$$

Apart from the condensate density  $n_c = |\Phi|^2$ , there is the thermal density  $n = \langle \hat{\phi}^{\dagger} \hat{\phi} \rangle$  and the anomalous density  $n_a = \langle \hat{\phi} \hat{\phi} \rangle$ . As was done for the pure case, it is beneficial to find a description in terms of the amplitude and phase of the condensate wave function (2.12). Multiplying the exact equation by  $\Phi^*$  and subtracting from the complex conjugate gives the generalized continuity equation

$$\frac{\partial n_c}{\partial t} + \nabla (n_c \mathbf{v}_s) = \frac{2g}{\hbar} \operatorname{Im} \left[ (\Phi^*)^2 n_a + \Phi^* \left\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \right\rangle \right].$$

Rather than having a conserved condensate density, a source/sink term is present

$$\frac{\partial n_c}{\partial t} + \nabla (n_c \mathbf{v}_s) = \boldsymbol{\sigma}$$

with  $\sigma(\mathbf{x},t) = \frac{2g}{\hbar} \operatorname{Im}\left[ (\Phi^*)^2 n_a + \Phi^* \langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \rangle \right]$ . The GP equation is indeed recovered by setting  $n_a = \langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \rangle = 0$ .

The phase variable evolves in time with a modified Josephson equation that allows to define the chemical potential and condensate energy. This is possible because the condensate wave function is only slowly dependent on time (slow with respect to the time necessary to average quantities like  $n_a$ ). Taking the product of  $\Phi^*$  and the GP equation and adding its complex conjugate we find

$$\begin{split} \hbar\partial_t \theta &= -\frac{\hbar^2 \nabla^2 \sqrt{n_c}}{2m\sqrt{n_c}} + V + gn_c + 2gn + \frac{g}{\hbar n_c} \operatorname{Re}\left[ (\Phi^*)^2 n_a + \Phi^* \left\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \right\rangle \right] + \frac{1}{2} m \mathbf{v}_s^2 \\ &= \mu_c + \frac{1}{2} m \mathbf{v}_s^2 = \varepsilon_c. \end{split}$$

In the last steps we defined the chemical potential  $\mu_c$  of the condensate

$$\mu_{c} = -\frac{\hbar^{2} \nabla^{2} \sqrt{n_{c}}}{2m \sqrt{n_{c}}} + V + gn_{c} + 2gn + \frac{g}{\hbar n_{c}} \operatorname{Re}\left[\left(\Phi^{*}\right)^{2} n_{a} + \Phi^{*} \left\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \right\rangle\right]$$

and use the interpretation of  $\varepsilon_c$  being the local energy of the condensate. Apart from the classically expected terms  $V + gn_c + 2gn$ , one has additionally the quantum pressure term

$$-rac{\hbar^2 
abla^2 \sqrt{n_c}}{2m \sqrt{n_c}}$$

which corresponds to the energy necessary to deform the amplitude of the many-body wavefunction. Further there is a new potential stemming from the anomalous terms, which we will show to be small ( $\sim g^2$ ). This sort of equation was first derived in [70, 71].

To decompose further, let us first look at the three-particle average using equation (3.3). The equation has two terms, one is the evolution under the Hartree-Fock Hamiltonian, the other stems from collisions that do not necessarily conserve particle number. Because the observable  $\hat{\phi}^{\dagger} \hat{\phi} \hat{\phi}$  by itself does not conserve the particle number, it is necessary for collision processes to provide a non-vanishing average. If we assume that at  $t_0$  no correlations are present and these are built up over time with the collisions, we can simplify the term, especially as these anomalous terms turn out to be small either way. Because we must have particle number conservation at all times, it is clear that only those parts of the Hamiltonian contribute where the sum of creation and annihilation fields exactly cancels the fields of  $\hat{\phi}^{\dagger} \hat{\phi} \hat{\phi}$ . Thus we have

$$\left\langle \hat{\phi}^{\dagger}(\mathbf{x},t) \hat{\phi}(\mathbf{x},t) \hat{\phi}(\mathbf{x},t) \right\rangle$$
  
=  $-i \operatorname{Tr} \hat{\rho}(t_0) \int_{t_0}^t dt' \hat{U}_0^{\dagger}(t',t_0) \left[ \hat{U}_0^{\dagger}(t,t') \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi}(\mathbf{x},t_0) \hat{U}_0(t,t'), \hat{H}_1 + \hat{H}_3 \right] \hat{U}_0(t',t_0)$ 

In this case, the relevant Hamiltonian terms are

$$\hat{H}_{1} = -\int d\mathbf{x}' g \left(2n\Phi + n_{a}\Phi^{*} + \left\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \right\rangle \right) \hat{\phi}^{\dagger} \approx -2g \int d\mathbf{x}' n\Phi \hat{\phi}^{\dagger}$$

and

$$\hat{H}_3 = g \int d\mathbf{x}' \Phi \hat{\phi} \hat{\phi}^{\dagger} \hat{\phi}^{\dagger}.$$

At the same time one has to make the hydrodynamic assumption, namely that at all points in time the averages are well defined, which necessitates that the collision times are short compared to the time scales over which averages change and that many collisions are necessary to have a significant effect. Since we study dilute weakly interacting gases this is indeed a good assumption. This means that the condensate density, the thermal density and the local Hartree-Fock potential are well defined. In the same way the condensate phase is assumed to be well defined over the distances we are observing, as the interaction potential is supposed to be very short-ranged, at least compared to the average inter-particle distance. To this end one can expand

$$\theta \left( \mathbf{x}', t' \right) \simeq \theta \left( \mathbf{x}, t \right) + \partial_t \theta \left( t' - t \right) + \nabla \theta \cdot \left( \mathbf{x}' - \mathbf{x} \right)$$
$$= \theta \left( \mathbf{x}, t \right) + \varepsilon_c \left( \mathbf{x}, t \right) \left( t' - t \right) + m \mathbf{v}_s \left( \mathbf{x}' - \mathbf{x} \right).$$

To evaluate the field terms, it is useful to switch again to the Fourier basis as interactions conserve momentum

$$\hat{\phi}(\mathbf{x},t_0) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} \hat{a}_{\mathbf{k}},$$

where V is a small, yet macroscopic, local volume over which we coarse grain and assume that the densities between neighboring volumes vary only little.

Evaluating the first commutator

$$\left[\hat{U}_0^{\dagger}(t,t')\hat{\phi}^{\dagger}\hat{\phi}\hat{\phi}(\mathbf{x},t_0)\hat{U}_0(t,t'),\hat{H}_1\right]$$

$$\simeq -\frac{2gn(\mathbf{x},t)\sqrt{n_c(\mathbf{x},t)}}{V}e^{i\theta(\mathbf{x},t)}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}e^{-i(m\mathbf{v}_s+\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)\cdot\mathbf{x}}e^{i(\varepsilon_c+\varepsilon_1-\varepsilon_2-\varepsilon_3)(t-t')}\times$$

$$\delta_{m\mathbf{v}_s,\mathbf{k}_4}\left[\hat{a}_{\mathbf{k}_1}^{\dagger}\hat{a}_{\mathbf{k}_2}\delta_{\mathbf{k}_3,\mathbf{k}_4}+\hat{a}_{\mathbf{k}_1}^{\dagger}\hat{a}_{\mathbf{k}_3}\delta_{\mathbf{k}_2,\mathbf{k}_4}\right].$$

In the above equation the  $\varepsilon_i$  are the energies of the thermal states in the Hartree-Fock approximation. In the last step, we took advantage that over the integration volume the hydrodynamic variables are well defined. The resulting form allows us to find a shortcut in generating the higher order terms, namely by substituting in the Hamiltonian  $\Phi = \sqrt{n_c(\mathbf{x},t)}e^{i\theta(\mathbf{x},t)}e^{-im\mathbf{v}_s\mathbf{x}}e^{i\varepsilon_c(t-t')}$  and using the Fourier expansion of the thermal fields plus a momentum conserving Kronecker delta. Additionally a factor of *V* is created by the real space integration over  $\mathbf{x}'$ . That is to some extent the local approximation of the Hamiltonian, justified by having a local interaction model. Inserting the commutator expression in the Kubo-like formula for the three-field average, we obtain

$$\left\langle \hat{\phi}^{\dagger}(\mathbf{x},t) \, \hat{\phi}(\mathbf{x},t) \, \hat{\phi}(\mathbf{x},t) \right\rangle_{(1)}$$

$$=i\frac{2gn(\mathbf{x},t)\sqrt{n_c(\mathbf{x},t)}}{V}e^{i\theta(\mathbf{x},t)}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\delta_{m\mathbf{v}_s,\mathbf{k}_4}e^{-i(m\mathbf{v}_s+\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)\cdot\mathbf{x}}\times$$
$$\int_{t_0}^t e^{i(\varepsilon_c+\varepsilon_1-\varepsilon_2-\varepsilon_3)(t-t')}\left[\left\langle \hat{a}_{\mathbf{k}_1}^{\dagger}\hat{a}_{\mathbf{k}_2}\right\rangle_{t'}\delta_{\mathbf{k}_3,\mathbf{k}_4}+\left\langle \hat{a}_{\mathbf{k}_1}^{\dagger}\hat{a}_{\mathbf{k}_3}\right\rangle_{t'}\delta_{\mathbf{k}_2,\mathbf{k}_4}\right],$$

where

$$\begin{split} \left\langle \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}'} \right\rangle_{t'} &= \mathrm{Tr} \hat{\rho}(t_0) \hat{U}_0^{\dagger} \left( t', t_0 \right) \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}'} \hat{U}_0 \left( t', t_0 \right) \approx \mathrm{e}^{i \left( \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} \right) \left( t' - t_0 \right)} \left\langle \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}'} \right\rangle (\mathbf{x}, t_0) \\ &= \mathrm{e}^{i \left( \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} \right) \left( t' - t_0 \right)} \delta_{\mathbf{k}, \mathbf{k}'} f \left( \mathbf{k}, \mathbf{x}, t_0 \right), \end{split}$$

and  $f(\mathbf{k}, \mathbf{x}, t_0)$  is the distribution function of the particles with momentum  $\mathbf{k}$  at position  $\mathbf{x}$ . This assumes, that the initial density matrix  $\hat{\rho}(t_0)$  is indeed diagonal in the momentum basis, which is a reasonable assumption, as decoherence times for the off-diagonal elements are short.

In the next step the time integral is performed. To this end, one introduces an infinitesimal convergence factor  $-\eta (t - t')$  in the exponent. When the difference in time becomes much longer than the collision time, one can formally set  $t_0$  to  $-\infty$  and the time integral becomes

$$\lim_{t_0\to-\infty}\int_{t_0}^t dt' \mathrm{e}^{i(\varepsilon_c+\varepsilon_1-\varepsilon_2-\varepsilon_3+i\eta)(t-t')} = iP\left(\frac{1}{\varepsilon_c+\varepsilon_1-\varepsilon_2-\varepsilon_3}\right) + \pi\delta\left(\varepsilon_c+\varepsilon_1-\varepsilon_2-\varepsilon_3\right),$$

as the integral is the Fourier transform of the Heaviside function.

Performing the analogous calculation for the third Hamiltonian  $\hat{H}_3$ , part of which cancel actually the contribution of the first Hamiltonian, and adding the two terms together gives finally

$$\left\langle \hat{\phi}^{\dagger}(\mathbf{x},t)\,\hat{\phi}(\mathbf{x},t)\hat{\phi}(\mathbf{x},t)\right\rangle$$

$$= -i2\pi \frac{g}{V^2} \Phi(\mathbf{x}, t) \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3} \left[ \delta\left(\varepsilon_c + \varepsilon_1 - \varepsilon_2 - \varepsilon_3\right) + \frac{i}{\pi} P\left(\frac{1}{\varepsilon_c + \varepsilon_1 - \varepsilon_2 - \varepsilon_3}\right) \right] \\ \times \delta_{m\mathbf{v}_s + \mathbf{k}_1, \mathbf{k}_2 + \mathbf{k}_3} \left[ f_1 \left(1 + f_2\right) \left(1 + f_3\right) - \left(1 + f_1\right) f_2 f_3 \right],$$

where  $f_i \equiv f(\mathbf{k}_i, \mathbf{x}, t)$ . This term is proportional to  $\sqrt{n_c}$  and vanishes thus when the condensate vanishes. One can perform an analogous calculation for the anomalous moment  $n_a = \langle \hat{\phi}(\mathbf{x}, t) \hat{\phi}(\mathbf{x}, t) \rangle$  and finds

$$n_{a}(\mathbf{x},t) = -i\pi \frac{g}{V} \Phi^{2} \sum_{\mathbf{k}_{1}\mathbf{k}_{2}} \delta_{\mathbf{k}_{1}+\mathbf{k}_{2},2m\mathbf{v}_{s}} \left[1+f_{1}+f_{2}\right] \left[\delta\left(\varepsilon_{1}+\varepsilon_{2}-2\varepsilon_{c}\right)+\frac{i}{\pi} P\left(\frac{1}{\varepsilon_{1}+\varepsilon_{2}-2\varepsilon_{c}}\right)\right].$$

This is a useful result, as it shows that for  $\mathbf{v}_s = 0$  and local thermal equilibrium when the  $f_i$  are the thermal Bose functions, the imaginary part vanishes and  $n_a$  is purely real. This is of course only valid for this particular approximation, and there might be higher orders in g that contribute. Needless to say that also  $n_a(\mathbf{x},t)$  vanishes when the local condensate vanishes.

Now we can also find the collision term in the quantum Boltzmann equation (3.5) using the same method. Inserting the definition of the Wigner operator (3.4) and the interaction Hamiltonian  $\hat{H}_{nc}$  into the Kubo formula (3.3), it becomes clear that there are two non-vanishing contributions, namely from  $\hat{H}_3$  and  $\hat{H}_4$  which by replacing the condensate terms with the polar representation can be locally approximated as

$$\hat{H}_{3}(\mathbf{x},t) \approx \frac{g\sqrt{n_{c}}}{\sqrt{V}} \sum_{\mathbf{k}_{1}\mathbf{k}_{2}\mathbf{k}_{3}} \delta_{m\mathbf{v}_{s}+\mathbf{k}_{1},\mathbf{k}_{2}+\mathbf{k}_{3}} \left[ e^{-i\theta(\mathbf{x},t)} e^{i\varepsilon_{c}(t-t')} e^{im\mathbf{v}_{s}\cdot\mathbf{x}} a_{\mathbf{k}_{1}}^{\dagger} a_{\mathbf{k}_{2}} a_{\mathbf{k}_{3}} + \text{h.c.} \right]$$
$$\hat{H}_{4}(\mathbf{x},t) \approx \frac{g}{2V} \left( \sum_{\mathbf{k}_{1}\mathbf{k}_{2}\mathbf{k}_{3}\mathbf{k}_{4}} \delta_{\mathbf{k}_{1}+\mathbf{k}_{2},\mathbf{k}_{3}+\mathbf{k}_{4}} a_{\mathbf{k}_{1}}^{\dagger} a_{\mathbf{k}_{2}}^{\dagger} a_{\mathbf{k}_{3}} a_{\mathbf{k}_{4}} - 4n \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \right).$$

Clearly, the first term does not conserve the thermal particle number because the number of creation and annihilation operators is not the same, whereas the second term does. So we will associate the first term with collision processes that involve the condensate, whereas the second term leads to equilibration within the thermal gas without a condensate.

The collision term can thus be decomposed into two contributions

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = C_{\Phi}\left[\Phi, f\right] + C_{th}\left[f\right]$$

There is a weak dependence of f on the condensate as well, but  $\Phi$  does not appear directly in the second collision term. The first term, using similar procedures as for the calculation of  $\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \rangle$  as well as those results for triple averages, is given by

$$C_{\Phi} [\Phi, f] = \frac{1}{i\hbar} \operatorname{Tr} \rho (t) \left[ \hat{f} (\hbar \mathbf{k}, \mathbf{x}, t_0), \hat{H}_3(t) \right]$$
  
=  $4\pi \frac{g^2 n_c}{V} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3} \delta (\varepsilon_c + \varepsilon_1 - \varepsilon_2 - \varepsilon_3) \, \delta_{m \mathbf{v}_s + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3}$   
 $\times \left[ \delta_{\mathbf{k}_1, \mathbf{k}} - \delta_{\mathbf{k}_2, \mathbf{k}} - \delta_{\mathbf{k}_3, \mathbf{k}} \right] \left[ (1 + f_1) \, f_2 f_3 - f_1 \left( 1 + f_2 \right) (1 + f_3) \right].$ 

One can see already the strong similarity with the term  $\Phi^* \langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \rangle$ , as these terms really describe the same collisions. For completeness we shall state the term  $C_{th}[f]$ 

$$C_{th}[f] = \frac{\pi g^2}{V^2} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \mathbf{k}_4} \delta\left(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4\right) \delta_{\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4} \\ \times \left[\delta_{\mathbf{k}_1, \mathbf{k}} + \delta_{\mathbf{k}_2, \mathbf{k}} - \delta_{\mathbf{k}_3, \mathbf{k}} - \delta_{\mathbf{4}_3, \mathbf{k}}\right] \left[f_1 f_2 \left(1 + f_3\right) \left(1 + f_4\right) - \left(1 + f_1\right) \left(1 + f_2\right) f_3 f_4\right].$$
(3.6)

As this term describes the collisions between particles and how they can change the occupations of said states, one would have to assume that in equilibrium, and if the system is unperturbed, the term  $C_{th}[f] = 0$ , which means that as many particles are scattered into a particular state as are scattered out of it. The distribution function for which this is true should be thermal, as this is what statistical physics predict. Indeed, as the Bose function  $f_B(x) = 1/(\exp[x] - 1)$  fulfills the equation

$$1 + f(x) = -f(-x),$$

the thermal Bose function makes the collision term disappear and confirms again that the Bose distribution is the correct equilibrium description of the gas. This means that the collision term really is only relevant when the particles are perturbed away from an equilibrium distribution.

We can use these results to find the growth rates of the condensate. First we can reduce to good approximation  $\sigma$  to

$$\sigma \approx \frac{2g}{\hbar} \mathrm{Im} \left[ \Phi^* \left\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \right\rangle \right],$$

just because to this order in g the anomalous density  $n_a$  is purely real.

It is this term that changes the number of condensate particles, because the number of thermal creation operators is not equal to the thermal annihilation operators, and must thus be a collision term. As such it depends on the state of the condensate and the occupation of thermal states.

Further we see that there is only a small offset of the Hartree Fock potential, which is either way dominated by the term 2gn close to transition. The effective source term can be incorporated into equation (2.10) to have an approximation for the growth dynamics of the condensate. The resulting equation is called the generalized Gross-Pitaevskii equation (GGP)

$$i\hbar\partial_t\Phi = \left[-\frac{\hbar^2\nabla^2}{2m} + gn_c + 2gn - iR\right]\Phi$$

where

$$R(\mathbf{x},t) = -\frac{g}{n_c(\mathbf{x},t)} \operatorname{Im}\left[\Phi^*(\mathbf{x},t)\left\langle \hat{\phi}^{\dagger} \hat{\phi} \hat{\phi} \right\rangle(\mathbf{x},t)\right].$$

An important insight is, that  $R(\mathbf{x},t)$  does not depend on the mean condensate density  $n_c$ 

$$R(\mathbf{x},t) = 2\pi \frac{g^2}{V^2} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \delta\left(\varepsilon_c - \varepsilon_1 - \varepsilon_2 - \varepsilon_3\right) \delta_{m\mathbf{v}_s + \mathbf{k}_1,\mathbf{k}_2 + \mathbf{k}_3}$$
$$\times \left[f_1\left(1 + f_2\right)\left(1 + f_3\right) - \left(1 + f_1\right)f_2f_3\right].$$

This suggests that this quantity is well-defined even at temperatures above criticality, when the system is in equilibrium and  $mv_s = 0$ . Let us assume in an ansatz, that even above the critical temperature we do have a fluctuation of the form

$$\Phi = \mathrm{e}^{(i\omega - \Gamma)t} \Phi(\mathbf{k}) \,.$$

Then, following the generalized GP equation, above  $T_c$ 

$$-\hbar\omega - \hbar\Gamma i = -\frac{\hbar^2 k^2}{2m} + 2gn - Ri$$

or

$$\Gamma = \frac{1}{\tau_0} = \frac{R}{\hbar},$$

the collision term R controls the lifetime of fluctuations. Next we want to argue that such an equation can be generalized to a Ginzburg-Landau functional that can even track some of the time-dependent behaviour of the order parameter of this specific transition.

### **3.2** The Ginzburg-Landau functional

We want to obtain an effective equation describing the fluctuations close to equilibrium, as part of a generalized Ginzburg-Landau functional. We then have to show that fluctuations can become significant close to equilibrium, so that their effects have to be estimated to get a full physical discription of the system.

The Ginzburg-Landau  $F[\Phi]$  functional describes the effective fluctuations of the macroscopic parameter  $\Phi$  and can formally be derived by the integration of the non-condensate fluctuations. For the partition function we know that

$$Z = \int d\Phi d\Phi^* d\phi d\phi^* e^{S[\Phi,\phi]} = \int d\Phi d\Phi^* e^{-\beta [F[\Phi] + F_0]}.$$

We know already that the generalized GP and the generalized Boltzmann equation is a good approximation to the action (at least to first order in g), so we can use this information to find a good estimate of  $F[\Phi]$ , which then is used to find the magnitude of the fluctuations by using the thermal properties.

The equilibrium action  $S[\Phi]$  is a sum over Matsubara frequencies. We can consider the action in terms of the original Bose fields  $\phi_B = \Phi_B + \phi$  in the complex field representation

$$\int d\Phi d\Phi^* d\phi d\phi^* e^{S[\Phi,\phi]} = \int d\Phi d\Phi^* d\phi d\phi^* e^{\int d\tau \phi_B^* (i\partial_\tau - H)\phi_B}$$
$$= \int d\Phi d\Phi^* d\phi d\phi^* e^{\int d\tau \left[\phi_B^* (i\partial_\tau - H)\phi_B + \langle H \rangle_{\phi} - \langle H \rangle_{\phi}\right]}$$
$$\approx \int d\Phi d\Phi^* e^{-\int_0^\beta \langle H \rangle_{\phi}} \int d\phi d\phi^* e^{\int d\tau \Delta S}$$
(3.7)

where  $\langle H \rangle_{\phi} = \int d\mathbf{x} \left[ \frac{\hbar^2 |\nabla \Phi|^2}{2m} - \mu |\Phi|^2 \right]$  is the GP Hamiltonian and we used that, as the field  $\Phi$  is only slowly evolving, the sum of the Matsurbara frequencies can be cut off to contain only the lowest Matsubara component n = 0, as it dominates the statistical behaviour. This approximation of the Bose field as a purely classical one is certainly only true for interacting bosons which are in a different universality class that the non-interacting bosons [72]. We showed previously that perturbations to  $\langle H \rangle_{\phi}$  are small  $\sim g^2$ . Thus the effective Ginzburg-Landau functional is

$$\beta F_{GL}[\Phi] = \int_0^\beta \langle H \rangle_\phi \, d\tau = \beta \int d\mathbf{x} \left( \frac{\hbar^2 |\nabla \Phi|^2}{2m} - \mu |\Phi|^2 \right),$$

whereas the remaining action is that of the thermal gas, depending for large T only weakly on  $\Phi$ . From that

action one can see, that the different **k** components of the slow condensate field have non-vanishing expectation values even if no condensate exists. These fluctuations are usually strongly suppressed, however as we will see shortly, close to criticality they are very soft and can become quite large. Indeed, because of the non-linear form of the GP equation ( $\mu$  contains the condensate field as  $gn_c = g|\Phi|^2$ ), the free energy functional can be approximated as

$$F[\Phi] = \int d\mathbf{x} \left[ \frac{\hbar^2}{2m} |\nabla \Phi|^2 + A[\tau] |\Phi|^2 + g |\Phi|^4 \right], \qquad (3.8)$$

where A is a function of the temperature in terms of the parameter  $\tau$ 

$$\tau = \frac{T - T_c}{T_c}.$$

A functional of that form was first phenomenologically introduced for conventional superconductors [73]. In statistical mechanics non-trivial solutions  $\Phi_{eq}$  to the saddlepoint equation  $\frac{\delta F[\Phi]}{\delta \Phi^*} = L[\Phi] = 0$  determine whether a condensate exists, which in the uniform case must be at  $\mathbf{k} = 0$ . As the free energy functional depends necessarily on powers of  $|\Phi|^2$  one can find for the condensate density

$$\frac{\partial F}{\partial |\Phi|^2} = A + 2g |\Phi|^2 = {}^! 0$$
$$\rightarrow n_c = |\Phi_{eq}|^2 = \frac{-A}{2g}.$$

This means that below the transition, A < 0 so that non-trivial solutions exist, and above the transition A > 0. Very close to the transition A becomes small, and the specific behaviour depends on the microscopics of the system

$$A \sim f(\tau).$$

In the following we will denote the  $\delta$  without index as a small parameter depending on  $\tau$ 

$$\boldsymbol{\delta}=f\left(\boldsymbol{\tau}\right).$$

#### CHAPTER 3. BOSONIC FLUCTUATIONS CLOSE TO CRITICALITY

Next we use the free energy (3.8) to find the fluctuations of the order parameter

$$\left\langle \left| \Phi_{\mathbf{k}}^{2} \right| \right\rangle = \frac{2mT}{\mathbf{k}^{2} + \xi_{0}^{-2} \delta}.$$
(3.9)

We have to keep in mind, that although above  $T_c$ ,  $\langle \Phi \rangle = 0$ ,  $\langle \Phi^2 \rangle$  can become significantly large. In reality the finite size of the system would limit the extent of the divergence. One also has to keep in mind that, close to criticality where the fluctuations become large, interactions among them cannot be neglected and one needs renormalization techniques to find the exact limiting exponent of divergence [74].

For some applications, like finding dynamic properties such as a quasi-conductivity, it is useful to extend the time-independent Ginzburg-Landau equations to contain time-like effects.

We want to show that the statistical fluctuations can be approximated by a dynamic Ginzburg-Landau equation that drives large fluctuations of the order parameter back to its equilibrium value, because this means that we have a stable system. The form of such an equation would be

$$-\gamma \frac{\partial \Phi(\mathbf{x},t)}{\partial t} = \frac{\delta F}{\delta \Phi^*}(\mathbf{x},t) + \zeta(\mathbf{x},t).$$
(3.10)

The left hand side of the equation is the time dependence of relaxation processes and depends on the parameter  $\gamma$ , which we have to infer from our microscopic observations. Additionally on the right-hand side we added a noise term  $\zeta(\mathbf{x},t)$ , which is necessary to allow for non-zero averages  $\langle |\Phi_k|^2 \rangle$ . Such a term can be derived in the Keldysh formalism [32] and stems from the collisions of non-thermal particles that spontaneously create a condensate droplet. Such a derivation is fairly elaborate and does not add much physical insight, as the size of the fluctuations predicted by equilibrium statistical physics (3.7) must be the same as the size predicted by the stochastic equation (3.10). This is a special case of an Einstein relation, that relates dynamical properties with equilibrium statistical properties.

To better motivate the equation, we have to look at the Boltzmann equation, especially the collision terms. We know that the collision integral (3.6) for the collisions between thermal particles,  $C_{th}$  vanishes when the particles are distributed according to the Bose distribution. Assuming that the thermal cloud is indeed thermal with a Bose distribution governed by the Hartree-Fock potential

$$f^{0}(\mathbf{k},\mathbf{x}) = \frac{1}{e^{\beta \left[\hbar^{2}\mathbf{k}^{2}/2m + U_{HF} - \mu\right]} - 1}$$

lets us approximate the cloud-condensate collision term as

$$R = \frac{g^2}{(2\pi)^2 \hbar} \int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 \delta \left(m\mathbf{v}_s + \mathbf{k}_1, \mathbf{k}_2 + \mathbf{k}_3\right)$$
$$\times \delta \left(\varepsilon_c - \varepsilon_1 - \varepsilon_2 - \varepsilon_3\right) \left(1 + f_1^0\right) f_2^0 f_3^0$$
$$\times \left[e^{\beta(\varepsilon_c - \mu)} - 1\right].$$

We see that the last term vanishes if  $\varepsilon_c = \mu$ . So to approximate the collision term we write

$$R \approx \frac{\hbar}{\tau_0} \left[ \mathrm{e}^{\beta[\varepsilon_c - \mu]} - 1 \right]$$

where

$$\frac{1}{\tau_0} \approx \frac{g^2}{(2\pi)^2 \hbar} \int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 \delta\left(m\mathbf{v}_s + \mathbf{k}_1, \mathbf{k}_2 + \mathbf{k}_3\right)$$
$$\times \delta\left(\varepsilon_c - \varepsilon_1 - \varepsilon_2 - \varepsilon_3\right) \left(1 + f_1^0\right) f_2^0 f_3^0.$$

Especially close to equilibrium we expect that  $\varepsilon_c$  is close to  $\mu$  which allows us to approximate even further

$$R \approx rac{\beta\hbar}{ au_0} \left[ arepsilon_c - \mu 
ight].$$

Now quite generally the time evolution of the order parameter can be written as

$$\frac{1}{\Phi}\partial_t \Phi = -\partial_t \theta + \frac{i}{2}\partial_t \log n_c.$$

We can recursively approximate the solution to the GP equation by using the Josephson relation,  $\dot{\theta} = \mu$ , in *R* 

$$R \approx \frac{\beta \hbar}{\tau_0} \left[ \frac{1}{\Phi} \partial_t \Phi - \mu \right]$$

and using this expression in the GP equation with the subsequent rotation  $\Phi \rightarrow e^{-i\mu t}$  to obtain

$$i[\hbar + i\gamma]\partial_t \Phi = \left[-\frac{\hbar^2 \nabla^2}{2m} + U_{HF} - \mu\right] \Phi = \frac{\delta F}{\delta \Phi^*},$$

where  $\gamma = \hbar \beta / 2\tau_0$ . A similar equation was first derived by Gardiner and Zoller [75]. If we now project this equation onto its real part we indeed obtain the time dependent Ginzburg-Landau equation where the time constant is microscopically identified. This also shows the close relationship between the GP description and the more phenomenological Ginzburg-Landau approach.

We have to question though, how reliable the equation is close (but not too close) to the transition. We have to confirm that the dynamics are not anomalous, i.e. that they do not freeze out at the transition and that  $\gamma$  becomes not too small. This calculation is done in the appendix and confirms the validity of the generalized Ginzburg-Landau functional, which shows that fluctuations are not as long lived and relaxation processes are actually quite fast due to an enhancement of the collision integral because of the bosonic nature of the particles. Importantly, no kinetic hindrance due to the thermal bosons is expected.

We can use the specific model (3.8) to get a better understanding of the fluctuations. For the time being we know that *A* at criticality is small. It also has the units of an energy. So we set  $A = T_c \delta$ , where  $T_c$  is again the critical temperature and a good reference energy and  $\delta$  is a small dimensionless parameter that depends on  $\tau$ . As we will show later, the actual function depends on the overall trapping. Rewriting the stochastic equation leaves us with

$$-\gamma \frac{\partial}{\partial t} \Phi(\mathbf{x},t) = \left(T_c \delta - \frac{\nabla^2}{2m}\right) \Phi(\mathbf{x},t) + \zeta(\mathbf{x},t),$$
$$\left[\gamma \partial_t + \left(T_c \delta - \frac{\nabla^2}{2m}\right)\right] \Phi = \zeta$$
$$\Phi = \frac{1}{\gamma} \left(\partial_t + \frac{1}{\tau_0} \left(\delta - \xi_0^2 \nabla^2\right)\right)^{-1} \zeta$$

where  $\tau_0 = \gamma/T_c$  is the time scale of the problem, whereas  $\xi_0$  is the typical lengthscale. In this context when using the critical temperature dependence of the uniform gas,  $\xi_0$  becomes the healing length of the condensate, or in a trap the healing length of the condensate in the center of the trap (apart from a numerical factor and of course the additional dependence on the trapping potential  $V(\mathbf{x})$ ).

#### CHAPTER 3. BOSONIC FLUCTUATIONS CLOSE TO CRITICALITY

Taking the Fourier transform

$$\Phi(\mathbf{k},\omega) = \frac{1}{\gamma} \left( i\omega + \frac{1}{\tau_0} \left( \delta + \xi_0^2 \mathbf{k}^2 \right) \right)^{-1} \zeta(\mathbf{k},\omega),$$

where we assumed that a noise spectrum exists. This equation allows us to relate the spectrum of the order parameter fluctuations to the spectrum of the semi-classical (white) noise term (which has no correlations between the different **k** and  $\omega$  components)

$$\left\langle \Phi^{*}\left(\mathbf{k},\omega\right)\Phi\left(\mathbf{k}',\omega'\right)
ight
angle =rac{\delta_{\mathbf{k},\mathbf{k}'}\delta_{\omega,\omega'}}{\left(\omega^{2}+rac{1}{ au_{0}^{2}}\left(\delta+\xi_{0}^{2}\mathbf{k}^{2}
ight)^{2}
ight)}rac{\left\langle |\zeta\left(\mathbf{k},\omega
ight)|^{2}
ight
angle }{\gamma^{2}}.$$

On the other hand we know by observation of the equilibrium free energy (3.8) that

$$\left\langle |\Phi_{\mathbf{k}}|^{2} \right\rangle = \frac{1}{2\pi} \int d\omega \left\langle |\Phi(\mathbf{k},\omega)|^{2} \right\rangle = \frac{1}{\left(\delta + \xi_{0}^{2} \mathbf{k}^{2}\right)},$$

from which the spectrum of  $\zeta$  can be inferred (Einstein relation) to be

$$\left\langle \left| \zeta \left( \mathbf{x}, \boldsymbol{\omega} \right) \right|^2 \right\rangle = 2T\gamma,$$

and that

$$\left\langle \left| \Phi_{\mathbf{k},\omega} \right|^2 \right\rangle = \left\langle \left| \Phi_{\mathbf{k}} \right|^2 \right\rangle \frac{2\tau_{\mathbf{k}}}{1 + \omega^2 \tau_{\mathbf{k}}^2}$$

where  $\tau_k = \tau_0 / (\delta + \xi_0^2 \mathbf{k}^2)$ . Using the Wiener-Khintchine theorem [76, 77], which relates the spectrum of a function to its autocorrelation, it follows that the spatial fluctuations decay with a **k** dependent life time

$$\left\langle \Phi_{\mathbf{k}}^{*}\left(0\right)\Phi_{\mathbf{k}}\left(t\right)\right\rangle =\left\langle \left|\Phi_{\mathbf{k}}\right|^{2}\right\rangle \mathrm{e}^{-\tau/\tau_{\mathbf{k}}}.$$

As one would expect, fluctuations with large spatial variation have not only a smaller amplitude, they also decay faster. Because  $\tau_0$  becomes rather small (see appendix), it is really only the static properties that should be experimentally accessible.

## 3.3 Trap specific properties

Whereas uniform systems are perhaps the easiest to calculate with, in reality almost all cold gas experiments involve some form of trapping. It is thus important to study how the traps might alter the physical observables.

As mentioned earlier, close to criticality the *A* term in the Gibzburg-Landau equation becomes small as  $A \sim T_c \delta$  where

$$\delta = f(\tau).$$

At this point we want to understand how  $f(\tau)$  behaves for different scenarios above the critical temperature.

The  $\tau$  behavior of the term *A* is dominated by the dependence of the chemical potential close to criticality. Even though the chemical potential at condensation is generally not zero when interactions are present, the behaviour of the chemical potential close to transition can be approximated by the free case. That is because thermodynamic quantities must converge when the interactions go to zero. The *A* term is independent of the overall offset of the chemical potential and for weak interactions the quasiparticles are well described by almost free bosons.

The condensation condition was such that at the transition the excited states are completely filled with all available particles in such a way, that any additional particle would occupy the ground state. Thus

$$N = C \int_0^\infty \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}} d\varepsilon = \left(\frac{T}{\hbar\omega_0}\right)^{d_\varepsilon} \mathrm{Li}_{d_\varepsilon}\left(\mathrm{e}^{\beta\mu}\right),$$

where C is a normalization constant and  $d_{\varepsilon}$  the energetic dimension as discussed previously.

The critical point is determined by  $\text{Li}_{d_{\varepsilon}}(1)$ . If the temperature is increased, then the chemical potential must change, as still the same total number of particles is in the excited states, as the ground state occupation can be

safely neglected. Thus

$$\begin{split} \Delta N &= N\left(T_{c}\right) - N\left(T_{c}\left(1+\tau\right)\right) = 0 \\ &= \left(\frac{T_{c}}{\hbar\omega_{0}}\right)^{d_{\varepsilon}} \left(\operatorname{Li}_{d_{\varepsilon}}\left(1\right) - (1+\tau)^{d_{\varepsilon}}\operatorname{Li}_{d_{\varepsilon}}\left(e^{\delta}\right)\right) \\ &\approx \left(\frac{T_{c}}{\hbar\omega_{0}}\right)^{d_{\varepsilon}} \left(\operatorname{Li}_{d_{\varepsilon}}\left(1\right) - (1+d_{\varepsilon}\tau)\operatorname{Li}_{d_{\varepsilon}}\left(1+\delta\right)\right) \\ &\approx \left(\frac{T_{c}}{\hbar\omega_{0}}\right)^{d_{\varepsilon}} \left(\operatorname{Li}_{d_{\varepsilon}}\left(1\right) - \operatorname{Li}_{d_{\varepsilon}}\left(1+\delta\right) - d_{\varepsilon}\tau\operatorname{Li}_{d_{\varepsilon}}\left(1\right)\right) \end{split}$$

Thus

$$\tau = -\frac{1}{d_{\varepsilon}} \frac{\operatorname{Li}_{d_{\varepsilon}}(1+\delta) - \operatorname{Li}_{d_{\varepsilon}}(1)}{\operatorname{Li}_{d_{\varepsilon}}(1)}.$$

The expansion of the polylogarithm depends on the dimension  $d_{\varepsilon}$ .

In general the polylogarithm can be expanded as [78]

$$\operatorname{Li}_{\alpha}(\mathbf{e}^{x}) = \Gamma(1-\alpha)(-x)^{\alpha-1} + \sum_{k=0}^{\infty} \frac{\zeta(\alpha-k)}{k!} x^{k}.$$

Slightly nontrivial is the case  $\alpha$  = integer, as here the  $\Gamma$  and  $\zeta$  function diverge, the divergences however cancel and

$$\operatorname{Li}_{\alpha}(\mathbf{e}^{x}) = \sum_{n=0}^{\infty'} \zeta(m-n) \frac{x^{n}}{n!} + \frac{x^{m-1}}{(m-1)!} [\psi(m) - \psi(1) - \log(-x)]$$
  

$$\to \sum_{n=0}^{\infty'} \zeta(m-n) \frac{x^{n}}{n!} + \frac{x^{\alpha-1}}{(\alpha-1)!} \left[ \sum_{h=1}^{\alpha-1} \frac{1}{h} - \log(-x) \right],$$

where the prime ' in the sum indicates that the term  $n = \alpha - 1$  is omited. The digamma function  $\psi = \frac{d \log \Gamma(z)}{dz}$  is the derivative of the logarithm of the gamma function.

For us of special interest is the case  $\alpha = d_{\varepsilon} = 2$ , as this is the only case where the logarithmic correction really is relevant. For the direct calculation of the  $\alpha = 2$  case we refer to the appendix. For the trapped gas in

Energetic dimension $d_{\varepsilon}$	Critical Temperature $T_c/\hbar\omega_0$	$\delta \mu/T_c$
1/2	n.a	n.a.
1	0	-
3/2	$\zeta^{-2/3}(3/2)N^{2/3}$	$-rac{1}{\pi}\left(rac{3\zeta(3/2)}{4} ight)^2 au^2$
2	$\sqrt{6}/\pi N^{1/2}$	$\sim  au / \log  au$
5/2	$\zeta^{-2/5}(5/2)N^{2/5}$	$-rac{5}{2}rac{\zeta(5/2)}{\zeta(3/2)} au$
3	$\zeta^{-1/3}(3)N^{1/3}$	$-rac{3\zeta(3)}{\zeta(2)} au$

Table 3.1: The most common trapping scenarios and the behaviour of the chemical potential close to criticality.

three dimensions  $\alpha = d_{\varepsilon} = 3$  and the chemical potential behaves as

$$rac{\delta\mu}{T_c}=\delta=-rac{3\zeta(3)}{\zeta(2)} aupprox-2.2 au.$$

For the uniform gas  $\alpha = d_{\varepsilon} = 3/2$  and the highest order term in the expansion of the polylogarithm is the square root. Then

$$\frac{\delta\mu}{T_c} = \delta = -\frac{1}{\pi} \left(\frac{3\,\zeta(3/2)}{4}\right)^2 \tau^2 \approx -1.2\,\tau^2.$$

One can see that both situations have a very different behaviour for the chemical potential, which might seem on first sight counter-intuitive, as locally in the trap center the system looks similar to the uniform system. But, because these are thermodynamic quantities that sample the whole system and equilibration to temperature  $T_c(1 + \tau)$  has to be achieved among all parts of the system, this is not a contradiction. We have seen earlier that the order parameter fluctuations grow as  $\delta^{-1}$ , which suggests that the temperature dependence in both systems is in fact different.

We have to mention the case  $d_{\varepsilon} = 5/2$ , which corresponds to a three-dimensional system that is harmonically trapped in two dimensions and free to move in the third dimension (like a cylindrical potential, however the trap strengths do not have to be equal). Expansion leads again to a linear behavior

$$\frac{\delta\mu}{T_c} = -\frac{5}{2} \frac{\zeta (5/2)}{\zeta (3/2)} \tau \approx -1.28\tau.$$

It is convenient to tabulate these findings 3.1.

How reliable are these models? Certainly the Ginzburg-Landau model only holds when fluctuations are a sufficiently small perturbations to the system as a whole. The necessary condition is better known as the Ginzburg-Levanyuk criterion [11, 79]. It is equivalent to stating that the overall effect of the Ginzburg-Landau action

$$S[\Phi] = \frac{1}{T} \int d\mathbf{x} \left( \frac{\hbar^2 |\nabla \Phi|^2}{2m} - \delta \mu |\Phi|^2 + \frac{g}{2} |\Phi|^4 \right)$$

is only a small perturbation with respect to the total action of the system. This action is indeed the zeroth Matsubara frequency component. As discussed earlier and in reference [72] it is only this term that contributes to the singular  $\tau$  behaviour close to transition, so this semiclassical approximation is justified for a weakly interacting dilute bosonic gas, but not for an ideal Bose gas.

As the fluctuation contribution is of the order  $e^{-S[\Phi]}$ , it is convenient to cast the action into the form

$$S = \chi \tilde{S}$$

with dimensionless action

$$\tilde{S} = \int d\mathbf{y} \left( |\nabla \Psi|^2 - |\Psi|^2 + |\Psi|^4 \right)$$

and the prefactor

$$\chi = \frac{2\sqrt{|\delta\mu|}}{gT_c} \left(\frac{\hbar^2}{2m}\right)^{3/2}.$$

If  $\chi \gtrsim 1$ , the fluctuations are relatively small. If we substitute the values of  $T_c$  and  $\delta \mu$  for the different scenarios we can find the Ginzburg number Gi. This gives for the uniform three dimensional case

$$\chi \equiv \frac{\tau}{\mathrm{Gi}},$$
 
$$\mathrm{Gi} \approx 20an^{1/3},$$

for the three dimensional harmonic trap and

$$\chi \equiv \left(\frac{\tau}{\text{Gi}}\right)^{1/2}$$
$$\text{Gi} \approx 30an^{1/3}$$

for the uniform gas.

It is not surprising that the unitless Ginzburg number depends on the dimensionless gas parameter  $an^{1/3}$  in both cases, as this is the defining dimensionless parameter of the system. However it is very remarkable that the prefactor to the small gas parameter is so large. It means that fluctuations are much stronger in the bosonic system than in conventional superconductors, where Gi is typically of the order of Gi  $\sim 10^{-12} \div 10^{-14}$  [11], which renders the superconducting fluctuation observation practically impossible (other fluctuation mechanisms are observable though). On the other hand for the typical dilute Bose gas with  $n \sim 10^{12} \div 10^{13}$  cm<sup>-3</sup> [11] and the scattering length  $a \sim 10^2$ nm, the Ginzburg number is generally larger than 1. Luckily in many experimental Bose systems the interactions can be finetuned via a Feshbach resonance (e.g. in [16]) such that *a* becomes very small indeed and the perturbative behaviour becomes observable.

Fluctuations tend to be more important in lower dimensional systems. Heuristically one can explain this with the fact that the fluctuations have less freedom and are hence more likely to add up to produce significant effects on observables. It is thus experimentally even more interesting to look at an anisotropically layered trap where the particles are either harmonically trapped or free within a layer and can tunnel between the different layers, as this system has a 2d-3d crossover. The model action for this system could be well approximated by a bosonic Lawrence-Doniach model [80]

$$S[\Phi] = \sum_{l} \int d\mathbf{x}^{2} \left( \frac{\hbar^{2}}{2m} |\nabla_{\parallel} \Phi_{l}|^{2} - \delta \mu |\Phi_{l}|^{2} + \frac{g}{2} |\Phi_{l}|^{4} + J |\Phi_{l+1} - \Phi_{l}|^{2} \right),$$

where l is the index of the layer and J is the tunneling term. If one zooms out of the system, then one basically recovers an anisotropic system. As the different layers are coupled and large differences in neighboring layers are energetically prohibited, one can in the limit of small distances and strong coupling between the layers

replace the absolute difference by a derivative along the z axis of the coarse grained system,

$$J \left| \Phi_{l+1} - \Phi_l \right|^2 \approx J \left| \ell \partial_z \Phi \right|^2 \equiv \frac{\hbar^2}{2m_z} \left| \partial_z \Phi \right|^2,$$

where  $\ell$  is the distance between layers and

$$m_z = \frac{\hbar^2}{2J\ell^2},$$

is the quasi mass in the z direction, which grows as the coupling between the layers becomes weaker.

Using that analogy, the critical temperature in the uniform case can be directly generalized

$$T_{c} = \frac{2\pi}{\left(\zeta\left(3/2\right)\right)^{3/2}} \frac{\hbar^{2} n^{2/3}}{\sqrt[3]{m^{2}m_{z}}} = T_{c}^{i} \left(\frac{m}{m_{z}}\right)^{1/3},$$

where the index *i* denotes the isotropic case.

As expected, weaker coupling between the planes lowers the critical temperature up to the point where no Bose condensation is expected (we avoid a discussion of phase transitions of the Kosterlitz-Thouless type, which could still happen in the resulting two dimensional system. This means we keep the coupling J strictly larger than zero).

We can next also find the Ginzburg-Levanyuk criterion which goes indeed as

$$\operatorname{Gi} = \operatorname{Gi}^{i} \left( \frac{m}{m_{z}} \right)^{1/6} \approx 22 \left( \frac{mJ\ell^{2}}{\hbar^{2}} \right)^{1/6}$$

This estimation will prove valuable in the estimation of crossover effects.

### 3.3.1 Comparison with fermionic superconductors

We would like to understand how the bosonic fluctuations relate to their fermionic counterparts. As the fluctuational contribution tends to be generally impossible to calculate exactly very close to the transition where interactions between fluctuations cannot be neglected and only perturbative solutions like the  $\varepsilon$  expansion (see [29]) exist, we want to focus on the one case that can be exactly calculated, namely the so-called zero-dimensional grain. If the size of the grain  $\ell$  on which the condensate sits is much smaller than the coherence length  $\xi$  of the fluctuations, then within the system variations of the order parameter do not matter and the action can be approximated as

$$S = \beta \left( -T_c \delta |\Phi|^2 + \frac{g}{2V} |\Phi|^4 \right),$$

where V is the volume of the grain and  $T_c \approx \hbar^2 N^{2/3} / 2m\ell^2$ . The partition function becomes

$$Z = \int d^{2} \Phi e^{-S[\Phi]} = \pi \int_{0}^{\infty} d|\Phi|^{2} e^{-\beta T_{c} \delta |\Phi|^{2} - \frac{\beta g}{2V} |\Phi|^{4}}$$
$$= \pi \sqrt{\frac{2V}{g\beta}} \int_{0}^{\infty} dx e^{-\beta T_{c} \delta \sqrt{\frac{2V}{g}} x - x^{2}}$$
$$= \pi \sqrt{\frac{2V}{g\beta}} e^{\left(\beta T_{c} \delta \sqrt{\frac{V}{2g\beta}}\right)^{2}} \int_{0}^{\infty} e^{-\left(x + \beta T_{c} \delta \sqrt{\frac{V}{2g\beta}}\right)^{2}}$$
$$= \sqrt{\frac{\pi^{3} V}{2g\beta}} e^{\left(\beta T_{c} \delta \sqrt{\frac{V}{2g\beta}}\right)^{2}} \left(1 - \operatorname{erf}\left(\beta T_{c} \delta \sqrt{\frac{V}{2g\beta}}\right)\right)$$

where  $\operatorname{erf}(x) = 2 \int_0^x e^{-t^2} dt / \sqrt{\pi}$  is the gaussian error function.

Naturally, we do not expect a real transition because the fluctuations smear out the transition at such low dimension, however we do expect a crossover between the small T and the high T case. Such a crossover can be expected in observables, like the heat capacity. For a real transition the heat capacity has a jump or at least a discontinuity. This can be explained by observing that while the thermal density barely changes, the condensate density varies sharply at the transition (2.4). The heat capacity per particle changes only slowly for the thermal phase, whereas particles in the condensate do not contribute, as the condensate occupies a single state which according to Nernst's theorem has no entropy and can thus not contribute to the heat capacity. The change in heat capacity thus comes directly from taking excitable particles and dropping them into the condensate. From a thermodynamical point of view, it is the discontinuity in  $\mu$  at the transition that is responsible. Since

$$\delta E = \left(rac{\partial E}{\partial T}
ight)_{\mu} \delta T + \left(rac{\partial E}{\partial \mu}
ight)_{T} \delta \mu$$

and the first term is smooth, whereas the second term jumps. Using  $C = (\partial E / \partial T)_V$ , it is clear that the jump



Figure 3.1: The heat capacity of the zero-dimensional system in terms of  $x = \beta T_c \delta \sqrt{\frac{V}{2g\beta}}$ .

across the transition is

$$\Delta C = \left(\frac{\partial E}{\partial \mu}\right)_T \left(\frac{\partial \mu}{\partial T}\right)\Big|_{T_{c^+}} - \left(\frac{\partial E}{\partial \mu}\right)_T \left(\frac{\partial \mu}{\partial T}\right)\Big|_{T_{c^-}} = \left(\frac{\partial E}{\partial \mu}\right)_T \left(\frac{\partial \mu}{\partial T}\right)\Big|_{T_{c^+}},$$

since  $\mu = \text{const}$  for  $T < T_c$ , at least in the non-interacting case, but changes only weakly in the interacting case (2.15). This behaviour is generally shared by the fermionic condensation, which is why here a comparison is reasonable.

Returning to the zero dimensional system, we can numerically differentiate the partition function to find the heat capacity  $C \sim T^2 \left( \frac{\partial^2 Z}{\partial \beta^2} \right)$  which is plotted in figure 3.1.

The transitional behaviour approximately happens in the interval  $-1 \le \beta T_c \delta \sqrt{\frac{V}{2g\beta}} \le 1$ , which means that in this particular case the Ginzburg-Levanyuk criterion can be approximated for  $\beta \approx T_c^{-1}$ 

$$\delta_c \sim \sqrt{\frac{E_{int}}{T_c}} \sqrt{\frac{\xi_0^3}{V}},$$

where  $\xi_0$  is the zero temperature healing length and  $E_{int} = gn_c$  the condensate energy. This approximation can be compared to the fermionic case [81]

$$\delta_c \sim \left(rac{T_c}{arepsilon_F}
ight) \sqrt{rac{\xi_0^3}{V}}.$$

Here it becomes clearer why for comparable systems the bosonic case has much stronger fluctuations, namely because the relevant energy scale in the system is much lower then in the Fermi case, where  $T_C/\varepsilon_F \sim 10^{-12} \dots 10^{-14}$ . There, fluctuations are just a small effect on top of a large Fermi sea, whereas in the bosonic system all the energy scales are easily of comparable size and the fluctuations become dominant, especially since the healing length is independent of the critical temperature. That being said, the Fermi systems usually studied are metallic electron systems, with very high Fermi energies. On the other hand, in a dilute cold gas context one can easily imagine conventional attractive fermionic systems that show also relatively large fluctuations, as the densities and therefore the Fermi energy is stronger decreased than the critical temperature .

We can investigate how the fluctuational corrections behave in real space. For instance, when we look at the correlation function in the GL approach (3.8)

$$egin{aligned} &\left\langle \phi(0)\phi^{\dagger}(\mathbf{x})
ight
angle &pprox rac{1}{V}\sum_{\mathbf{k}}\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}}\left\langle \left|\Phi_{\mathbf{k}}\right|^{2}
ight
angle \\ &pprox \sum_{\mathbf{k}}rac{\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}}}{\mathbf{k}^{2}+\xi_{0}^{-2}\delta}. \end{aligned}$$

It becomes clear that for smaller and smaller  $\delta$ , the  $\mathbf{k} = 0$  contribution becomes more and more important. If one turns the sum over the  $\mathbf{k}$  into an integral and extends to the complex plane, then it is the approach of the poles of  $(\mathbf{k}^2 + \xi_0^{-2}\delta)^{-1}$  towards the real axis that gives the large contribution. The outcome of the correlation function depends on the dimension (again Mermin-Wagner), but in three dimensions the above summation can be approximated to

$$\left\langle \phi(0)\phi^{\dagger}(\mathbf{x})\right\rangle \approx \int \frac{d^{3}\mathbf{k}}{(2\pi)^{3}} \frac{\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}}}{\left(k^{2}+\xi_{0}^{-2}\delta\right)} = \frac{\mathrm{e}^{-|\mathbf{x}|\sqrt{\delta}/\xi_{0}}}{4\pi|\mathbf{x}_{0}|}.$$

So the closer to transition, the longer the  $\phi$  correlations become, though they are not yet truly long-range. We want to identify which quantity in a fermionic superconductor is responsible for these long range correlations, so that we can better see where similarities and differences lie. As we previously observed, dilute fermionic gases have fluctuations of the same order of magnitude as the bosonic systems. It is not unreasonable to assume at this point that the fermionic and bosonic fluctuations can be related to each other in weakly dilute systems.

By looking at how fermions create the fluctuations we can learn about their potential relation to bosonic fluctuations. Fermions are principally different from bosons, namely that, depending on our starting point, either their annihilation and creation operators anticommute  $\{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^{\dagger}, \hat{c}_j^{\dagger}\} = 0$ ,  $\{\hat{c}_i, \hat{c}_j^{\dagger}\} = \delta_{ij}$ , or that their field representation is done via Grassmann fields rather than complex fields (see appendix for a short

introduction).

In the fermionic action with short range attractive interactions, one has to introduce a spin index  $\sigma = \uparrow, \downarrow$ (since otherwise a direct contact interaction is impossible due to  $\psi(\mathbf{x})^2 = 0$ )

$$S\left[\bar{\psi},\psi\right] = \int_{0}^{\beta} d\tau \int d\mathbf{x} \left[\bar{\psi}_{\sigma} \left(\partial_{\tau} - \frac{\nabla^{2}}{2m} - \mu\right) \psi_{\sigma} - gV \bar{\psi}_{\uparrow} \bar{\psi}_{\downarrow} \psi_{\downarrow} \psi_{\uparrow}\right].$$

This is the celebrated BCS action [6]. In normal BCS superconductors, the attractive interaction exists only in a band of width  $\omega_D$ , the Debye frequency, around the Fermi level which is due to the mechanism of phonon assisted attraction [82]. However, in a non-electronic system the attractive interaction can be different and an effective cut-off in momentum space does appear if the interaction is equipped with a finite range.

It is quite common that the fermions are charged and are coupled to an electromagnetic field. This coupling is generally very interesting, as it introduces a theory with local gauge invariance. But, as we are interested in the principal importance of the fluctuations, we skip this discussion. Furthermore, for experimental systems, neutral fermions that do not couple to the electromagnetic field are available, like  $^{40}$ K.

To deal with the quartic interaction one can introduce a complex field  $\Phi(\Phi(0, \mathbf{x}) = \Phi(\beta, \mathbf{x}))$  by way of a Hubbard-Stratonovich transformation

$$\mathrm{e}^{-g\int d\tau d\mathbf{x}\bar{\psi}_{\uparrow}\bar{\psi}_{\downarrow}\psi_{\downarrow}\psi_{\uparrow}} = \int D\Phi D\Phi^{*}\mathrm{e}^{-\int d\tau d\mathbf{x}\left[\frac{1}{gV}\Phi^{*}\Phi - \left(\Phi^{*}\psi_{\downarrow}\psi_{\uparrow} + \Phi\bar{\psi}_{\uparrow}\bar{\psi}_{\downarrow}\right)\right]},$$

which decouples the interaction term and leaves an action that is quadratic in the fermionic fields  $\psi_{\uparrow/\downarrow}$ . Here we already chose tentatively the Cooper channel via the field coupling  $\Phi \bar{\psi}_{\uparrow} \bar{\psi}_{\downarrow}$ . Recollecting the terms in the exponential into a matrix form for the so-called Nambu spinor  $\Psi = (\psi_{\uparrow}, \bar{\psi}_{\downarrow})^T$  leads to the partition function

$$Z = \int D\Phi D\Phi^* D\Psi D\bar{\Psi} \exp\left\{-\int d\tau \int d\mathbf{x} \left[\frac{1}{gV}\Phi^*\Phi - \bar{\Psi}\mathbf{G}^{-1}\Psi\right]\right\}$$
(3.11)

with

which is also called the Gorkov Green's function. Integrating over the Grassmann fields using (5.1) for the

discretized paths of the Grassmann fields and reexponentiating the determinant using the identity

$$\ln \det \mathbf{G}^{-1} = \mathrm{Tr} \ln \mathbf{G}^{-1}$$

gives the purely bosonic problem

$$Z = \int D\Phi D\Phi^* \exp\left[-\frac{1}{gV}\int d\tau d\mathbf{x}\Phi^*\Phi + \operatorname{Tr}\ln\mathbf{G}^{-1}\right].$$

This effective bosonic action can now be used to obtain a mean field solution for  $\Phi = \Phi_0 = \text{const.}$ , including Gaussian fluctuations that will mirror the bosonic Ginzburg-Landau equation for small amplitudes (3.8), and is in fact the original Ginzburg-Landau equation. To get there, we want to first take the saddle-point approximation by varying the action with respect to  $\Phi$ . Using that

$$\frac{\delta}{\delta\Phi} \operatorname{Tr} \ln \mathbf{G}^{-1} = \operatorname{Tr} \left( \mathbf{G} \frac{\delta}{\delta\Phi} \mathbf{G}^{-1} \right)$$

we find that

$$\begin{split} \Phi_0^* &= gV \operatorname{Tr} \left[ \begin{pmatrix} -\partial_{\tau} + \frac{\nabla^2}{2m} + \mu & \Phi \\ \Phi^* & -\partial_{\tau} - \frac{\nabla^2}{2m} - \mu \end{pmatrix}^{-1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right] \\ &= gV \operatorname{Tr} \left( \frac{\Phi_0^*}{\partial_{\tau}^2 + (-\nabla^2/2m - \mu)^2 + |\Phi_0|^2} \right) \\ &= gT \sum_{\mathbf{k}, \omega_n} \frac{\Phi_0^*}{\omega_n^2 + (\mathbf{k}^2/2m - \mu)^2 + |\Phi_0|^2}. \end{split}$$

Clearly  $\Phi_0 = 0$  is a valid solution, however, non trivial solutions are possible for small enough temperatures. One can find the temperature by performing the summation over the  $\omega_n$  as described in the appendix. Directly at the transition the order parameter is very small, so that  $|\Phi_0|^2$  can be set to zero and one obtains the saddle-point equation

$$1 = g \sum_{\mathbf{k}} \frac{1 - 2n_F(\boldsymbol{\xi}_{\mathbf{k}})}{2\boldsymbol{\xi}_{\mathbf{k}}} = g \sum_{\mathbf{k}} \frac{\tanh(\boldsymbol{\xi}_{\mathbf{k}})}{2\boldsymbol{\xi}_{\mathbf{k}}},$$

where  $\xi_{\mathbf{k}} = \mathbf{k}^2/2m - \mu$ . This saddle point approximation is clearly a function of  $\mu$  and  $T_c$  and one can find both



Figure 3.2: A cartoon that visualizes the relationship between the bosonic and fermionic fluctuations close to criticality. On the left hand side the attraction between the fermions is only weak and the Fermi surface is intact. Close to criticality Cooper resonance scattering becomes significant and couples fermions of opposite spin close to the Fermi edge. Below  $T_c$  the Cooper pairs condense and form a macroscopic condensate, though most fermions are still part of the Fermi sea. On the right hand side the fermions have been strongly coupled to create bosons consisting of fermions of opposite spin. It is known how the bosons behave above and below  $T_c$ . To find the relevant fluctuational contributions there are two ways to approach the problem (arrows), starting directly from the bosonic picture or transitioning from the fermionic fluctuational terms over to the strongly coupled bosonic side. We show that both approaches give the same result and the interacting Bose gas close to criticality can be viewed as a dilute system in which bosons form spontaneously unstable condensate droplets that have longer range coherences. Below  $T_c$  the bosons form the well-known long-range condensate.

in appropriate limits.

The important insight that helps us to understand bosonic fluctuation, is that very strongly attractive fermions become bound state bosons and that this transition is analytical. This is the famous BCS-BEC theory [83, 84], which also has been observed experimentally [85]. In one limit we have a purely fermionic gas with Fermi energy  $\varepsilon_F = (3\pi^2 n_F)^{2/3}/2m = k_F^2/2m$  and a weak effective coupling that destabilizes the Fermi surface only close to  $\varepsilon_F$ . In the opposite limit the pairs are strongly coupled and all the fermions are transformed into strongly bound composite bosons (see cartoon figure 3.2).

At each point the transition temperature is an analytic function of the effective scattering length a that is

related in three dimensions (e.g. [86]) to the bare interaction parameter g as

$$\frac{m}{4\pi a} = -\frac{1}{g} + \sum_{\mathbf{k}} \frac{1}{2\varepsilon_{\mathbf{k}}},$$

where  $\varepsilon_{\mathbf{k}}$  measures the energy above the chemical potential. Inserting this into the saddle-point equation allows us to derive the saddle-point condition including the tunable parameter *a* 

$$\frac{m}{4\pi a} = \sum_{\mathbf{k}} \left[ \frac{1}{2\epsilon_{\mathbf{k}}} - \frac{\tanh\left(\xi_{\mathbf{k}}/2T_{c}\right)}{2\xi_{\mathbf{k}}} \right].$$
(3.12)

Now we can take the limits. For very weak but attractive interactions, a < 0 and  $|k_F a| \ll 1$ , we know that the energy scale of the chemical potential is close to the Fermi energy  $\mu \approx \varepsilon_F$  and the critical temperature for a BCS system is recovered

$$\frac{m}{4\pi a} = \int d\varepsilon v(\varepsilon) \left[ \frac{1}{2\varepsilon} - \frac{\tanh\left[\left(\varepsilon - \varepsilon_F\right)/2T_c\right]}{2\left(\varepsilon - \varepsilon_F\right)} \right] = -\frac{mk_F}{2\pi^2} \ln\left(\frac{8\gamma\varepsilon_F}{\pi e^2 T_c}\right),$$

with  $v(\varepsilon) = m^{3/2}\sqrt{\varepsilon}/\sqrt{2\pi^2}$  and  $\gamma$  is the Euler constant. The critical temperature then becomes

$$T_c = \frac{8\gamma}{\pi e^2} \varepsilon_F \mathrm{e}^{-\pi/2|k_F a|}.$$

We have to keep in mind that the systems we are talking about are very dilute, so that  $\varepsilon_F$  is considerable smaller than in the usual metallic systems, where the overall scale of the critical temperature is instead given by  $\omega_D$ .

Now we want to expand the term  $Tr \ln G^{-1}$  for small  $\Phi$ , so we can get a picture of the system close to criticality. If we denote by  $G_0$  the  $\Phi = 0$  limit of G, then we can decompose

$$\operatorname{Tr}\ln\mathbf{G}^{-1} = \operatorname{Tr}\ln\left[\mathbf{G}_{0}^{-1}\left(1+\mathbf{G}_{0}\mathbf{Z}\right)\right]$$

where

Since  $\det \mathbf{Z}$  is small the expansion goes as

$$\begin{aligned} \operatorname{Tr}\ln\left[\mathbf{G}_{0}^{-1}\left(1+\mathbf{G}_{0}\mathbf{Z}\right)\right] &= \operatorname{Tr}\ln\mathbf{G}_{0}^{-1} + \operatorname{Tr}\ln\left(1+\mathbf{G}_{0}\mathbf{Z}\right) \\ &= \operatorname{Tr}\ln\mathbf{G}_{0}^{-1} - \sum_{n=0}^{\infty} \frac{1}{2n} \operatorname{Tr}\left(\mathbf{G}_{0}\mathbf{Z}\right)^{2n}, \end{aligned}$$

where the trace operation keeps only the even terms. This expansion was pioneered by Gorkov [87]. The first term is merely a constant and keeps the normalization and a finite constant  $F_0$  in the free energy. The quadratic term of the Hubbard-Stratonovich transformation can be combined with the second order term of (3.11)

$$\frac{1}{2}\mathrm{Tr}\left(\mathbf{G}_{0}\mathbf{Z}\right)^{2} = \frac{1}{2}\mathrm{Tr}\left(\mathbf{G}_{0,11}\Phi\mathbf{G}_{0,22}\Phi^{*}\right) = \sum_{\mathbf{q}}\frac{T}{V}\sum_{\mathbf{k}}G_{\mathbf{k}}G_{-\mathbf{k}+\mathbf{q}}\Phi^{*}\left(q\right)\Phi\left(q\right),$$

where  $G_p$  are the single particle fermionic Green's functions  $G(\mathbf{k}) = (i\omega_n - \mathbf{k}^2/2m + \mu)^{-1}$  to give

$$\sum_{\mathbf{q}} \left( \frac{1}{gV} - \sum_{\mathbf{k}} \frac{T}{V} G_{\mathbf{k}} G_{-\mathbf{k}+q} \right) \Phi^* \Phi(\mathbf{q}).$$

Again, for the case of fermions where all the action is concentrated around the Fermi level we substitute the relationship (3.12). It can be expanded in **q** to give

$$\left[A\tau+Cq^2\right]|\Phi(q)|^2$$

where  $A = v(\varepsilon_F)$  and  $C = v(\varepsilon_F) \frac{7\zeta(3)}{48\pi^2} \left(\frac{v_F}{T}\right)^2$ . The higher order terms of the expansion are well behaved and go as  $v(\varepsilon_F) T\left(\frac{|\Phi|^2}{T^2}\right)^n$ . So in this way one indeed recovers the Ginzburg-Landau equation with a well-defined transition. But more importantly we can get an understanding of what is happening on the microscopic level as the sum

$$\frac{1}{gV} - \frac{T}{V}\sum_{\mathbf{k}} G_{\mathbf{k}} G_{-\mathbf{k}+q}$$


Figure 3.3: The Dyson equation for the Cooper pair. The wavy line is the Cooper pair propagator, the solid lines belong to the single particle fermions. For each bubble the fermions have to have opposite spins, otherwise the interaction vertex (dot) would be zero. It is this propagator that causes the leading order fluctuational corrections in the BCS limit and in the strongly coupling limit.

has a well-defined meaning in the electron picture. Its inverse

$$\Gamma_q = \frac{gV}{1 - gT\sum_{\mathbf{k}} G_{\mathbf{k}+q}G_{-\mathbf{k}}}$$

diverges at the critical temperature and it is the Cooper vertex function describing the correlation function

$$C(q,\tau) = \frac{1}{V^2} \sum_{\mathbf{k},\mathbf{k}'} \left\langle \bar{\psi}_{\mathbf{k}+q,\uparrow}(\tau) \bar{\psi}_{-\mathbf{k},\downarrow}(\tau) \psi_{\mathbf{k}'+\mathbf{q},\downarrow}(0) \psi_{-\mathbf{k}',\uparrow}(0) \right\rangle$$

which signals the creation of new quasi-particles (see figure 3.3).

At the transition this correlation function diverges, similarly to the bosonic correlation function, as the result of an infinite sum of resonant scatterings close to the Fermi surface [88].

The two fermions with opposite spins weakly couple to form quasi-particles, the so-called Cooper pairs, and it is those contributions that are mainly responsible for fluctuational corrections above  $T_c$ . Because of the BEC-BCS analyticity we thus can find the bosonic fluctuations by replacing any Cooper vertices in the diagrams responsible for the fluctuational contributions by the standard bosonic propagator, for the boson is made up of the two fermions, as the Hubbard-Stratonovich transformation suggests.

We want to study the full propagator in three dimensions

$$\Gamma^{-1}(\mathbf{q},\omega_n) = \frac{1}{gV} - \frac{T}{V} \sum_{\mathbf{k}} G_{\mathbf{k}+q} G_{-\mathbf{k}}$$
  
=  $\frac{m}{4\pi a} - \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\tanh\left(\xi(\mathbf{k})/2T_c\right) + \tanh\left(\xi(\mathbf{k}-\mathbf{q})/2T_c\right)}{2\left(\xi(\mathbf{k}) + \xi\left(\mathbf{k}-\mathbf{q}\right) - i\omega_n\right)} - \frac{m}{\mathbf{k}^2},$  (3.13)

where  $q = (\mathbf{q}, \omega_n)$  and  $\omega_n$  is bosonic, because it is the difference of two fermionic Matsubara Green's functions and as usual  $\xi(\mathbf{k}) = \mathbf{k}^2/2m - \mu$ . Equation (3.13) can be evaluated in the strong coupling limit (a < 0) where the two fermions bind into one boson with binding energy  $E_B = 1/ma^2$ . The chemical potential approaches  $\mu \rightarrow -E_B/2$ , the binding energy per fermion, and for large binding energies we take the limit where the binding energy strongly exceeds the temperature ( $\mu/T \rightarrow -\infty$ ) and in the limit the vertex becomes

$$\Gamma(\mathbf{q},\omega_n) = \frac{m^2 a}{4\pi} \frac{\left(i\omega_n - \frac{\mathbf{q}^2}{4m} + (2\mu + E_B)\right)}{1 + \sqrt{1 + \frac{\left(-i\omega_n + \mathbf{q}^2/2m - \mu_B\right)}{E_B}}},$$
$$\stackrel{\mathrm{E}_{\mathrm{B}\to\infty}}{\to} \frac{m^2 a}{8\pi} \left(i\omega_n - \frac{\mathbf{q}^2}{4m} + (2\mu + E_B)\right)$$

which is exactly the inverse of a bosonic propagator for a particle of mass 2m, indicating a composite of two fermions, and an effective chemical potential that does not contain the binding energy anymore but is instead the weakly interacting boson chemical potential (the effective scattering length between the bosons is small in that limit  $a_{\text{eff}} \sim |a|$  [89, 90]). This limiting propagator was first described in this context in [90].

This first of all shows, that the fluctuational corrections we previously expected are just continuations of the fermionic theory of Aslamazov-Larkin (AL) type contributions [13] and therefore hardly surprising, the Ginzburg-Landau theory should be sufficient to describe their effects. On the other hand it can also be used to justify why other diagrams that are responsible for anomalous contributions of observables in disordered superconductors, for instance the Maki-Thomson contribution [14, 15] in the case of conductivity, will not appear in the bosonic case, since those diagrams cannot be contracted into bosonic diagrams, as they rely on the temporary splitting of Cooper pairs.

We are left to check that the leading order corrections are indeed as expected and that the subleading order corrections are suppressed. To generate the boson response we have to start from the current response function [33] where some couplings of the bosons to the external fields have been defined. The couplings themselves are not as interesting (we are looking for applications of non-charged bosons), but we can generate the corresponding fermionic response by replacing the boson propagators with the fluctuation propagator and connecting the free ends in all possible ways so that the number of internal fermions and spin are conserved. For the leading contribution there is one diagram (depicted in figure 3.4) that contributes with fourfold degeneracy.



Figure 3.4: The leading order contribution when the bosonic propagator in the polarisation bubble is replaced by the fluctuation propagator. Due to the internal spins of the constituting electrons, the diagram has a degeneracy factor of 4. The bubbles with the letter E symbolize the bosonic coupling to external fields.

One of the fluctuation propagators carries the four-momentum q, the other the four momentum q+Q, where Q is the externally transmitted momentum. Apart from the fluctuational propagators, there are two triangular Fermi structure that are contracted into a point for the pure bosonic case, with each giving the same contribution

$$T(q,Q) = T \sum_{\omega_n} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{2(\mathbf{k}+\mathbf{q}) + \mathbf{Q}}{2m} G(-k)G(k+q)G(k+q+Q)$$
$$= 2\frac{\mathbf{q}+\mathbf{Q}}{2m}C(q,Q).$$

The factor C(q,Q) vanishes quickly as  $E_B$  grows and leads to leading order in the limit  $\mu/T \to -\infty$  to

$$C(0,0) = -\frac{m^{3/2}}{16\pi} \frac{1}{\sqrt{2\,|\mu|}}$$

The prefactors of the strongly bound bosons contribute as  $\sim a^{-2}$ , whereas the two triangles go as  $\sim \mu^{-1} \sim E_B^{-1} \sim ma^2$ , so the resulting diagram returns the bosonic response coming from the bosonic Ginzburg-Landau action without any remnants of the underlying fermionic structure.

On the other hand one should check that the terms that are subleading but important in the fermionic case (see figure 3.5) vanish in the strong coupling limit. These terms only contain one fluctuation propagator and hence no bosonic counterpart exists.

Interestingly, these terms do not vanish in the strongly bound limit. However, their contributions  $\sim n/m$  exactly cancel each other in the clean system [91, 17]. For fermionic disordered systems these terms generally do not cancel though [92, 93]. The effects rely on the Cooper pair temporarily dissociating and the single fermions staying close enough to each other to interfere (hence the dependence on the disorder). We cannot expect effects like that for purely bosonic systems, as these do lack the internal structure for such processes.



Figure 3.5: Subleading fluctuation diagrams. a) The Maki-Thompson (MT) term and b) the DOS term. Both contain only one fluctuational propagator.

We can thus conclude that the close to criticality theory for interacting bosons is generally simpler than for fermions because fewer diagrams have to be taken into account. This can be specifically applied to the case of conductivity where anomalous corrections to the bosonic conductivity can be expected, but they are merely of the simpler Aslamasov-Larkin type. It should also be noted that the transport measurements neccessary to observe such contributions are very difficult, which is why we rather focus on the observation of the magnetic susceptibility in the next part.

## **3.4 Rotation and artificial magnetic fields**

In the history of the research of superconducting fluctuations, magnetic properties were the observable of choice, mostly because SQUID techniques allow for a very precise measurement of small quantities, like the fluctuational susceptibility (e.g. [94]).

Similar measurements will most likely be the forefront of bosonic fluctuational measurements as well, for flow and current transport measurements are currently difficult to control and as we will see, (quasi) magnetic/rotational measurements should be easier to implement.

To clarify the connection between magnetic and rotational properties we will essentially follow the argument in Leggett's book [26]. We will look at a uniformly rotating bosonic system and find its description in the rotating frame. The resulting Hamiltonian will in general contain extra terms that depend on the angular rotational frequency  $|\omega|$ . The derivation of the susceptibility is a generalization of the superconducting fluctuational response [95, 81].

Since we need the result later, we will consider here a general rotation that is not around the trap center, but rather the whole trap rotates around a point that is not the center of its coordinate system.

Let **R** be the position of the rotating center of the trap potential in the coordinate system (centered around that rotational point) in the frame that is at rest. Let us for now focus on a single particle. The velocity of that particle can be decomposed into the velocity of the moving rotation center  $\dot{\mathbf{R}}$  and the remainder  $\mathbf{v}'$ 

$$\mathbf{v} = \mathbf{v}' + \dot{\mathbf{R}}$$

We will perform two transformations. The first is the translation into the frame moving with velocity  $\dot{\mathbf{R}}$  that leads to the Lagrangian

$$L = \frac{m\mathbf{v}^2}{2} - m\ddot{\mathbf{R}} - V,$$

where the prime on the **v** was omitted.

The next step is to transform into a frame that rotates around the center of the trap. This time the velocity is split according to the prescription

$$\mathbf{v}' = \mathbf{v} + \boldsymbol{\omega} \times \mathbf{r},$$

with **r** being the position from the trap center.

The Lagrangian in the rotating frame becomes

$$L = \frac{m\mathbf{v}^2}{2} + m\mathbf{v} \cdot \boldsymbol{\omega} \times \mathbf{r} + \frac{m}{2} \left(\boldsymbol{\omega} \times \mathbf{r}\right)^2 - m\ddot{\mathbf{R}}\mathbf{r} - V.$$

As we are in a rotational frame, the vector **R** is rotating. If we let the operator of rotation be  $R_t$ , then

$$\mathbf{R}_t = R_t \mathbf{R}_0$$

and because it is a rotation

$$\ddot{\mathbf{R}} = \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{R}) = -\boldsymbol{\omega}^2 \mathbf{R}$$

In the rotating frame,  $\mathbf{r} \to R_t \mathbf{r}$ . This then also means that the scalar product  $\mathbf{\ddot{R}} \cdot \mathbf{r}$  is time independent. The rotating potential in the rest frame has the form

$$V\left(\mathbf{r}\right) = V_0\left(R_t^{-1}\left(\mathbf{r} - \mathbf{R}_t\right)\right)$$

which after the two transformations is also time-independent  $V(\mathbf{r}) = V_0(\mathbf{r})$ .

To obtain the proper prescription for the Hamiltonian we use the canonical momentum

$$\frac{\partial L}{\partial \mathbf{v}} = \mathbf{p} = m(\mathbf{v} + \boldsymbol{\omega} \times \mathbf{r})$$
$$\Rightarrow \mathbf{v} = \frac{\mathbf{p}}{m} - \boldsymbol{\omega} \times \mathbf{r}.$$

The full Hamiltonian is then

$$H = \mathbf{v}\mathbf{p} - L(\mathbf{v}[\mathbf{p}, \mathbf{r}], \mathbf{r})$$
  
=  $\frac{\mathbf{p}^2}{2m} - \omega(\mathbf{r} \times \mathbf{p}) - m\omega^2 \mathbf{R}_0 \mathbf{r} + V(\mathbf{r}).$ 

This can be put into the form of an effective vector potential

$$H = \frac{(\mathbf{p} - m(\boldsymbol{\omega} \times \mathbf{r}))^2}{2m} - \frac{m}{2}\omega^2 \mathbf{r}^2 - m\omega^2 \mathbf{R}_0 \mathbf{r} + V(\mathbf{r}).$$

We see that the potential the particle feels is weakened by the term  $-\frac{m}{2}\omega^2 \mathbf{r}^2$ , which is the equivalent of the centrifugal force that distorts the trap. The third term just shifts the center of the trap slightly.

Of prime interest for us is the artificial gauge potential

$$m(\boldsymbol{\omega} \times \mathbf{r}) \equiv \mathbf{A}(\mathbf{r}) = \frac{1}{2} (\mathbf{B} \times \mathbf{r}),$$

where the last equivalence is merely a convenient choice of gauge. This leads to the correspondence

$$\mathbf{B} = 2m\omega$$
.

Interestingly, the cyclotron frequency of the magnetic field  $\omega_B = B/m$  is twice the rotation frequency

$$\omega_B = 2\omega$$
,

something not immediately obvious.

The generalization to the multi-particle interacting Hamiltonian is straightforward

$$H[\{\mathbf{r}_i, \mathbf{p}_i\}] = \sum_i \left(\mathbf{p}'_i - m(\boldsymbol{\omega} \times \mathbf{p}_i)\right)^2 / 2m + \sum_i V_i(\mathbf{r}_i) + \frac{1}{2} \sum_{ij} U\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right),$$

where the  $V_i$  are the weakened and shifted potentials, and U is the interaction term, which is invariant under rotations.

This shows us that a rotation can simulate a magnetic field (up to an overall potential, that can be counteracted by fine tuning the trap). In the next step we calculate the magnetic susceptibility of the fluctuations and find a suitable interpretation.

# 3.5 Calculation of the magnetic susceptibility

We first start with the case of the magnetic susceptibility in the anisotropic case. The susceptibility per particle is defined as

$$\chi_{fl} = -\frac{1}{N} \frac{\partial^2 F_{fl}}{\partial \omega_B^2} = -\frac{1}{4N} \frac{\partial^2 F_{fl}}{\partial \omega^2} = -\frac{1}{4N} I_{fl},$$

where  $F_{fl}$  is the fluctuational contribution to the free energy,  $\omega$  the equivalent rotational frequency, and  $I_{fl}$  is the moment of inertia in the rotating frame. We thus are looking for corrections to the moment of inertia of the bosonic system. Namely a superfluid resists an external rotation and the contribution we are about to calculate,  $\chi_{fl}$  is the fluctuational precursor of the Hess-Fairbanks effect, which is the equivalent of the Meissner effect in superconducting systems. We want to look at a system that is layered in one direction and continuous in the other two directions. Such a system in of great interest, as it is experimentally feasible and, as we show later, lets us explore different dimensionalities. To obtain the fluctuational free energy, we diagonalize the Lawrence-Doniach action with magnetic field applied along the z-direction  $B\mathbf{e}_z = \nabla \times \mathbf{A}$ 

$$S[\Phi] = \sum_{l} \int d\mathbf{x}^{2} \left( \frac{\hbar^{2}}{2m} \left| \left( \nabla_{\parallel} - \mathbf{A} \right) \Phi_{l} \right|^{2} - \delta \mu \left| \Phi_{l} \right|^{2} + \frac{g}{2} \left| \Phi_{l} \right|^{4} + J \left| \Phi_{l+1} - \Phi_{l} \right|^{2} \right),$$
(3.14)

and then integrate out the various modes. The wave functions that diagonalize the uniform system ( $\delta \mu = -c_2 T_c \tau^2$ ) with an applied uniform magnetic field are the well known Landau functions [96]. Per definition the magnetic field is applied perpendicular to the layers of the system, that is along the *z* - axis. Because the system is periodic along the *z*-direction, the  $k_z$  are good quantum numbers as well. We thus expand the order parameter / wave function as

$$\Phi(\mathbf{x}) = \sum_{n,k_z} \Phi_{n,k_z} \phi_n(\rho) e^{ik_z z}, \qquad (3.15)$$

where  $\phi_n$  is the wave function of the *n*th Landau level and  $\rho$  is the position vector within the layer. The  $k_z$  are restricted to the first Brillouin zone. Substituting (3.15) into (3.14), the energy of each state in terms of the quantum numbers is

$$E_{n,k_z} = -\delta\mu + \hbar\omega_B \left(n + 1/2\right) + 2J\cos\left(k_z\ell\right),$$

with  $\omega_B$  being the cyclotron frequency in terms of the artificial magnetic field. As the action is quadratic, we may use that

$$Z = e^{-F_{fl}/T_c} = \int D\Phi D\Phi^* e^{-\Phi^* G\Phi}$$
$$= \det G^{-1}$$

so that the fluctuation free energy of the independent fluctuational modes becomes

$$F_{fl} = \frac{BA}{\Phi_0} T_c \sum_{n,k_z} \log \frac{\pi T_c}{\delta \mu + \hbar \omega_B \left(n + 1/2\right) + 4J \sin^2\left(k_z \ell/2\right)},$$

where A is the effective surface of the layers that are probed by the field (as the free energy is extensive and we

probe just a small part of the bulk system, we do not care about boundary effects) and  $\Phi_0 = 2\pi\hbar$  is the elementary flux known from standard quantum mechanics [96]. As the sum itself is divergent, one has to introduce a cutoff level  $n_c \sim T_c/\hbar\omega_B \sim 1/h$ , which corresponds roughly to the highest states that are considerably occupied at temperature  $T_c$ . Here *h* is the reduced magnetic field

$$4h \equiv \frac{\hbar B}{mT_c c_2},$$

where  $c_2$  is the proportionality factor between the chemical potential and the small parameter  $\tau^2$  close to transition. We can use that  $\sum \log(...) = \log \prod(...)$ . As the formulas become more involved, we introduce for short hand

$$\kappa = \tau^2 + \frac{\eta_2}{2} \left( 1 - \cos(k_z \ell) \right)$$

with

$$\eta_2 = \frac{4J}{T_c c_2}$$

is an anisotropy parameter which is small for a very two-dimensional system.

Next one uses the identity [78]

$$\Gamma(z) = \lim_{n_c \to \infty} \frac{n_c! n_c^{z-1}}{z(z+1)(z+2)\cdots(z+n_c-1)}$$

to obtain the following approximation for the free energy

$$F_{fl} \approx \frac{BA}{\Phi_0} T_c \sum_{k_z} \left\{ n_c \log\left[\frac{\pi}{4hc_2}\right] + \log\left[\Gamma\left(\frac{1}{2} + \frac{\kappa}{4h}\right) - \log\left[n_c! n_c^{\kappa/4h-1/2}\right]\right] \right\}.$$

Because we are only interested in the magnetic contribution, but not so much in the overall offset, so it is useful to expand in terms of the reduced magnetic field h

$$F(h) - F(0) = \frac{AN_{\ell}T_{c}}{\pi\xi_{0}^{2}} \int_{-\pi/\ell}^{\pi/\ell} \frac{\ell dk_{z}}{2\pi} \frac{h^{2}}{3\kappa} = \frac{AN_{\ell}T_{c}h^{2}}{3\pi\xi_{0}^{2}} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \left(\tau^{2} + \frac{\eta_{2}}{2}\left(1 - \cos\left(\theta\right)\right)\right)^{-1},$$

where we have again a lengthscale of the fluctuations  $\xi_0^2 = \hbar^2/2mc_2T_c$  and  $N_\ell$  is the number of layers that are

probed. The remaining integral can be evaluated [78]

$$\int_0^{\pi} \frac{d\theta}{2\pi} \left( \tau^2 + \frac{\eta_2}{2} \left( 1 - \cos(\theta) \right) \right)^{-1} = \left[ \tau^2 \left( \tau^2 + \eta_2 \right) \right]^{-1/2}.$$

Thus we can see that

$$F(h) - F(0) = \frac{AN_{\ell}T_{c}h^{2}}{3\pi\xi_{0}^{2}} \frac{1}{\sqrt{\tau^{2}(\tau^{2} + \eta_{2})}}$$
  

$$\rightarrow \chi = -\frac{1}{N_{\ell}}\frac{\partial^{2}F}{\partial h^{2}} = \frac{2AT_{c}}{3\pi\xi_{0}^{2}}\frac{1}{\sqrt{\tau^{2}(\tau^{2} + \eta_{2})}}.$$
(3.16)

This is indeed very interesting. Not only is the fluctuation contribution to an actual observable divergent (one has to keep in mind that in order to apply the GL theory one has to have that  $\tau > \text{Gi}$ ), it also diverges in a different power law compared to the superconducting case, where it goes as  $\sim [\tau(\tau + \eta)]^{-1/2}$ . We observe that the dimensionality of the trap is important. For  $\tau^2 \gg \eta_2$ , the system is essentially two-dimensional and  $\chi \sim 1/\tau^2$ , whereas for  $\tau \ll \eta_2$  the coherence along the *z* direction is increasing and extends beyond the layers, therefore making the system more three-dimensional with  $\chi \sim 1/\tau$ . This comes along with another important observation, namely that the powerlaw exponent in higher dimension tend to be smaller and in general there will be a dimension for which the fluctuations will not diverge, the upper critical dimension [11].

Next we look at the case of a two-dimensionally trapped system. First we have to diagonalize the action

$$S[\Phi] = \int d^2 \mathbf{x} \left( \frac{\hbar^2}{2m} \left| (\nabla - \mathbf{A}) \Phi \right|^2 - \delta \mu \left| \Phi \right|^2 \right),$$

where  $\mu \sim \tau/\log \tau$  for small  $\tau$ . We do know already from the previous observations, that the situation is very similar to a two dimensionally trapped system with an applied rotation. Thus the diagonalization of the action is equivalent to diagonalizing the two dimension harmonic oscillator  $H_{2d}$  with applied rotation

$$\begin{split} H &= H_{2d} - \omega L_z, \\ H_{2d} &= \frac{1}{2m} \left( p_x^2 + p_y^2 \right) + \frac{m\omega_0^2}{2} \left( x^2 + y^2 \right) = \hbar \omega_0 \left( \frac{P_X^2}{2} + \frac{P_Y^2}{2} + \frac{X^2}{2} + \frac{Y^2}{2} \right), \\ L_z &= x p_y - y p_x, \end{split}$$

where the coordinates and momenta are quantum operators with  $[x, p] = i\hbar$  and for convenience we shifted to the dimensionless spatial operators  $X/Y = \sqrt{\frac{m\omega_0}{\hbar}} x/y$  and the dimensionless momenta  $P_{X/Y} = \frac{1}{\sqrt{m\hbar\omega_0}} p_{x/y}$ . It is useful to introduce the creation and annihilation operators that diagonalize the harmonic action by defining the creation and annihilation operators of an harmonic excitation in x/y direction

$$a_x = \frac{X + iP_X}{\sqrt{2}}, a_x^{\dagger} = \frac{X - iP_X}{\sqrt{2}},$$
$$a_y = \frac{Y + iP_Y}{\sqrt{2}}, a_y^{\dagger} = \frac{Y - iP_Y}{\sqrt{2}}.$$

These operators fulfill the relation  $[a, a^{\dagger}] = 1$  while at the same time

$$H_{2d} = \hbar\omega_0 \left( a_x^{\dagger} a_x + a_y^{\dagger} a_y + 1 \right)$$

In that same basis, the angular momentum operator becomes

$$L_z = xp_y - yp_x = \hbar (XP_Y - YP_X)$$
$$= i\hbar (a_y^{\dagger}a_x - a_x^{\dagger}a_y).$$

One sees that the angular momentum mixes the x and y components. We introduce the mixed creation and annihilation operators

$$a_{\pm} = rac{a_x \pm i a_y}{\sqrt{2}}, \qquad \qquad a_{\pm}^{\dagger} = rac{a_x^{\dagger} \mp i a_y^{\dagger}}{\sqrt{2}},$$

for which

$$L_z = \hbar \left( a_+^{\dagger} a_+ - a_-^{\dagger} a_- \right),$$

while leaving the principal form of the harmonic oscillator intact

$$H_{2d} = \hbar \omega_0 \left( a_+^{\dagger} a_+ + a_-^{\dagger} a_- + 1 \right)$$

These diagonalize the Hamiltonian H

$$H = H_{2d} - \omega L_z$$
  
=  $\hbar (\omega_0 + \omega) a_-^{\dagger} a_- + \hbar (\omega_0 - \omega) a_+^{\dagger} a_+ + \hbar \omega_0.$ 

We thus have the degeneracy of the two levels of the Hamiltonian lifted by an application of a magnetic field, as  $\omega = \omega_B/2$ . We apply this diagonalization to the free energy (switch the indices  $\pm$  for better intuition)

$$F[\tau,B] = T_c \sum_{n_{\pm}} \log \frac{\pi T_c}{\hbar(\omega_0 + \omega)n_+ + \hbar(\omega_0 - \omega)n_- + \hbar\omega_0 - \mu(\tau)}.$$

It is useful to change to the new quantum numbers  $n = n_+ + n_-$  and  $m = n_+ - n_-$  where for each *n* the allowed *m* values are  $m \in \{-n, -n+2, ..., n-2, n\}$ , so there are n + 1 terms. Then

$$F[\tau, B] = T_c \sum_{n,m} \log \frac{\pi T_c}{\hbar \omega_0 n + \hbar \omega_B m + \hbar \omega_0 - \mu(\tau)}$$
$$= T \sum_{n,m} \log \frac{1}{An + Mm + C},$$

where  $A = \hbar \omega_0 / \pi T_c$ ,  $M = \hbar \omega / \pi T_c$  and  $C = (\hbar \omega_0 - \mu) / \pi T_c$ .

The susceptibility can thus be expressed as

$$\chi = T_c \left(\frac{\hbar}{2\pi m T_c}\right)^2 \left.\frac{\partial^2 F}{\partial B^2}\right|_{B\to 0}$$
$$= T_c \left(\frac{\hbar}{2\pi m T_c}\right)^2 \sum_{n,m} \frac{m^2}{An + Mm + C}.$$

The sum over the m terms can be performed by noticing that

$$\sum_{m} m^{2} = (-n)^{2} + n^{2} + (-(n-2))^{2} + (n-2)^{2} + \dots$$
$$= 2 \sum_{n'}^{n/2} (2n')^{2} = \frac{1}{3}n(n+1)(n+2),$$

independent of whether n is even or odd.

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The remaining sum over n can be approximated by the integral

$$\Xi \sim \frac{T}{3} \left(\frac{\hbar}{2\pi mT_c}\right)^2 \int_0^{n_c} dn \frac{n(n+1)(n+2)}{(An+C)^2},$$

where we reintroduced the cutoff  $n_c \sim T_c/\hbar\omega_0$ .

The question is now, of whether one could observe a significant contribution from the  $\tau$  dependence. For small  $\tau$  (and hence small *C*) and fixed  $n_c$  the integral is not vanishing. Noticing that  $n_c \sim A^{-1}$  we can easily see that the non *C* dependent contribution

$$\sum_{n}^{n_{c}} \frac{n^{2}}{\left(An+C\right)^{2}} \sim \frac{1}{A^{3}},$$

whereas the most divergent (in C) term goes as

$$\sum_{n=1}^{n_c} \frac{2}{(An+C)^2} \approx \frac{2}{A} \int_0^1 \frac{dy}{(y+C)^2} = \frac{2}{AC} \int_0^{1/C} \frac{dx}{(x+1)^2} \sim \frac{1}{AC}.$$

This means that the relative importance between the fluctuational part and the ordinary oscillator part goes as  $A^2 \sim \left(\frac{\hbar\omega_h}{T_c}\right)^2 \to 0$ , which goes to zero in the thermodynamic limit. The thermodynamic limit is defined as  $N \to \infty$  and  $\omega_0 \sim N^{-1/2}$  and  $T_c = \text{const.}$  Thus in the thermodynamic limit the fluctuation contribution vanishes which shows that for the harmonic oscillator d = 2 is the upper critical dimension! As d = 1 is the lower critical dimension for harmonic oscillators, these systems are technically never strongly fluctuating. This seems at first sight maybe counterintuitive, as the center of a flat trap can be approximated by a uniform system. However, the fluctuations will be cutoff at the point where the harmonic potential becomes sufficiently strong and, as we just showed, the majority of the contribution does come from the rest of the trap. In hindsight it is not surprising at all though. We know that a uniform system has an upper critical dimension d = 4, and as each harmonic confinement adds one degree of freedom to the Hamiltonian, so that the effective Hamiltonian degrees of freedom are 2*d*. Thus a critical dimension of 4 in the uniform system exactly corresponds to a critical dimension of 2 for the trapped system.

This however does not rule out that critical fluctuations cannot be observed, rather that the trap has to be selectively probed in the center where the system is quasi-uniform, instead of probing the total susceptibility of the trap. For the case of the system that is harmonically trapped in two dimensions while being in a layered configuration as in the Lawrence-Doniach model, the susceptibility density becomes, provided it is applied to the center region of the stack where the uniformity assumption holds,

$$\chi = \frac{2AN_{\ell}T_{c}h^{2}}{3\pi\xi_{0}^{2}}\frac{1}{\sqrt{\tau(\tau+\eta)}},$$
(3.17)

where  $\xi_0^2 = \hbar^2/2mc_2T_c$  with  $c = 5\zeta(5/2)/2\zeta(3/2) \approx 1.284$  and A is the area over which the system is probed.

One should of course keep in mind that all calculations of the susceptibility were done in the rotated frame. That means that in the original lab frame, the fluctuational contribution obtains an additional overall minus sign. This means that the system will react less drastically to the influence of the rotation. One can interpret these observations as an extension of the Hess-Fairbanks effect to the high temperature side of the transition, i.e. the superfluid part of the system resists an external rotation. This effect is certainly linked to the Meissner-Ochsenfeld effect and its fluctuational extension, where an external magnetic field induces a counter current that weakens the field inside the superconductor, an effect that for weak fields becomes perfect for large conductors below the critical temperature.

## **3.5.1** Observation of the susceptibility

Now that we have shown that suitable observables exist, it is necessary to specify how these can be probed. The invention of a scheme that is capable of doing exactly that is a large part of this thesis. Before we start getting into the scheme itself, it is necessary to give a small introduction to some key results from quantum electrodynamics and laser physics, as these build the fundamentals on which the scheme rests.

#### 3.5.1.1 Review of quantum electrodynamics

Many of the contents and reasoning inside this section are taken from the introductory books by Cohen-Tannoudji et al. [97, 46]. A good overview over the basic notions of artificial gauge fields is provided by the review of Dalibard et al. [98].

The main idea in quantum electrodynamics is that not only are the atomic parts of a system quantized, but also the electromagnetic fields that make up said system. These fields can be generally decomposed into harmonic modes with integer occupation states. These quanta of excitation are generally known as photons. The state space is thus a tensor product of the mechanical state  $|a\rangle$  and the Fock state of the occupation of the different modes  $|n_1, n_2, ...\rangle$  or superpositions thereof, just as for the material bosons. The coupling between matter and the photons comes via the minimal substitution. The Hamiltonian can be so chosen as to only contain a transverse vector field  $\mathbf{A} = \mathbf{A}_{\perp}$ , which means that the Fourier transform of the field satisfies  $\mathbf{k} \cdot \mathbf{A}_{\perp}(\mathbf{k}) = 0$ . This particular gauge where  $\nabla \cdot \mathbf{A} = 0$  is called the Coulomb gauge and we shall use it in the following. The Coulomb interaction term caused by the exchange of longitudinal photons, is called  $V_{\text{Coul}}$  and its exact form depends on the potential environment of the atom. The Hamiltonian describing the interaction of an electron in an atom with a laser light field becomes

$$H = \frac{\left(\mathbf{p} - e\mathbf{A}_{\perp}\right)^2}{2m} + V_{\text{Coul}} + H_R,$$

where  $H_R$  is the Hamiltonian of the radiation field, which for our purposes consists of a finite collection of harmonic oscillators  $H_R = \sum_i \omega_i \left(a_i^{\dagger} a_i + \frac{1}{2}\right)$ , where the  $a_i$  are the same modes that appear in the transverse vector potential with wave vector  $\mathbf{k}_i$ 

$$\mathbf{A}_{\perp}(\mathbf{x}) = \sum_{i} \sqrt{\frac{\hbar}{2\varepsilon_{0}\omega_{i}L^{3}}} \left[ a_{i}\varepsilon_{i} \mathbf{e}^{i\mathbf{k}_{i}\cdot\mathbf{x}} + a_{i}^{\dagger}\varepsilon_{i}\mathbf{e}^{-i\mathbf{k}_{i}\cdot\mathbf{r}} \right],$$

where the  $\varepsilon_i$  are polarization vectors with  $\varepsilon_i \cdot \mathbf{k}_i = 0$ .

In addition we neglected the term coupling the spin of the electron to the magnetic field created by the laser, because its effects tend to be an order of magnitude lower than the dipole interaction we want to describe.

We assume that the size of the atom is much smaller than the relevant wave length  $\lambda$  of the laser. Because the laser is assumed to be of high quality, we can reduce the ensemble of field modes to the one of the laser,  $a_i$ , as all other effects are supposed to be weaker. We use the gauge transformation

$$T = \mathrm{e}^{-\frac{i}{\hbar}e\mathbf{x}\cdot\mathbf{A}_{\perp}(0)} = \mathrm{e}^{\eta a - \eta^* a^{\dagger}},$$

where

$$\eta_i = \frac{ie}{\sqrt{2\varepsilon_0 \hbar \omega L^3}} \varepsilon \cdot \mathbf{x},$$

and evaluate the electric field operator only at the origin, i.e. the expansion of the transformation matrix only to first order. Higher orders would give electric quadrupole and higher interactions, which are interesting per se, but also considerably weaker than the dipole interaction.

The transformation acts on the system such that

$$T\mathbf{x}T^{\dagger} = \mathbf{x} \longrightarrow TV_{\text{Coul}}T = V_{\text{Coul}},$$
  
 $T\mathbf{p}T^{\dagger} = \mathbf{p} + e\mathbf{A}_{\perp}(0)$   
 $TaT^{\dagger} = a + \eta$   
 $Ta^{\dagger}T^{\dagger} = a^{\dagger} + \eta^{*}.$ 

The new Hamiltonian is

$$THT^{\dagger} = \frac{\mathbf{p}^2}{2m} + V_{\text{Coul}} + H_R - e\mathbf{x} \cdot \sqrt{\frac{\hbar}{2\varepsilon_0 (2\pi)^3}} \left(ia\varepsilon - ia^{\dagger}\varepsilon\right) + \frac{1}{2\varepsilon_o L^3} |\varepsilon \cdot e\mathbf{x}|^2.$$

Here the first two terms are just the atomic system without light interaction. The fourth term is equivalent to the product of the dipole operator  $e\mathbf{x}$  and the transverse electric field operator

$$\mathbf{E}_{\perp} = \sqrt{\frac{\hbar}{2\varepsilon_0 \left(2\pi\right)^3}} \left(ia\varepsilon - ia^{\dagger}\varepsilon\right),$$

of that laser mode. The last term is finally a dipole interaction term, which is in this approximation a constant.

We can now decompose the Hamiltonian into the relevant atomic states (the ones that are close enough in energy to couple to each other, or where the difference in energy is close enough to the photon energy of the laser). Assuming we have only two relevant states, we can write

$$\frac{\mathbf{p}^{2}}{2m} + V_{\text{Coul}} = \varepsilon_{1} \left| 1 \right\rangle \left\langle 1 \right| + \varepsilon_{2} \left| 2 \right\rangle \left\langle 2 \right|$$

In the same basis, the dipole operator  $e\mathbf{x}$  becomes the off-diagonal matrix

 $e\mathbf{x}\cdot\boldsymbol{\varepsilon} \rightarrow d_{12} \left|1\right\rangle \left\langle 2\right| + d_{12}^{*} \left|2\right\rangle \left\langle 1\right|,$ 

where  $d_{12} = \langle 1 | e \mathbf{x} | 2 \rangle$  and symmetry demands that  $\langle i | \mathbf{x} | i \rangle = 0$ . Note that the dipole moments can still be zero if certain selection rules are not complied with. If the laser mode is strongly occupied  $n \gg 1$ , the field essentially becomes a coherent state  $|\alpha\rangle$  of photons, i.e.

$$a(t) | \alpha \rangle = e^{i\omega t} a(0) | \alpha \rangle = e^{i\omega t} \alpha | \alpha \rangle,$$

such that the average

$$\langle \alpha | \mathbf{E} | \alpha \rangle = \mathbf{E}_{\omega} \frac{\mathrm{e}^{i\omega t} + \mathrm{e}^{-i\omega t}}{2i} = \mathbf{E}_{\omega} \sin(\omega t),$$

becomes a classic electromagnetic wave with field amplitude  $E_{\omega}$ . The resulting Hamiltonian is that of a twolevel system with a periodically time-dependent coupling between the states.

Now we want to investigate what happens when the perturbation acts weakly on the atomic system. Our atomic state can then be decomposed into a superposition of the two eigenstates of the unperturbed system

$$|\psi\rangle = c_1(t) |1\rangle + c_2(t) |2\rangle$$

Naturally the overlap of the perturbation will be in terms of the overlap elements

$$\langle 1|e\mathbf{x}\mathbf{E}_{\omega}\sin(\omega t)|2\rangle = d_{12}E_{\omega}\sin(\omega t).$$

The Schrödinger equation leads to

$$i\hbar \frac{dc_1}{dt} = \varepsilon_1 c_1 + d_{12} E_\omega \sin(\omega t) c_2$$
$$i\hbar \frac{dc_2}{dt} = \varepsilon_2 c_2 + d_{21} E_\omega \sin(\omega t) c_1$$

The explicit term  $\sim \varepsilon_i c_i$  can be eliminated by defining  $c_i(t) = b_n(t)e^{-i\varepsilon_i t}$ . The resulting system of equations is

then

$$i\hbar \frac{db_1}{dt} = \hbar \Omega_{12} \sin(\omega t) e^{i(\varepsilon_1 - \varepsilon_2)t/\hbar} b_2$$
$$i\hbar \frac{db_2}{dt} = \hbar \Omega_{12}^* \sin(\omega t) e^{i(\varepsilon_2 - \varepsilon_1)t/\hbar} b_1,$$

where  $\Omega_{12} = d_{12}E/\hbar$  is the Rabi frequency of the transition, which is evidently controlled by the laser intensity. One can see that the Bohr frequencies  $\omega_{ij} = (\varepsilon_i - \varepsilon_j)/\hbar$  naturally appear. A common approximation is the rotating wave approximation, which is based on the fact that the sine has two frequency components, one rotating with and one rotating against the Bohr frequency. As the anti resonance term is very quickly oscillating, it essentially cancels over the time scale in which the resonant term acts on the system. It is a good simplification to take into account only the slowly evolving terms

$$\sin(\omega t) e^{i\omega_{ij}t} = \frac{1}{2i} \left( e^{i(\omega_{ij}+\omega)t} - e^{i(\omega_{ij}-\omega)t} \right)$$
$$\approx \frac{i}{2} e^{i(\omega_{ij}-\omega)t}.$$

We will use this approximation and its generalization in the following, thereby discarding processes that change the overall manifold of the atom-lightfield dressed state and lead to decoherence. It has to be mentioned, that these equations are approximations, which need clean transitions and very long life-times of the excited state, which in practice can be a limitation. The extension of this system to a decaying system would mean going into a system of density matrices and master equations. The resulting Bloch equations describe the system more exactly. In the following we are mainly interested in the artificial magnetic fields which are already visible in our simplified system, so we will content ourselves with this simpler description.

## **3.5.1.2** The $\Lambda$ setup and its generalization

As mentioned earlier, we want to use artificial magnetic fields to probe the fluctuational susceptibility of bosonic systems. To this end we want to describe a setup that is able to create gradients of artificial magnetic fields, as these allow for a more precise measurement of these subtle effects. In the  $\Lambda$  setup the atomic system consists of three states, two ground states that are almost degenerate and one excited state (see figure 3.6).



Figure 3.6: The normal A scheme of two ground states  $|g_1\rangle$ ,  $|g_2\rangle$  which are coupled to an excited state  $|e\rangle$  with the Rabi fields  $\Omega_1$  and  $\Omega_2$  respectively.

Let us describe the amplitude of the two ground states with  $b_{1/2}$ , whereas we call the amplitude of the excited state  $b_e$ . Apart from the small difference in energy between the ground states, the system consists of two natural energies, namely the excitation (Bohr) energies

$$\hbar\omega_{e,g1/2}=\varepsilon_e-\varepsilon_{1/2},$$

where the  $\varepsilon_i$  are the energies of the respective internal states of the atom.

The point of our new scheme is to couple all three states to each other via three applied laser fields, each with frequency  $\omega_i$  and Rabi frequency  $\Omega_i$ . One couples the excited state to the first ground state, whereas the other two both couple the excited state to the second ground state (see figure 3.7).

As described in the previous section this leads, in the rotating wave approximation, to a time dependent system of equations of the form

$$\begin{split} & i\frac{db_1}{dt} = \frac{\Omega_1}{2i} e^{i(\omega_1 - \omega_{e1})t} b_e(t) \\ & i\frac{db_2}{dt} = \left(\frac{\Omega_2}{2i} e^{i(\omega_2 - \omega_{e2})t} + \frac{\Omega_3}{2i} e^{i(\omega_3 - \omega_{e2})t}\right) b_e(t) \\ & i\frac{db_e}{dt} = -\frac{\Omega_1^*}{2i} e^{-i(\omega_1 - \omega_{e1})t} b_1(t) - \left(\frac{\Omega_2}{2i} e^{-i(\omega_2 - \omega_{e2})t} + \frac{\Omega_3}{2i} e^{-i(\omega_3 - \omega_{e2})t}\right) b_2(t). \end{split}$$

At this point it is convenient to assume that the first laser is in tune with the first Bohr frequency, i.e.  $\omega_1 = \omega_{e2}$ .



Figure 3.7: The generalized  $\Lambda$  scheme. The second ground state is coupled to the excited state via two detuned lasers, each with its distinct Rabi field  $\Omega_{2/3}$ .

If we for a moment assume that  $\Omega_3 = 0$ , then the system can always be brought into a time-independent form by rotating the amplitudes around the chosen detunings  $\delta_i$ 

$$b_i(t) = e^{i\delta_i t} \tilde{b}_i$$
$$\longrightarrow \frac{db_i}{dt} = e^{i\delta_i t} \left( i\delta_i \tilde{b}_i + \frac{d}{dt} \tilde{b}_i \right).$$

For the simplified case with only two applied lasers, setting  $\delta_e = 0$  and  $\delta_2 = \omega_2 - \omega_{e2}$  will do the trick, however, at the cost of introducing diagonal factors in the previously purely off-diagonal system.

Returning to the more general case with three applied lasers, the introduction of the  $\delta_i$  gives (leaving out the tildes)

$$\frac{db_1}{dt} = -\frac{\Omega_1}{2}b_e - i\delta_e b_1,$$

$$\frac{db_2}{dt} = -\left(\frac{\Omega_2}{2} + \frac{\Omega_3}{2}e^{i(\delta_A - \delta_a)t}\right)b_e - i(\delta_e - \delta_a)b_2,$$

$$\frac{db_e}{dt} = \frac{\Omega_1^*}{2}b_1 + \left(\frac{\Omega_2^*}{2} + \frac{\Omega_3}{2}e^{-i(\delta_A - \delta_a)t}\right)b_2 - i\delta_e b_e,$$
(3.18)

where  $\delta_a = \omega_2 - \omega_{e2}$  and  $\delta_A = \omega_3 - \omega_{e2}$ . In addition we made the somewhat arbitrary choice  $\delta_e - \delta_2 = -\delta_a$ , which only matters for how the detunings are distributed about the rows. The important and intuitive thing to notice is that no matter which transformation is used, one always keeps a time dependence of frequency  $\omega_a - \omega_A = \omega_2 - \omega_3$ , the beating frequency between the lasers, in the system. Naturally when  $\omega_2 = \omega_3$ , the situation is the same as having only a single laser with amplitude  $\Omega_2 + \Omega_3$  interacting with the system.

Let us investigate that particular case of only two applied fields further. Without detuning we can write the Hamiltonian governing the previously derived time evolution in the form

$$H = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega_1 & 0 \\ \Omega_1^* & 0 & \Omega_2^* \\ 0 & \Omega_2 & 0 \end{pmatrix}.$$
 (3.19)

The Hamiltonian has three eigenstates,

$$|D
angle = rac{1}{\Omega} \left(-\Omega_2, 0, \Omega_1
ight)^T,$$

the so-called dark state with eigenenergy  $\varepsilon_D = 0$  and the two so-called bright states

$$|B_{\pm}
angle = rac{1}{\sqrt{2}\Omega} \left(\Omega_1, \pm \Omega, \Omega_2 
ight)^T$$

with energy  $\varepsilon_{B\pm} = \pm \hbar \Omega$ , where  $\Omega = \sqrt{|\Omega_1|^2 + |\Omega_2|^2}$ . The dark state is aptly named, as the eigenvalue suggests that atoms in that state do not directly couple to the lightfield and in addition also contain no excited state, which makes them very robust in experiments, as the excited state usually has a finite lifetime [99, 100]. These states are obviously not purely atomic in nature, but exists due to the interaction of light and atoms and they are commonly referred to as dressed states. Now clearly  $|\hbar \Omega|$  is the level splitting and sets an energy scale that can be compared to  $\delta = \delta_a - \delta_A$ . To do this, let us add a time-dependent perturbation of the form

$$\Delta H = \hbar \Omega_3 \mathrm{e}^{i\delta t} \left| e \right\rangle \left\langle 2 \right| + \hbar \Omega_3^* \mathrm{e}^{i\delta t} \left| 2 \right\rangle \left\langle e \right|.$$

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Thus the coupling between neighboring states has magnitude

$$V \equiv \langle D | \Delta H | B_{\pm} \rangle = \pm \hbar \frac{\Omega_1 \Omega_3}{\sqrt{2}\Omega} \mathrm{e}^{i \delta t}.$$

According to standard perturbation theory [96] the probability to transition from one state into the other for transversing a region where  $\Omega_3$  is very slowly turned on and off is given by

$$P_{\text{trans}} \approx \frac{1}{\hbar^2 \Omega^2} \left| \int_{-\infty}^{\infty} \frac{dV}{dt} e^{i\Omega t - \eta |t|} \right|^2 = \frac{\delta^2 |\Omega_1 \Omega_3|^2}{\Omega^4} \left| \int_0^{\infty} e^{i(\delta + \Omega + i\eta)t} \right|^2 \sim \frac{\delta^2}{\Omega^2}$$

So one should expect that for  $\delta^2/\Omega^2 \ll 1$ , the description of the system in terms of the eigenstates of the  $\delta = 0$  case is adequate. This is generally expected when the two time scales making up a process are widely different.

We will now use a more systematic method of finding a good approximation of the system when  $\delta$  is large, which is a common situation in laser physics. To do this we will expand our time dependent states in a Floquet basis and then use a transformation similar to the famous Schrieffer-Wolff transformation [101] to find a good effective description.

The use of the Floquet basis is easily motivated. The Hamiltonian and the equations of motion (3.18) are beating with the frequency  $\delta$ . For easier use we choose to have all the diagonal terms to be in the  $b_2$  evolution with detuning  $\delta_2$ . Now because the system is periodic, its eigenstates have to be periodic as well, essentially Floquet's theorem, which is very similar to Bloch's theorem, describing solutions in periodic potentials. The most general ansatz for such a periodic system is according to Floquet's theorem

$$b_i(t) = \mathrm{e}^{i\varepsilon t} \sum_n c_i^n \mathrm{e}^{in\delta t},$$

where the  $c_i^n$  are complex coefficients.

Using that

$$\frac{d}{dt}\left(e^{i\varepsilon t}\sum_{n}c_{i}^{n}e^{in\delta t}\right) = e^{i\varepsilon t}\left(\sum_{n}i\left(\varepsilon+n\delta\right)c_{i}^{n}e^{in\delta t}\right)$$

one finds via substitution into (3.18) and the overall fulfillment of time-independence of those states the follow-

ing set of equations for all integer n

$$\begin{aligned} (\varepsilon + n\delta) c_1^n &= \Omega_1 c_e^n \\ (\varepsilon + n\delta) c_2^n &= \delta_2 c_2^n + \Omega_2 c_e^n + \Omega_3 c_e^{n-1} \\ (\varepsilon + n\delta) c_e^n &= \Omega_1^* c_1^n + \Omega_2^* c_2^n + \Omega_3^* c_2^{n+1}. \end{aligned}$$

The equations can be ordered into blocks with the same *n*, that are coupled via the terms  $\sim \Omega_3$ . So when  $\Omega_3 \rightarrow 0$ , the proper time-independent scenario is recovered. Also one can see from the general structure, that solutions iterated from the *n* = 0 block have a large *n* behaviour of the form

$$c^n \sim \frac{\Omega_3}{n\delta} c^{n-1}$$
 for *n*positive,  
 $c^n \sim \frac{\Omega_3}{|n|\delta} c^{n+1}$  for *n*negative.

Looking at it closer, each block has essentially the matrix form

$$H_0^{n,n} = \hbar \left( egin{array}{ccc} n\delta & \Omega_1 & 0 \ \Omega_1^* & n\delta & \Omega_2^* \ 0 & \Omega_2 & n\delta \end{array} 
ight),$$

whereas the elements coupling the different blocks are

$$V^{n+1,n} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \Omega_3^* \\ 0 & 0 & 0 \end{pmatrix},$$
$$V^{n-1,n} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \Omega_3 & 0 \end{pmatrix}.$$

It is convenient to denote the *i*th eigenvector of the block  $H_0^{n,n}$  as  $|n,i\rangle$ , where the index *i* can take  $\pm 1$  or 0.

The eigenvalues in that system are

$$\begin{aligned} H_0^{n,n} | n, \pm 1 \rangle &= \hbar n \left( \delta \pm \Omega \right) \\ H_0^{n,n} | n, 0 \rangle &= \hbar n \delta, \end{aligned}$$

which shows that the energetic distance between neighboring manifolds is of order  $\delta$ , which is per assumption our largest energy scale. Our goal is to find an effective Hamiltonian for the states that evolve from the n = 0, block, as these are the ones that are naturally populated in a  $\Lambda$  scheme, and only upon increasing  $\Omega_3$  will the  $n = \pm 1$  part of the state space be occupied. We thus assume that the states  $|n, \pm 1/0\rangle$  are still good descriptions as long as  $\Omega_3 \ll \delta$ .

First we define the projector into the *n*th manifold as

$$P^n = \sum_i |n,i\rangle \langle n,i|.$$

For the effective Hamiltonian H' we have to demand that

a) H' is hermitian.

b) H' has the same eigenvalues as the original Hamiltonian and the same degeneracies

c) H' will have no matrix elements between the *unperturbed* manifolds.

The transformation should be of the form  $T = e^{iS}$ , where *S* is hermitian,  $S = S^{\dagger}$ . The new Hamiltonian is then  $H' = THT^{\dagger}$ . The last of the demands can be expressed as

$$P^n H' P^{n'} = 0$$
, for  $n \neq n'$ .

The effective Hamiltonian can then be decomposed into the sum of Hamiltonians for each manifold

$$H' = \sum_{n} P^{n} H'_{n}.$$

As the three requirements do not determine the transformation S completely, one can choose the simplifying

condition that the transformation only acts in between manifolds, i.e. that  $P^n SP^n = 0$ . The perturbation is then  $\lambda V$ , where  $\lambda$  is a small parameter. The transformation itself can be expanded in this small parameter

$$S = \lambda S_1 + \lambda^2 S_2 + \dots + \lambda^n S_n + \dots$$

Naturally the zeroth order should be zero, because to that order the Hamiltonian is already diagonal. Next one expands

$$H' = TH_0T^{\dagger} = H_0 + [iS, H_0] + \frac{1}{2!}[iS, [iS, H_0]] + \frac{1}{3!}[iS, [iS, [iS, H_0]]] + \dots$$

At the same time this means that because the small parameter  $\lambda$  is only present in *S*, the effective Hamiltonian can be expanded as well

$$H'=H_0+\lambda H_1+\lambda^2 H_2+\ldots.$$

It is useful to define the level shift operator

$$W = H' - H_0 = \lambda H_1 + \lambda^2 H_2 + \dots$$

Expanding the transformation with respect to  $\lambda$ 

$$W = \lambda [iS_{1}, H_{0}] + \lambda V$$
  
+  $[i\lambda^{2}S_{2}, H_{0}] + [iS_{1}, \lambda V]$   
+  $\frac{1}{2}[i\lambda S_{1}, [i\lambda S_{1}, H_{0}]] +$   
:  
+  $[i\lambda^{n}S_{n}, H_{0}] + [i\lambda^{n-1}S_{n-1}, \lambda V] +$   
+  $\frac{1}{2}[i\lambda^{n-1}S_{n-1}, [iS_{1}, H_{0}]] + ...$   
+  $\frac{1}{n!}[i\lambda S_{1}, [i\lambda S_{1}, ... [i\lambda S_{1}, H_{0}]]] +$   
:

Because the *n*th order of this equation only depends on  $S_n$  and the  $S_{n' < n}$ , one can solve iteratively starting with the first order by demanding

$$\lambda H_1 = \lambda \left( \left[ iS_1, H_0 \right] + V \right)$$

while additionally demanding that cross manifold terms are zero, i.e.

$$\langle n,i|i\lambda S_1|n',j\rangle\left(\varepsilon_{0j}^{n'}-\varepsilon_{0i}^n\right)-\langle n,i|\lambda V|n',j\rangle=0.$$

This gives alongside the previously mentioned zero intra block coupling a way to construct the matrix elements of  $S_1$ 

$$ig\langle n, i | i \lambda S_1 | n', j 
angle = rac{\langle n, i | \lambda V | n', j 
angle}{\left( arepsilon_{0j}^{n'} - arepsilon_{0i}^n 
ight)}$$
  
 $\langle n, i | i \lambda S_1 | n, j 
angle = 0.$ 

We want to approximate the effective Hamiltonian to second order in  $\lambda$ , i.e. find the matrix elements

$$\langle i|W|j\rangle = \langle i|\lambda V + i\lambda [S_1, V] + \frac{1}{2} [i\lambda S_1, [i\lambda S_1, H_0]]|j\rangle$$

Because the nondiagonal terms of the perturbation we have

$$[i\lambda S_1, H_0] + \lambda V = 0.$$

The last term is reduced to  $-[i\lambda S_1, \lambda V]/2$  and the approximation of the shift operator projection onto the *n* manifold is reduced to

$$H^n = P_n \lambda V P_n + \frac{1}{2} P_n \left[ i \lambda S_1, \lambda V \right] P_n.$$

The matrix elements of the commutator can be evaluated

$$\left\langle i | \frac{1}{2} P_n[i\lambda S_1, \lambda V] P_n | j \right\rangle = \sum_{k, n' \neq n} \left\langle n, i | \lambda V | n', k \right\rangle \left\langle n', k | \lambda V | n, j \right\rangle \left( \frac{1}{\varepsilon_{0i}^n - \varepsilon_{0k}^{n'}} + \frac{1}{\varepsilon_{0,j}^n - \varepsilon_{0,k}^{n'}} \right)$$

Because the perturbation only couples neighboring manifolds, we pick up only terms from  $n' = n \pm 1$ . Indeed, we can write the perturbation as

$$\lambda V = \sum_{n} \Omega_3 |n,2\rangle \langle n-1,e| + \Omega_3^* |n,e\rangle \langle n+1,2|,$$

which can be decomposed into the eigenstates of the  $\Lambda$  setup. Because of the coupling of neighboring manifolds we have that

$$rac{1}{arepsilon_i^n-arepsilon_k^{n\pm 1}}+rac{1}{arepsilon_i^n-arepsilon_k^{n\pm 1}}=rac{\mp\delta+2arepsilon_k+arepsilon_k+arepsilon_j}{(\mp\delta+arepsilon_i+arepsilon_k)\,(\mp\delta+arepsilon_j+arepsilon_k),}$$

where the  $\varepsilon_i$  are just the eigen energies of the  $\Lambda$  scheme. Of course, the denominators could become 0 when  $\delta \approx \varepsilon_i$ , but then the perturbation theory breaks down anyway and higher order terms including the coupling to higher order manifolds cannot be neglected anymore. However, in the regime were the perturbation theory is valid  $|\delta| \gg |\varepsilon_i|$ , the term essentially reduces to  $-1/\delta$ .

We can use these results to find the shifted energies of the n = 0 states. However, more interesting is the perturbation of the actual states, which we will need later to find the artificial magnetic fields. To lowest order the shifted states are given by

$$|\psi_n\rangle = |\psi_0\rangle + \sum_{p \neq n} \frac{\langle \psi_{0,p} | \lambda V | \psi_{0,n} \rangle}{\varepsilon_{0,n} - \varepsilon_{0,p}} |\psi_p\rangle + O(\lambda^2).$$
(3.20)

A lengthy calculation using the previously defined states shows that the perturbation of the dark state is given by

$$|D_{\delta}\rangle = \frac{1}{\Omega} \begin{pmatrix} -\Omega_{2}^{*} \\ 0 \\ \Omega_{1}^{*} \end{pmatrix} |0\rangle - \frac{\Omega_{3}^{*}}{\Omega\left(\delta^{2} - \Omega^{2}\right)} \begin{pmatrix} |\Omega_{1}|^{2} \\ \delta\Omega_{1}^{*} \\ \Omega_{1}^{*}\Omega_{2} \end{pmatrix} |-1\rangle.$$

The coupling mixes some manifolds and the perturbed states obtain a small beating frequency. In the next section we are going to introduce the concept of artificial gauge fields and how the perturbed states we just described can be used to create tunable artificial magnetic fields.

## 3.5.2 Artificial magnetic fields

We showed in the previous part that one can create states of the atoms, dressed states, which are explicitly dependent on  $\Omega$ , the Rabi frequency. We also argued that, because of the separation of energy scales, to a very good approximation the particles stay in their dressed state and follow it adiabatically if the perturbative potential acting on the system changes slowly in time. Next one lets  $\Omega$  vary spatially, i.e.  $\Omega \rightarrow \Omega(\mathbf{x})$ . This can create interesting effects, specifically artificial gauge fields may appear [102, 103, 104].

The atom-light system is still formally in a superposition of the orthonormalized dressed states, i.e.

$$egin{aligned} \ket{\psi} &= \sum_{\mathrm{i}} \psi_{\mathrm{i}} \ket{\psi_{\mathrm{i}}(\mathbf{x})} \ &= \psi_{0} \ket{\psi_{0}(\mathbf{x})} + \sum_{\mathrm{i}' 
eq 0} \psi_{\mathrm{i}'} \ket{\psi_{\mathrm{i}'}} \end{aligned}$$

,

where  $|\psi_0\rangle$  is the state which we want to adiabatically occupy for the time of the experiment, and the *i'* are all the states that are not this state. In addition at each point in space we have the decomposition of the identity  $I(\mathbf{x}) = \sum_i |\psi_i(\mathbf{x})\rangle \langle \psi_i(\mathbf{x})|$ . Because the overlap of the orthonormal states does not change as one moves in real space, the equation

$$abla \left\langle \psi_i | \psi_j \right\rangle = 0 = \left\langle 
abla \psi_i | \psi_j \right\rangle + \left\langle \psi_i | 
abla \psi_j \right\rangle,$$

wjere  $|\nabla\psi\rangle \equiv \nabla |\psi\rangle$  is a vector in the state space that constitues the atomic system, holds. Thus when the full momentum operator is applied to the state for which only  $\psi_0(\mathbf{x}) \neq 0$ , one finds

$$egin{aligned} \mathbf{P} egin{aligned} & \mathbf{\Psi} egin{aligned} & \mathbf{\Psi} & \mathbf{\Psi} egin{aligned} & \mathbf{\Psi} & \mathbf{\Psi} egin{aligned} & \mathbf{\Psi} & \mathbf{\Psi} & \mathbf{\Psi} egin{aligned} & \mathbf{\Psi} & \mathbf{\Psi} & \mathbf{\Psi} & \mathbf{\Psi} & \mathbf{\Psi} \ & \mathbf{\Psi} &$$

However, the behaviour is dictated by the function  $\psi_0$ . Since the system is always locally in that state, one can take the quantum mechanical average over  $|\psi_0(\mathbf{x})\rangle$  and finds the local formula for the (wavefunction) momen-

tum

$$\mathbf{P}\psi_0 = (\mathbf{p} - i\hbar \langle \psi_0 | \nabla \psi_0 \rangle) \psi_0$$
  
 $\equiv (\mathbf{p} - \mathbf{A}) \psi_0.$ 

One has thus introduced a vector potential  $\mathbf{A} = i\hbar \langle \psi_0 | \nabla \psi_0 \rangle$ , which, due to the orthonormality of  $\psi$  is real and the operator  $\mathbf{p}$  acts only on the wavefunction, which means it represents the orbital angular momentum rather than the whole momentum. Likewise, the whole Hamiltonian containing the external potential  $U(\mathbf{x})$  as well as the light-atom interaction can be projected onto the state  $|\psi_0(\mathbf{x})\rangle$  to give the effective Hamiltonian that determines the dynamics of the wave-function  $\psi_0$  as

$$H_0 = \frac{(\mathbf{p} - \mathbf{A})^2}{2m} + \varepsilon_0 + U + W,$$

where  $W = \sum_{i'} \frac{\hbar^2}{2m} |\langle \psi_{i'} | \nabla \psi_0 \rangle|^2$  is an effective potential created by the non-zero overlap between  $\nabla |\psi_0\rangle$  with the other states during the introduction of the identity. In the following we should not worry too much about this, as it can always be absorbed into U and in the cases we consider it can in fact be tuned away by adjusting U accordingly.

The potentials introduced are geometric potentials, i.e. different paths in space acquire a phase dependent on the direction travelled. Physically this means that a particle moving along a certain path is more likely to absorb a photon from the laser beam when it moves along a certain direction to the beam. It is this velocity dependent absorption that simulates an effective magnetic field without actually being one, which is why it can be used to simulate situations that one would not observe normally, like magnetic monopoles [104, 105].

We want to focus for now on configurations that are to give a constant magnetic field. If we keep in mind the equivalence of rotation and a magnetic field, as well as consider the laser field  $\Omega$  as a stirring device, it seems natural to investigate the scenario with non-trivial phase evolution in the plane of rotation. An important class of light fields that have such properties and also can be implemented in a lab are the Gauss-Laguerre beams. With the aid of holographic masks, almost arbitrary phase patterns can be imprinted onto a lightfield (see e.g. [106]). To accommodate the non-zero rotation of the light field, the intensity at the origin has to be zero and the

phase ill-defined. The beams can be parametrized in the form

$$\Omega_{i}(\rho,\phi) = \Omega_{i,0} \left(\frac{\rho}{\rho_{0}}\right)^{\ell_{i}} \mathrm{e}^{i\ell_{i}\phi} \mathrm{e}^{-\rho^{2}/w_{i}^{2}}$$

The radius  $\rho_0$  as well as the waist *w* generally are set by the beam width and tend to be of a similar order of magnitude. For the two-beam standard  $\Lambda$  scheme we can use the prescription

$$\mathbf{A} = i\hbar \left\langle D | \nabla D \right\rangle$$

and the convenient parametrization of the ground-state

$$|D\rangle = rac{1}{\sqrt{1 + x^{2(\ell_1 - \ell_2)}}} \left( egin{array}{c} -1 \\ 0 \\ x^{(\ell_1 - \ell_2)} \mathrm{e}^{i(\ell_1 - \ell_2)\phi} \end{array} 
ight),$$

with  $x = \rho / \rho_0$  and where it was assumed that the widths of the envelopes of the beams are equal, i.e.  $w_1 = w_2$ and an overall phase factor was taken out, so it becomes clearer that the result can only depend on  $\ell_1 - \ell_2$ .

The next step is to find the magnetic field

$$\mathbf{B} = \nabla \times \mathbf{A}$$

with

$$\mathbf{A} = i\hbar \left\langle D | \nabla D \right\rangle = \frac{\hbar \left(\ell_2 - \ell_1\right)}{\rho_0} \frac{x^{2(\ell_1 - \ell_2) - 1}}{1 + x^{2(\ell_1 - \ell_2)}} \mathbf{e}_{\phi}$$

where  $\mathbf{e}_{\phi}$  is the unit vector in azimuthal direction. The effective magnetic field becomes then

$$\mathbf{B} = \nabla \times \mathbf{A}$$
  
=  $\frac{1}{\rho} \frac{\partial}{\partial \rho} (\rho A_{\phi}) \mathbf{e}_{z}$   
=  $\frac{2\hbar\ell^{2}}{\rho_{0}^{2}} \frac{x^{2(\ell-1)}}{(1+x^{2\ell})^{2}} \mathbf{e}_{z},$ 



Figure 3.8: The artificial magnetic field for different values of transferred momentum,  $\ell = 2$  in red,  $\ell = 3$  in blue and  $\ell = 4$  in green.

with  $\ell = \ell_1 - \ell_2$ . We see that the principal magnitude of the magnetic field is given by  $\hbar \ell^2 / \rho_0^2$ , i.e. the smaller the beam waists are, the stronger the field becomes. Some field distributions for different  $\ell$  are shown in figure 3.8.

For  $\ell = 1$  the maximum of the magnetic field is in the center of the beam, for  $\ell$  larger than 1 it is slightly shifted to the value

$$x_{\max} = \frac{\rho_{\max}}{\rho_0} = \left(\frac{\ell - 1}{\ell + 1}\right)^{1/2\ell}$$

These results for the artificial magnetic field seems slightly counter-intuitive, as the strength of the field seem not to depend on the magnitude of the Rabi frequency at all. To find an answer, let us introduce a small detuning to the stationary scheme as a weak ( $\delta \ll \Omega$ ) perturbation of the form

$$\delta V = \hbar \delta \left( egin{array}{ccc} -1 & 0 & 0 \ 0 & 0 & 0 \ 0 & 0 & +1 \end{array} 
ight).$$

Using again the standard expression (similar to eq. (3.20)) for a perturbed state

$$\ket{\psi} = \ket{\psi_0} + \sum_{i 
eq 0} rac{\langle \psi_i | \delta V | \psi_0 
angle}{arepsilon_0 - arepsilon_i} \ket{\psi_i},$$

where the states over which we sum are unperturbed and not degenerate with respect to the state  $|\psi_0\rangle$ .

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Applying this to the dark state we find after normalization

$$|D_{\delta}\rangle = \frac{1}{\sqrt{1+\delta^2/2\Omega^2}} \left( |D\rangle + \frac{(\Omega_1\Omega_2^* + \Omega_1^*\Omega_2)}{\sqrt{2}\Omega^2} \frac{\delta}{\Omega} \left( |B_+\rangle - |B_-\rangle \right) \right).$$

For symmetry reasons the added magnetic field must be zero. This becomes obvious when one observes that

$$\partial_{\phi}\ket{B_+}=\partial_{\phi}\ket{B_-}$$

and both contributions to the vector potential **A** cancel. The magnetic field is weakened because the new dark state (though technically not quite dark anymore) has less weight on a magnetic contribution and the new magnetic field  $|\mathbf{B}_{\delta}|$  relates to the unperturbed magnetic field  $|\mathbf{B}_{0}|$  as

$$|\mathbf{B}_{\delta}| = \frac{1}{1 + \delta^2/2\Omega^2} |\mathbf{B}_0|.$$

Now we can understand the importance of the magnitude of the Rabi frequency for the amplitude of the artificial magnetic field. The stronger the Rabi field, the less sensitive the magnetic field becomes to very small fluctuations of the detuning. Thus a very weak Rabi field is unlikely to yield a quasi magnetic field, as the level of fine-tuning that is necessary becomes impossible to achieve realistically.

We should also look at the opposite case of a very large detuning such that  $\delta \gg \Omega$ , where we still consider the standard two-laser scheme as reference. Here we take for the unperturbed state the strong detuning limit

$$H_0 = \hbar \left( egin{array}{ccc} -\delta & 0 & 0 \ 0 & 0 & 0 \ 0 & 0 & +\delta \end{array} 
ight)$$

and the perturbation is (3.19). The eigenstates of the unperturbed Hamiltonian are simply the states  $|1\rangle$ ,  $|2\rangle$ ,  $|e\rangle$ . If we start the system in say the excited state  $|e\rangle$ , to lowest order the pertubation becomes

$$|e_{\delta}\rangle = \frac{1}{\sqrt{1+2\Omega^2/\delta^2}} \left(|e\rangle + \frac{\Omega_1}{\delta} \left|1\rangle - \frac{\Omega_2}{\delta} \left|2\rangle\right).$$

Indeed, this state is slightly magnetic since

$$\langle D|e_{\delta}\rangle \approx \frac{\delta}{\Omega}$$

with field strength

$$|\mathbf{B}_{e\delta}| \sim rac{\Omega^2}{\delta^2} |\mathbf{B}_0| \ll |\mathbf{B}_0|$$
 .

We have thus good reason to postulate

$$\mathbf{B}_{\boldsymbol{\delta}} = \mathbf{B}_0 f\left(\boldsymbol{\delta}^2/\Omega^2\right) = \frac{2\hbar\ell^2}{\rho_0^2} \frac{x^{2(\ell-1)}}{\left(1+x^{2\ell}\right)^2} \mathbf{e}_z f\left(\boldsymbol{\delta}^2/\Omega^2\right),$$

where f is a well behaved analytical function that can in principle be found explicitly, and of which we know the limits

$$\lim_{x \to 0} f(x) = \frac{1}{(1 + x^2/2)}$$

and

$$\lim_{x\to\infty}f(x)=\frac{1}{2x^2}.$$

Now we can return to the generalized 3-beam  $\Lambda$  setup. We found previously that adding a strongly detuned third laser with  $\delta \ll \Omega$  perturbs the dark state (we approximate  $\delta^2 - \Omega_2^2 \approx \delta^2$ )

$$|D_{\delta}
angle = rac{1}{\Omega} \left( egin{array}{c} -\Omega_2^* \\ 0 \\ \Omega_1^* \end{array} 
ight) |0
angle - rac{\Omega_3^*}{\Omega\delta^2} \left( egin{array}{c} |\Omega_1|^2 \\ \delta\Omega_1^* \\ \Omega_1^*\Omega_2 \end{array} 
ight) |-1
angle.$$

Now even though the added component is oscillating in time, it still contains spatial information for a geometric field in  $\Omega_3^*$ . Indeed, because the perturbation is in a different manifold, the effective vector field terms in  $\mathbf{A} = \langle D_{\delta} | \nabla D \rangle$  are additive since  $\langle 0 | -1 \rangle = 0$  and one can consider them as essentially belonging to different artificial magnetic field schemes that are superposed, one being in tune with the atomic frequencies and resultant magnetic field  $B \sim \hbar (\ell_2 - \ell_1)^2 / \rho_0^2$ , the other being far detuned from resonance and with field amplitude  $B = \hbar (\ell_3 - \ell_1)^2 / \rho_0^2$  and suppressed by the factor  $\Omega^2 / \delta^2$ . It is often more convenient and also practically easier to

leave  $\Omega_1$  with  $\ell_1 = 0$  so that the actual artificial magnetic field stems from  $\ell_2$  and  $\ell_3$ .

How can this be incorporated in a scheme that can actually create a linear gradient of the magnetic field? We know that for all practical purposes the generalized  $\Lambda$  scheme can be viewed as a superposition of two standard  $\Lambda$  schemes. The next step is to take the second ground state  $|g_2\rangle$  as Zeeman sensitive (see figure 3.7), which means it can be shifted by the application of a *real* magnetic field. This real magnetic field can influence the artificial magnetic field strength exerted by each  $\Lambda$  setup by moving the transition closer or further away from resonance. Assuming one starts with a large enough detuning between the  $\Omega_2$  and  $\Omega_3$  lasers, where the origin of the *z* axis the system is in resonance with the  $\Lambda$  setup of the field  $\Omega_2$  creating a magnetic field with strength  $\sim \ell_2^2$ . To understand how a linear real field gradient can give a linear artificial field dependence, let us look at a simplified picture. If the real magnetic field changes linearily along the *z* axis, i.e.  $\delta \sim z$ , then the magnetic field loses its strength approximately in a quadratic manner

$$B_2 \approx B_0 rac{\ell_2^2}{1+rac{\delta^2}{2\Omega^2}} \approx B_0 \ell_2^2 \left(1-rac{\delta^2}{2\Omega^2}\right).$$

At the same time as the system becomes out of tune with the first  $\Lambda$  setup, it gets closer to resonance with the second  $\Lambda$  setup, originally detuned by  $\delta_0$ , with effective field proportional  $\ell_3^2 > \ell_2^2$ . As it moves closer, the field effect grows also approximately quadratically

$$B_3 \approx B_0 \frac{\ell_3^2 \Omega^2}{2\left(\delta_0 - \delta\right)^2} \approx \frac{B_0 \ell_3^2 \Omega^2}{2\delta_0^2} \left(1 + \frac{\delta}{\delta_0}\right)^2 \approx \frac{B_0 \ell_3^2 \Omega^2}{2\delta_0^2} \left(1 + \frac{2\delta}{\delta_0} + \frac{\delta^2}{\delta_0^2}\right).$$

Obviously, the field curvatures created by the two  $\Lambda$  schemes have opposite signs. By choosing an appropriate  $\delta_0$ , one can make the sum of their artificial magnetic fields curvature free

$$\frac{d^2}{d\delta^2} (B_2 + B_3) = B_0 \left( -\frac{\ell_2^2}{\Omega^2} + \frac{\ell_3^2 \Omega^2}{\delta_0^4} \right) \equiv 0$$
$$\rightarrow \delta_0 = \left( \frac{\ell_3}{\ell_2} \right)^{1/2} \Omega.$$

Of course this is just an approximation and in reality one would rather have a plateau of considerable size in which a linear real change in magnetic field is turned into a linear gradient in artificial magnetic field, as seen in



Figure 3.9: The gradient of the artificial magnetic field  $dB/d\delta$  in units of  $\Omega$  for different detunings  $\delta_a - \delta_A = \delta_0$  of the field beams with  $\Delta \ell = 2$ . The upper (blue) line is for an initial detuning of  $\delta_a - \delta_A \approx 2\Omega$ , the lowest (green) for  $\delta_0 \approx 2.8\Omega$ . The red line in the middle is tuned such that the two curvatures cancel and a plateau of width  $\approx \Omega$  is formed for  $\delta_0 \approx 2.5\Omega$ . In that region a linear gradient of a *real* magnetic field translates into a linear gradient of the artificial magnetic field.

figure 3.9.

The actual steepness of the field gradient then depends on the gradient of the real magnetic field and the value  $\ell_2/\ell_3$ . One might argue that as one gets close to the condition where  $\delta/\Omega \approx 1$ , this should not be a principle problem, as the function  $f(\delta^2/\Omega^2)$  is analytic. One can however justify the use of the limiting factors in practice. One has a bit of freedom in choosing the ratio of converted angular momentum, i.e.  $\ell_2/\ell_3$ . One can find the approximate values for which the plateau exists roughly as  $\Omega/\delta_0 = 0.7$  for  $\Delta \ell = 1$ ,  $\Omega/\delta_0 = 0.4$  for  $\Delta \ell = 2$  and  $\Omega/\delta_0 = 0.32$  for  $\Delta \ell = 3$ . Moreover, the plateau is fairly wide  $\approx \Omega$ , and robust, as small changes in the detuning  $\delta_0$  barely effect the overall gradient.

## 3.5.3 Observation of the susceptibility

It is very difficult to observe the fluctuational susceptibility using a constant artificial magnetic field, as small fluctuations of the field would lead to a direct error in measurement. Using a gradient however could make a relative measurement possible, which is in theory much more precise, as global fluctuations of any involved parameter become unimportant.

Let us combine the generalized  $\Lambda$  setup with the layered bosonic system that is essentially non-interacting, i.e. a = 0, in such a way that the laser beam is perpendicular to the layers (see figure 3.10 for a sketch). If

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Angular Momentum Transfer

Real Magnetic Gradient

Figure 3.10: A cartoon of the scheme for the observation of fluctuational effects. The different layers of the cloud gather different angular momenta, dependent on their position in the generalized  $\Lambda$  scheme.

the bosonic system has the additional harmonic trapping potential in x - y direction, we have to make sure that  $\rho_0 < a_0 \sim \sqrt{\hbar/m\omega_0}$ , i.e. we want the focus on the region where the energy of the fluctuations is larger than any trapping potential. On the other hand it is desired to stay in the weak field regime where our predictions using the unrenormalized Ginzburg-Landau model hold, though it is not strictly necessary. This means that  $\hbar\omega_B \ll T$ , or alternatively  $\rho_0 n^{1/3} \gg 1$ , where *n* is the particle density at the center of the trap. In practice this translates into a beam width  $\rho_0$  of a few microns.

Upon turning on the  $\Lambda$  scheme, the radiated layer of the cloud obtains locally the angular velocity

$$\omega(z) = \frac{B_{\rm art}(z)}{2m}.$$

It follows that in a short period of time the internal illuminated part rotates and picks up the angular momentum

$$L = N_{\parallel}(\rho_0) \chi(\rho_0) \omega(z)$$

where  $N_{\parallel}(\rho)$  is the number of particles in a disk of radius  $\rho$ 

$$N_{\parallel}(\rho) = \pi n d\rho^2$$
,

with d being the thickness of a layer of the "stack of pancakes"-like structure. The susceptibility comes from the addition of two contribution, the "classical" contribution of a number of thermal particles rotating, and
a contribution due to the fluctuations that effectively reduce the overall susceptibility, because the superfluid droplets resist rotation. The classical susceptibility is derived from the classical free energy of rotation

$$F_{\rm cl} = -\frac{1}{4}m\rho_0^2 N_{\parallel}\left(\rho_0\right)\omega_{\rm rot}^2,$$

when it is considered that  $\omega_{\rm rot} = \omega_B/2$  such that the susceptibility per particle becomes

$$\chi_{\rm cl} = -\frac{1}{N_{\parallel}} \frac{\partial^2 F}{\partial \omega_B^2} = \frac{1}{8} m \rho_0^2.$$

This susceptibility can be compared to the fluctuational susceptibility (3.16), (3.17)

$$\frac{\chi_{\rm fl}}{\chi_{\rm cl}} = -\frac{2}{3N_{\parallel}} \begin{cases} c_1^{-1} \left[ \tau \left( \tau + \eta_1 \right) \right]^{-1/2}, & \text{trapped gas} \\ c_2^{-1} \left[ \tau^2 \left( \tau^2 + \eta_2 \right) \right]^{-1/2} & \text{uniform gas.} \end{cases}$$

Their contributions are added

$$\chi = \chi_{\rm cl} + \chi_{\rm fl}.$$

At this point the center of each layer should rotate with its individual frequency.

A subtle but important point is that the magnetic field imposes angular velocity, rather than angular momentum, even though angular momentum is naturally transferred from the laser beam onto the cloud. In order to measure the susceptibility, one has to somehow perform a measurement of the momentum. There are certainly many ways to do just that. One possible way is to ramp up the interactions for a short period of time and let the angular momentum spread over the whole layer of radius *R*. Because  $R \gg \rho_0$  the entire layer is essentially classical with respect to its angular momentum. After equilibration and subsequent return to the low-interaction regime the angular velocity of the layer becomes

$$\begin{split} \omega(z) &= \frac{N_{\parallel}\left(\rho_{0}\right)\chi\left(\rho_{0}\right)}{N_{\parallel}\left(R\right)\chi\left(R\right)}\frac{\omega_{B}(z)}{2} \\ &= \frac{\rho_{0}^{4}}{R^{4}}\left[1 + \frac{\chi_{\mathrm{fl}}}{\chi_{0}\left(\rho_{0}\right)}\right]\frac{\omega_{B}(z)}{2} \end{split}$$

Now the gradient can be used to measure a phase difference between neighboring layers. First after rotation the whole cloud can be squeezed such that the cross section of the cloud becomes elongated (e.g. in [63]). One can now wait for a certain time t and make a projective measurement along the z axis. If no time has passed since the squeeze, the projection should be an oval as well. However with increasing time, this projection will become round, as the relative phases between the layers evolve at different speeds. The estimated time for loss of contrast will be

$$t_0 \sim \frac{2\pi}{\Delta\omega_{\rm outer}}$$

where  $\Delta \omega_{\text{outer}}$  is the difference in angular velocity of the outermost layers. This time  $t_0$  is measurable and can be observed at different temperatures in the vicinity of  $T_c$ . For  $\tau \approx 1$  the fluctuational contribution is totally negligible and can thus be used as a calibration. Measuring for different  $\tau$  can show the critical powerlaw dependence of  $\chi_{fl}$ 

$$\frac{t_0(\tau)}{t_0(1)} - 1 = -\frac{\chi_{\mathrm{fl}}(\tau)}{\chi_{\mathrm{cl}}}.$$

Also it is quite useful to note that the method does not depend on whether one is in the Ginzburg-Landau regime during the application of the magnetic field or not. In principle one can observe the critical exponents very close to the transition [74]. This method could then be used to interpolate the exact critical temperature by interpolating the power law. Experiments on the critical properties of trapped boson systems have already been performed [16] and box-like potentials to simulate uniform systems are available [107].

### **3.6 Outlook**

Observing the fluctuational behaviour close to a regular Bose-Einstein transition is exciting. As mentioned in the general introduction, fermionic fluctuational effects have been observed not only in low-dimensional

systems but also in disordered materials. This begs the question whether disorder can also drive a transition in bosonic systems and if so, what are the properties of such a transition. The theory for such transition, typically called the bosonic superfluid-insulator transition (SIT) exists [47], yet so far no direct experimental observation, especially with cold bosonic gases, has been made.

The model system for the superconducting insulator transition is a two-dimensional array of traps or pockets that each contain a condensate with a large number of particles  $N_i$  and a well defined phase  $\Phi_i$ . Such systems are believed to appear naturally, as in granulated superconductors or poreous media filled with liquid helium <sup>4</sup>He.

A somewhat intuitive picture can be obtained from the Bose-Hubbard model (2.7). Let us assume that two neighboring sites, *i* and *j*, are strongly coupled to each other. It is intuitively clear and a mean-field calculation can show [108] that the Fock states are not a good description, as particles are very likely to tunnel in between the two sites. Instead it is better to describe the states with coherent semi-classical states (2.5) with phases  $\theta_i$ and  $\theta_j$ , where we in addition assume that the mean field potentials on both sites are similar so the same particle mean numbers *N* is expected. Under these conditions the tunneling element in the Bose-Hubbard model takes the form

$$\left\langle \theta_i | -J\left(\hat{a}_i^{\dagger} \hat{a}_j + \hat{a}_j^{\dagger} \hat{a}_i\right) | \theta_j \right\rangle = -JN \left( e^{i\left(\theta_i - \theta_j\right)} + e^{i\left(\theta_j - \theta_i\right)} \right)$$
$$= -2JN \cos\left(\theta_i - \theta_j\right)$$
$$\equiv -E_J \cos\left(\theta_i - \theta_j\right),$$

where  $E_J$  is the Josephson energy of a Josephson junction, literally a junction that connects two reservoirs with well defined phases. Obviously the coupling energy is minimized when  $\theta_i - \theta_j = 0$ , (technically  $2\pi n$ , where n is integer, but in a collection of strongly coupled sites the phase-difference of 0 is preferred). In particular one could imagine many of those single sites being strongly coupled which then form grains each with well defined phase  $\Theta_i$ . This coarse graining procedure provides one with the effective grain Hamiltonian, which is very similar to the original Bose-Hubbard Hamiltonian. Expanding around the mean field and integrating out the remaining fluctuations gives for only nearest neighbor interactions [109, 110]

$$\hat{H}_{\rm gr} = \sum_{i} \frac{U}{2} \hat{N}_{i} \hat{N}_{i} - \sum_{\langle ij \rangle} J_{ij} \cos\left(\Theta_{i} - \Theta_{j}\right).$$

Naturally these grains are still coupled to their nearest neighbors. Such graining happens naturally in disordered Bose-Hubbard models, even at zero temperature, as the interactions and couplings are tuned and the onsite chemical potentials are disordered  $\mu \rightarrow \mu_i$ . In both, ordered or disordered, scenarios one expects a phase transition. In these transitions one basically transforms from the state where the particles are localized on their grains, or in the case of disorder on clusters of coupled grains, to a state where the particles are delocalized effectively leasing to macroscopic superfluidity [47]. To avoid unnecessary complications resulting from the Mermin-Wagner theorem and a lengthy discussion of the Berezinskii-Kosterlitz-Thouless transition and related effects [41], let us take the three dimensional case and let us look how a rotating trap setup might help to distinguish between different phases. The main idea is that different phases have a different moment of inertia. One could compare the situation with the rotation of a cup with cubes of ice (insulating state), which behave quite distinctly from a rotating cup filled with liquid (superfluid state). Something similar holds true for quantum states where localized particles behave differently under rotation than delocalized systems. To be more specific we prove the almost trivial quantum version of Steiner's theorem, namely that the moment of inertia of non-overlapping system is additive and contains a component of the mean angular momentum.

#### Inset: Steiner's theorem for quantum mechanical systems

Quite generally, when a physical system consists of several non-overlapping, non-entangled subsystems, i.e. the wave function is vanishing in between the different subsets, then any local operator  $\hat{O}$  average can be decomposed into the average over the subsystems

$$\left\langle \hat{O} \right\rangle = \sum_{i} \left\langle \hat{O}_{i} \right\rangle,$$

where  $\hat{O}_i$  is the operator  $\hat{O}$  projected onto the physical space over which the *i*th many-body wave function is

non-vanishing. Let us call these subsets grains. This of course holds true for the angular momentum operator

$$\hat{L} = m\hat{\mathbf{r}} \times \hat{\mathbf{p}}.$$

Let us decompose the position vector of a grain into

$$\hat{\mathbf{r}}=\hat{\mathbf{r}}'+\mathbf{R},$$

where **R** is the classical vector describing the center of mass of the grain and  $\mathbf{r}'$  is the position operator in the center of mass coordinate system of the grain. Thus for a single grain

$$\begin{split} \langle \mathbf{L} \rangle &= \left\langle \left( \hat{\mathbf{r}}' + \mathbf{R} \right) \times \hat{\mathbf{p}} \right\rangle \\ &= \left\langle \hat{\mathbf{r}}' \times \hat{\mathbf{p}} \right\rangle + \left\langle \mathbf{R} \times \hat{\mathbf{p}} \right\rangle \\ &= \left\langle \hat{\mathbf{r}}' \times \hat{\mathbf{p}} \right\rangle + \mathbf{R} \times \left\langle \hat{\mathbf{p}} \right\rangle. \end{split}$$

For a rotation with angular velocity  $\omega$  we know that  $\langle \mathbf{p} \rangle = mN_{\rm gr}\dot{\mathbf{R}} = mN_{\rm gr}\omega \times \mathbf{R}$ .

The angular momentum of a singular grain thus becomes

$$\langle \mathbf{L} \rangle = \langle \hat{\mathbf{r}} \times \hat{\mathbf{p}} \rangle_{\mathrm{cm}} + m N_{\mathrm{gr}} \mathbf{R}^2 \boldsymbol{\omega},$$

where the  $\langle \ldots \rangle_{cm}$  denotes averaging with respect to a coordinate system centered around the center of mass.

The moment of inertia is defined as

$$I = \lim_{\omega \to 0} \frac{\langle \mathbf{L} \rangle}{\omega}.$$

If we define the rest frame moment of inertia of a grain to be

$$I_{\rm gr} \equiv \lim_{\omega \to 0} \frac{\langle \hat{\mathbf{r}} \times \hat{\mathbf{p}} \rangle_{\rm cm}}{\omega},$$

then we have that for a grain not rotated around its center of mass

$$I_{\rm tot} = I_{\rm gr} + M_{\rm gr} \mathbf{R}^2$$

where  $M_{\rm gr}$  is the total mass that rotates around the grain.

Especially for a system of non-overlapping grains, each with center of mass vector  $\mathbf{R}_i$ , holds

$$I_{\mathrm{tot}} = \sum_{i} \left( I_{\mathrm{gr},i} + M_{\mathrm{gr},i} R_{i}^{2} \right),$$

which is the extension of the classical Steiner's theorem. This allows us to describe the moment of inertia of a more complicated quantum mechanical system, provided of course that its subcomponents are clearly separated in space.

We estimate now that a granular system can have up to two significant drops in moment of inertia when cooled down or the coupling is changed. The first drop appears when the bosons in the grains condense. Let us assume, that the grains are disks of radius *D*. Then the classical moment of inertia, if the disk is in equilibrium with the rotating trap, is

$$I_{\mathrm{cl},disk} = \frac{mN_{\mathrm{disk}}}{8}D^2,$$

where  $N_{\text{disk}}$  is the number of particles on a grain of disk shape. More generally the classical moment of inertia is given by

$$I_{\rm cl} = mN\left\langle x^2 + y^2\right\rangle.$$

Now when a grain becomes superfluid, its center of mass moment of inertia is diminished. Though the superflow is rotationless,  $\nabla \times \mathbf{v}_s = 0$ , it still can carry angular momentum if the trap is anisotropic, as the system is not rotation symmetric anymore. For the approximation of anisotropic harmonic traps one has [111]

$$I_{\rm cond} = \delta^2 I_{\rm cl},$$

where

$$\delta = \frac{\left\langle y^2 - x^2 \right\rangle}{\left\langle y^2 + x^2 \right\rangle}.$$

So in the case of a truly round disk the condensate moment of intertia does vanish, but anisotropies gives it a residual moment of inertia. Steiner's theorem then tells us that a system of  $N_{\text{grain}}$  identical grains will experience a drop

$$\Delta I_1 = m N_{\text{grain}} N_{\text{disk}} \left( 1 - \delta^2 \right) \left\langle x^2 + y^2 \right\rangle.$$

In the ideal case of round disks the remaining moment of inertia comes merely from the center of mass motion

$$I_{\rm cm} = \sum_i m N_{\rm disk} R_i^2.$$

One can approximate this value for the limit of densely packed grains. If the total radius of the rotating set of grains is *R*, then there are R/D layers. The *n*th layer has 6n grains and the radius of the distance to the center of the *n*th layer is  $R_n = nD$  giving a total moment of intertia of the *n*th ring to be  $I_n = 6n^3mN_{\text{disk}}D^2$ . After the summation one finds that the the maximum expected drop of

$$\Delta I_2 = \frac{3}{2} m N_{\rm disk} R^2 \left(\frac{R}{D}\right)^2.$$

This might look odd at first sight, as R/D could become fairly large at constant R, however for small D also the number of particles on a grain become smaller  $\sim (D/R)^2$ .

So one would expect that for perfectly round disks one has two separate drops of ratio

$$\frac{\Delta I_1}{\Delta I_2} = \frac{1}{12} N_{\text{grain}} \left(\frac{D}{R}\right)^4 \sim \left(\frac{D}{R}\right)^2,$$

so the relative effect becomes smaller for larger systems, as is expected. Now it should be noted that this effect might not be as clean in reality. For once one needs a clear separation between the transitions, which in principle should be possible by making the grain potentials deep enough to assure an early condensation there. Next one would like to look at the disordered case, where by chance neighboring grains might interlock. This

state would be similar to the Bose-Glass state, where neighboring states might, or might not be in resonance. This however means that upon increasing disorder, one cannot expect a clean drop of the moment of inertia. Instead this will depends highly on the disorder configuration and as we just showed, making the system larger to have more effective disorder averages would take away at least one of the signatures that shows that one indeed has a superconductor insulator transition. Also there might be considerable moment of inertia in the full superfluid state simply because of the geometric orientation of the grains, where the holes between the grains act as effective impurities that distort the superflow. One would need alternative ways to access that condensates appear in the grains.

However this still opens up some exciting new pathways for probing small systems. Such systems could be realized with microchips that carry a condensate that can be slowly rotated. Such chips can have almost arbitrary potential landscapes and can simulate the grains, as well as disorder up to a certain extent [112].

### **3.7** Summary of Results for Bosonic Fluctuations

In this part of the thesis we have elucidated the relationship between superconducting fluctuations and bosonic fluctuations and showed that there are strong similarities for the most part, but also some differences that can be observed experimentally. We have argued that a Ginzburg-Landau like approach is applicable for bosons as well because even above the critical temperature a generalized Gross-Pitaevskii equation holds. We looked at a system of fermions with tunable interactions. In the strong coupling limit, these fermions form composite bosons. We derived the bosonic limit of the fermionic fluctuation propagator and showed that it coincides with a bosonic operator of the low energy fields, as a naive guess would have predicted. This and more has however been done before in [17], as we found out later. Pure bosonic fluctuation theory in clean systems is simpler than the fermionic equivalent, because pair-splitting contributions (like Maki-Thompson) do not need to be taken into account. On the other hand care has to be taken as interactions are necessary to allow for a Ginzburg-Landau like description, which certainly does not hold for the non-interacting Bose gas.

We are the first to describe how fluctuational effects on observables differ between trapped and untrapped systems, especially in the case of a quasi-magnetic susceptibility of an anisotropically layered system. We expect stronger divergences in the uniform scenario, as for small  $\tau$  the coherence length diverges as  $\xi \sim \tau^{-1}$  compared to slower growth  $\xi \sim \tau^{-1/2}$  in trapped systems. We found for the layered three-dimensional anisotropic system a cross-over from 2D to 3D fluctuational behaviour as the coherence length grows close to the transition. We further observed that d = 2 is the upper critical dimension for trapped bosonic systems, but concluded that local probes are still able to access fluctuational observables.

Arguably the main contribution is a scheme that creates constant gradients of artificial magnetic fields for cold atom systems. We discussed that such a scheme is robust to small phase fluctuations when tuned into the proper region in parameter space and how it allows to measure the characteristic power-law behaviour of the fluctuational magnetic susceptibility.

Lastly we have argued how the rotational behaviour of small traps might allow for an experimental measurement of the characteristics of the different phases of a bosonic superfluid-insulator transition. For this we generalized Steiner's theorem to the case of disjoint quantum systems. Because the three phases, normal state, superfluid grains and total superfluid system have different moment of inertia, measuring the rotational properties can give evidence of such a layered transition. The caveat is that these observations will only be clear in small traps and as disorder driven transitions often require large systems to realize instances in which the disordered phase shows specific characteristics, like finite compressibility for the disordered Mott-insulator to superfluid transition [47].

## Chapter 4

# **Binary one-dimensional mixtures**

One dimensional systems are very special. Already in the previous chapters we saw that in one dimension the critical temperature for bosonic condensation is reduced to zero and that true long-range behaviour cannot be expected. On the other hand these systems are very appealing from a theoretical point of view, because at least in the limit of low energies they can be solved exactly, even with interactions. We will use the next chapter to give a small introduction to one-dimensional systems, bosonic and fermionic, which is based on the introductory texts by Giamarchi and Cazalilla [113, 114]. We argue that the low energy theories for bosons and fermions look very similar and that correlations, though not infinite in range, can still be power-law like and, for all practical purposes, quasi-long range.

Afterwards we present original research in the matter of one-dimensional mixtures. We especially investigate how the bosonic and fermionic dynamical structure factor changes when interactions are turned on.

## 4.1 Introduction to One-Dimensional Systems

To understand the nature of one-dimensional systems, we have to understand the fact that only in one dimension it is possible to enumerate particles in a non-arbitrary and continuous fashion, as a continuous mapping of a higher dimensional space onto a one-dimensional line is not possible. Though the particles themselves might be identical, they are always positioned on a line. If the line is directional, let us call it the *x*-axis, it is always possible to say that one particle is "ahead" of another particle if its position is further down the positive *x*-axis. This seems not very significant at first, but it allows us to describe the system in a very distinct way. The approach goes back to Haldane [21]. A labelling field  $\phi_l(x)$  is introduced. This field changes in between two particle positions by the value  $2\pi$ , such that  $(\phi_l(x') - \phi_l(x))/2\pi$  rounded to the lower integer value tells the number of particles in the interval x' - x. The field is so defined that at the position of the *k*th particle (here we need that the particle has definite position with respect to the other particles, which is only possible in one dimension) the labelling field has the value  $\phi_l(x_k) = 2\pi k$ . We can also assign to each particle the equilibrium position  $x_{k,0} = n_b^{-1}k$  and describe the displacement of the particle from that position  $u_k = x_k - x_{k,0}$ . Next we can replace the particle density

$$\rho(x) = \sum_{i} \delta(x - x_i)$$

by the field  $\phi_l$ , as we know that at the particle positions the label field is a multiple of  $2\pi$ 

$$\rho(x) = \sum_{i} \delta(x - x_{i}) = \sum_{k} |\partial \phi_{xl}(x)| \,\delta(\phi_{l}(x) - 2\pi k) = \frac{\partial_{x} \phi_{l}(x)}{2\pi} \sum_{p} e^{ip\phi_{l}(x)},$$

where in the last step the Poisson formula was used. Introducing the field relative to the equilibrium position  $\theta(x) = (2\pi n_b x - \phi_l(x))/2$ , the density becomes

$$\rho(x) = \left[n_b - \frac{1}{\pi}\partial_x \theta(x)\right] \sum_p e^{i2p(\pi nx - \theta(x))}.$$
(4.1)

We can see that the exponential terms are fluctuating fast compared to the p = 0 term and tend to average out over longer distances, so that a good approximation to the density is

$$\rho(x) \approx n - \frac{1}{\pi} \partial_x \theta(x),$$

which invites the interpretation of  $\partial_x \theta / \pi$  as a density fluctuation. First we want to describe the bosonic creation and annihilation operators using the new fields. To do this we use the amplitude-phase representation (2.12),

but to avoid naming confusion we replace the phase by the letter  $\phi$ 

$$\psi_b(x) = \sqrt{\rho(x)} \mathrm{e}^{-i\phi(x)}$$

where the density can be expressed in terms of the fields (4.1). To obtain a complete representation in terms of the fields  $\phi$  and  $\theta$  we have to deduce their commutation relationships. Because for bosons

$$\left[\psi_{b}(x),\psi_{b}^{\dagger}(x')\right]=\delta\left(x-x'\right),$$

and given (4.1), the commutation relation must be

$$\left[\frac{1}{\pi}\partial_{x}\theta(x),\phi(x')\right] = -i\delta(x-x').$$

We can define  $\Pi \equiv -\partial_x \theta / \pi$  as the canonically conjugate momentum to  $\phi(x)$ . Again, we have a choice here of whether we want  $\theta$  the field and  $\partial_x \phi$  the conjugate momentum. For the resultant theory it is of course inconsequential as the low energy Hamiltonian is symmetric with respect to  $\phi \leftrightarrow \theta$  and an appropriate rescaling.

Naturally one can do the same thing for fermions, i.e. defining a labelling field etc. However, in order for the fermion field to be anticommutative one has to perform a Jordan-Wigner transformation of the bosonic field, which essentially is a multiplication by the labeling field

$$\psi_f^{\dagger}(x) = \psi_b^{\dagger}(x) \mathrm{e}^{i\frac{1}{2}\phi_l(x)}$$

This leads finally to the Haldane representation of the bosonic and fermionic fields in terms of the new fields  $\theta$  and  $\phi$ 

$$\Psi_b^{\dagger} = \left[ n_b - \frac{\partial_x \theta_b(x)}{\pi} \right]^{1/2} \sum_p e^{i2p(\pi n_b x - \theta_b(x))} e^{-i\phi_b(x)}$$

$$\Psi_f^{\dagger} = \left[ n_f - \frac{\partial_x \theta_f(x)}{\pi} \right]^{1/2} \sum_p e^{i(2p+1)(\pi n_f x - \theta_f(x))} e^{-i\phi_f(x)}$$
(4.2)

where  $n_{b/f}$  are the equilibrium values of the respective densities.

The low energy Hamiltonian can be found phenomenologically. It has to be an expansion in powers of  $\partial_x \theta$  and  $\partial_x \phi$ . In an inversion symmetric system,  $\rho(x) \rightarrow \rho(-x)$  and  $\psi(x) \rightarrow \psi(-x)$  must hold. This leads to the conditions that  $\partial_x \theta(x) \rightarrow \partial_x \theta(-x)$  and  $\partial_x \phi(x) \rightarrow -\partial_x \phi(-x)$ . Thus a Hamiltonian cannot contain the term  $\partial_x \theta \partial_x \phi$ , as it is odd under inversion and would break the inversion symmetry. The Hamiltonian that describes the effective low energy properties of a massless one-dimensional system can only contain even powers of the operators. Its most general form is thus

$$H = \frac{v}{2} \int dx \left[ \frac{K}{\pi} \left( \partial_x \phi \right)^2 + \frac{\pi}{K} \Pi^2 \right],$$

where the choice of v and K as independent parameters is motivated by the observation that the speed of sound of such a system is indeed v. K is the so called Luttinger parameter and contains all the information about the interactions. For repulsive bosons, K > 1 and becomes smaller for increasing interactions. For repulsive fermions K < 1, and only for the free case K = 1. This leads to the insight that hardcore bosons, which means bosons with infinitely strong short range repulsions, are equivalent to free fermions in one dimension, which can be verified using exact solutions [20].

The action that is associated with such a Hamiltonian is

$$S = \int_0^\beta d\tau \int dx \left[ i \frac{1}{\pi} \partial_x \phi \, \partial_t \theta - \frac{v}{2} \left( \frac{K}{\pi} \left( \partial_x \phi \right)^2 + \frac{\pi}{K} \left( \partial_x \theta \right)^2 \right) \right]$$

Substituting the Fourier basis for real fields and applying the standard integration of bosonic Gaussian fields we arrive at the following correlator

$$\langle \boldsymbol{\theta}^*(k_1) \boldsymbol{\theta}(k_2) \rangle = \frac{\pi v K \delta_{k_1,-k_2} L \beta}{\omega_n^2 + v^2 k_1^2},$$

where the denominator shows that the excitations are indeed phononic, for after analytic continuation the poles

are at  $\omega = vk$ . Using similar results for  $\phi$  we can find the correlation functions for the fields

$$\left\langle \begin{bmatrix} \boldsymbol{\theta} \left( \boldsymbol{r} \right) - \boldsymbol{\theta} \left( \boldsymbol{0} \right) \end{bmatrix}^{2} \right\rangle = KF_{1}\left( \boldsymbol{r} \right),$$

$$\left\langle \begin{bmatrix} \boldsymbol{\phi} \left( \boldsymbol{r} \right) - \boldsymbol{\phi} \left( \boldsymbol{0} \right) \end{bmatrix}^{2} \right\rangle = K^{-1}F_{1}(\boldsymbol{r}),$$

$$\left\langle \boldsymbol{\theta} \left( \boldsymbol{r} \right) \boldsymbol{\phi} \left( \boldsymbol{0} \right) \right\rangle = \frac{1}{2}F_{2}(\boldsymbol{r}),$$

where  $r = (x, \tau)$  and [113]

$$F_1(r) = \frac{1}{2} \log \left[ \frac{x^2 + (v|\tau| + \alpha)^2}{\alpha^2} \right],$$
  
$$F_2(r) = -i \arg \left[ v\tau + \alpha \operatorname{Sign}(\tau) + ix \right],$$

with  $\alpha$  being a small cutoff parameter. Since we can deconstruct fields in the Haldane representation (4.2), we are interested in correlators of the type

$$\left\langle \mathrm{e}^{iA[\theta(r)-\theta(0)]}\mathrm{e}^{iB[\phi(r)-\phi(0)]}\right\rangle,$$

which according to the Debye-Waller relation for a quadratic action is the same as

$$\exp\left[-A^{2}\left\langle \left[\theta\left(r\right)-\theta\left(0\right)\right]^{2}\right\rangle -B^{2}\left\langle \left[\phi\left(r\right)-\phi\left(0\right)\right]\right\rangle ^{2}-2AB\left\langle\theta\left(r\right)\phi\left(0\right)\right\rangle \right].$$

The last exponent creates merely a phase factor we want to neglect as it can be absorbed into the definition of the operators we want to average over. More interestingly, the  $F_1$  functional causes the correlation to fall of in a power-law fashion

$$\left\langle \mathrm{e}^{iA[\theta(r)-\theta(0)]}\mathrm{e}^{iB[\phi(r)-\phi(0)]}\right\rangle \sim \left(\frac{\alpha^2}{x^2+(\nu|\tau|+\alpha)^2}\right)^{\frac{AK}{2}+\frac{B}{2K}}.$$

This is a very general result and shows that low energy systems in one dimension seem to be always in a critical state with power-law correlators, but non-universal exponents. This coincides with the fact that there is no real

phase transition in one dimension (Mermin-Wagner) as there cannot be true long range order. For practical purposes there is a long-range order though, as with thermal fluctuations taken into account, correlations fall off exponentially for distances larger than  $\xi \sim v\beta$ . If  $\beta$  is large, then  $\xi$  can easily outgrow the finite size of the system. If the correlator is decaying slowly enough, we have quasi long-range order. Moreover, phases can be characterized by the operator *O* associated with the order parameter for which the susceptibility

$$\chi(k,\omega_n) = \int_0^\beta d\tau \int dx \langle O^{\dagger}(x,\tau) O(0,0) \rangle e^{-ikx+i\omega_n\tau}$$

diverges the strongest. Quite generally when  $\langle O^{\dagger}(r)O(0) \rangle \sim r^{-\nu}$ , then  $\chi \sim (\max[k, \omega_n])^{\nu-2}$ , as we can see by dimensional analysis. Thus the strongest divergence of the susceptibility corresponds to the slowest decaying correlator. Though at each point all correlators fall off as power-laws, one can define phase diagrams with phase boundaries where there are qualitative changes in the long-range behaviour. We can imagine the system trying to order, which however is not allowed in one dimension. But, if the system is copied and weakly linked to its nearest neighbors to form a three-dimensional system of tubes, then operators with a divergent susceptibility can form order under the weakest link to neighbors and the system exhibits transition into a phase. In this way one can already classify one dimensional phases by their would-be behaviour when generalized to three dimensions. By changing microscopic parameters the slowest decaying correlator may change, which in return can be considered a 1D quantum phase transition. In the next section we investigate a system where long range correlations are dominated by composite operators, so-called polarons.

## 4.2 One-dimensional mixtures

We want to investigate the edge-state singularity of a one-dimensional mixture of bosons and fermions. The quantities that can describe the excitation spectrum are the dynamical structure factors, the susceptibility of the system with respect to perturbations that couple to the density, where we have to differentiate between a bosonic

#### CHAPTER 4. BINARY ONE-DIMENSIONAL MIXTURES

and a fermionic dynamical structure factor (DSF)

$$S_{b}(q,\omega) = \int dx dt e^{i(\omega t - qx)} \langle \rho_{b}(x,t) \rho_{b}(0,0) \rangle,$$
  
$$S_{f}(q,\omega) = \int dx dt e^{i(\omega t - qx)} \langle \rho_{f}(x,t) \rho_{f}(0,0) \rangle.$$

This is a convenient quantity, as it is experimentally accessible via different methods such as Bragg scattering or photoemission spectroscopy (see e.g. [115, 116]). In an ideal Luttinger liquid the excitation spectrum of density waves should lead to DSF of the form

$$S(q,\omega) \sim |q| \delta(\omega - v |q|),$$

which indeed holds for small momenta q. However broadening has to be taken into account even at small q and zero temperature to understand such phenomena as Coulomb drag [117].

Another case for comparison are free fermions with dispersion  $\varepsilon(k) - \mu = (k^2 - k_F^2)/2m$ , where the DSF can be directly calculated to give for  $q < 2k_F$ 

$$S_{0,f}(q,\omega) = \frac{m}{|q|} \Theta\left(q^2/2m - |\omega - v_F q|\right) = \frac{m}{|q|} \Theta\left(\omega - \omega_-(q)\right) \Theta\left(\omega_+(q) - \omega\right),$$

where  $v_F = k_F/m$  is the Fermi velocity. Clearly for a given q there exist threshold frequencies  $\omega_{\pm}$ , where  $\omega_- = v_F q - q^2/m$  is the minimum energy necessary to remove a particle from the bottom of the Fermi sea under momentum conservation and  $\omega_+ = (k_F + q)^2/2m - k_F^2/2m$  is the maximum energy where the system can be excited by taking fermions right at the Fermi edge and exciting them to momentum  $k_F + q$ . In between these values the DSF is a constant and outside it vanishes. However, it has been shown that the clear features of the free DSF are broadened into power-law behaviour when interactions are present for  $\omega > \omega_-$  as  $|\omega - \omega_-|^{-\alpha}$  and for  $\omega$  close to  $\omega_+$  as  $|\omega - \omega_+|^{\beta}$ , which are known as Fermi-edge singularities [118, 119]. We want to study how these singularities, which essentially appear due to the excitation of low-energetic modes close to the Fermi surface, behave in mixtures.

#### CHAPTER 4. BINARY ONE-DIMENSIONAL MIXTURES

The starting point for the interacting 1D dilute gas is a Hamiltonian of the form [22]

$$H_{\text{tot}} = \int dx \sum_{\alpha=f,b} \left[ \frac{1}{2m_{\alpha}} \partial_x \psi_{\alpha}^{\dagger}(x) \partial_x \psi_{\alpha}(x) - \mu \rho_{\alpha}(x) \right] + \frac{1}{2} \sum_{\alpha,\beta} \int dx \tilde{g}_{\alpha,\beta} \rho_{\alpha}(x) \rho_{\beta}(x)$$

It is convenient to replace the operators by their Haldane representation (4.2), which then gives the Hamiltonian

$$H_{\text{tot}} = \frac{v_b}{2} \int dx \left[ \frac{K_b}{2} \left( \partial_x \phi_b \right)^2 + \frac{\pi}{K_b} \Pi_b^2 \right] + \frac{v_f}{2} \int dx \left[ \frac{K_f}{2} \left( \partial_x \phi_f \right)^2 + \frac{\pi}{K_f} \Pi_f^2 \right] \\ + \frac{g\pi}{2\sqrt{K_bK_f}} \int dx \left[ \Pi_b \Pi_f + n_f n_b \cos\left(2\left(\theta_f - \theta_b\right) + \pi\left(n_f - n_b\right)x\right) \right],$$

where only the most relevant terms were kept. The terms where only a single species occured were put into Luttinger form, and the interspecies interaction term was replaced by  $\tilde{g}_{fb} \rightarrow g/\sqrt{K_bK_f}$  for future convenience. We can see that the last term, which describes the back-scattering between fermions and bosons, makes the Hamiltonian look locally like a sine-Gordon Hamiltonian and oscillates very fast in space when  $|n_f - n_b|$  becomes large, so that we can neglect it compared to the  $\Pi_b \Pi_f$  terms. In the following we will assume this assumption to hold. The effective Hamiltonian then becomes

$$\begin{split} H_{\text{tot}} &= \frac{v_b}{2} \int dx \left[ \frac{K_b}{2} \left( \partial_x \phi_b \right)^2 + \frac{\pi}{K_b} \Pi_b^2 \right] + \frac{v_f}{2} \int dx \left[ \frac{K_f}{2} \left( \partial_x \phi_f \right)^2 + \frac{\pi}{K_f} \Pi_f^2 \right] \\ &+ \frac{g\pi}{2\sqrt{K_b K_f}} \int dx \Pi_b \Pi_f. \end{split}$$

The Hamiltonian can be diagonalized (see appendix) into two uncoupled, polaronic modes (see below) [23, 22]

$$H_{\text{tot}} = \frac{v_a}{2} \int dx \left[ \frac{1}{2} \left( \partial_x \phi_a \right)^2 + \pi \Pi_a^2 \right] + \frac{v_A}{2} \int dx \left[ \frac{1}{2} \left( \partial_x \phi_A \right)^2 + \pi \Pi_A^2 \right], \tag{4.3}$$

where

$$v_{a/A}^2 = \frac{1}{2} \left( v_b^2 + v_f^2 \right) \pm \frac{1}{2} \sqrt{\left( v_f^2 - v_b^2 \right) + g^2 v_f v_b}.$$

One can see that for too strong interactions, one of the two modes becomes unstable, i.e. acquires an imaginary component. For very strong repulsive interactions this would mean a physical separation (demixing) of the two

liquids, whereas for very strong attractive interactions this would mean the formation of boson-fermion dimers [22].

One could ask, what are the operators that correspond to the new modes. A good ansatz are the dressed particle states [23]

$$\tilde{f} = \mathrm{e}^{-i\lambda\phi_b(x)}\psi_f(x), \quad \tilde{a} = \mathrm{e}^{-i\eta\phi_f(x)}\psi_b(x),$$

which are composite operators and describe polarons [119] with yet undetermined real parameters  $\eta$  and  $\lambda$ . Their correlators can be straightforwardly calculated using the techniques from the previous section and the Hamiltonian 4.3. Their correlators are of the form

$$\langle \tilde{a}(x)\tilde{a}^{\dagger}(0)\rangle \sim |x|^{-\frac{1}{2}(A\eta^2 - 2V\eta + C)}$$

where the constants *A*, *B* and *C* are functions of the Luttinger parameters of the original fluids and their mixing angle  $\tan 2\psi$  (see appendix for more details (5.3)). One can maximize the exponent to find the longest range correlations, which in the limit of weak interactions are

$$\eta_c 
ightarrow rac{2g_{\widetilde{b}f}}{\pi v_b}, \quad \lambda_c 
ightarrow rac{\widetilde{g}_{bf}}{\widetilde{g}_{bb}}.$$

The physical intuition for this result is that a boson, through its nearest neighbor interaction, locally enhances or supresses a cloud of  $\eta_c$  fermions and a fermion locally enhances or suppresses a cloud of  $\lambda_c$  bosons, depending on the sign of the interaction.

We want to investigate the edge state spectrum. Physically this means that with a probe bosons or fermions are excited and the resultant spectrum is measured. Such a probe transfers energy and momentum into the system and can thus be be quantified by a characteristic excitation frequency  $\omega$  and momentum vector q. In principle there are large areas in  $q - \omega$  space that allow for excitation, however they tend to be very difficult to describe analytically, because the amount of possible dynamic processes is large. The situation is however different at the edge of the spectrum, where the excess energy on top of the principal impurity excitation energy  $\varepsilon_d$  is small, at least small enough to only excite the lowest lying modes of the system, namely the Luttinger modes.

In fact we can postulate an impurity Hamiltonian that describes the impurity, the two Luttinger modes and interactions between the impurity and the low energy modes [24, 25]

$$H_{\text{tot}} = H_a + H_A + H_{\text{imp}} + H_{\text{int}}$$

$$H_{a/A} = \frac{v_{a/A}}{2} \int dx \left[ \frac{1}{2} \left( \partial_x \phi_{a/A} \right)^2 + \pi \Pi_{a/A}^2 \right]$$

$$H_{\text{imp}} = \int dx d^{\dagger}(x) \left[ \varepsilon_k - i v_d \partial_x \right] d(x)$$

$$H_{\text{int}} = \int dx \left[ V_{A, \Phi} \partial_x \phi_A + V_{a, \Phi} \partial_x \phi_a + V_{A, \Pi} \Pi_A + V_{a, \Pi} \Pi_a \right] d^{\dagger} d(x).$$
(4.4)

In the Hamiltonian  $\varepsilon_k$  is the dispersion relation of the impurity and  $v_d = \partial_k \varepsilon_k$  is the group velocity. The  $V_{a/A,\phi/\Pi}$  are constants that we have to determine.

#### 4.2.1 Description of the impurities

We want to describe what happens when one impurity is immersed in two liquids. This step is not strictly necessary to find the behaviour of the dynamical structure factors for the edge-state singularity, it is nonetheless an interesting exercise to gain physical insight. In general a fluid without impurity can be described by its entropy functional

$$S = S(E, P, N_1, N_2, V, v_{s1}, v_{s2}) = S(\varepsilon, g, \rho_1, \rho_2, v_{s1}, v_{s2})$$

which only depends on the energy density  $\varepsilon$ , momentum density g, the superfluid particle densities  $\rho_{1,2}$  and the superfluid velocities  $v_{s1,2}$  [96]. That has the important implication that an interacting mixture of fluids has only one normal component (because the momentum transfers are coupled and only one momentum density gexists) rather than a normal component for each fluid. Additionally there are up to two superfluid components, characterized by a local phase  $\Psi_{1/2}(x)$ . One might ask whether the description by superfluid is relevant in one dimension. That impurities can move in a one-dimensional system without dissipation follows from the quasi-order and the appearance of a critical velocity [120].

The Lagrangian of two non-interacting liquids is given in the hydrodynamical description by ([28])

$$\begin{split} L_0 &= \int dx \left[ \dot{\phi}_1 n_1 - \varepsilon_1 \left( n_1 \right) + \dot{\phi}_2 n_2 - \varepsilon_2 \left( n_2 \right) \right] \\ &= \int dx \left[ \mu_1 n_1 - \varepsilon_1 \left( n_1 \right) + \mu_2 n_2 - \varepsilon_2 \left( n_2 \right) \right] \\ &= L_0 \left( \mu_{1,2}, n_{1,2} \right). \end{split}$$

Here  $\varepsilon$  is the energy density of the fluid and in equilibrium

$$\mu_i = \mu_i \left( n_i \right) = \frac{\partial \varepsilon_i}{\partial n_i}$$

The grandcanonical potential for such an equilibrium fluid is

$$\Omega_0(\mu_{1,2}) = -L_0(\mu_{1,2}, n_{1,2}).$$

To describe the impurity, it is convenient to focus on its effect on the fluid. If the impurity is small, which means its scale is  $\ll \xi$ , and it equilibrates fast with its immediate environment, i.e.  $\frac{1}{\tau} \gg \frac{c}{\xi}$ , the equilibration time scale  $\tau$  is much smaller than the time scale of the phonons surrounding it, then the effect of the impurity is merely to deplete locally particles  $N_{1,2}$  out of the superfluids and to cause phase  $\Psi_{1,2}$  drops along the superfluid [121, 122]. We want to find a model that describes these variables in terms of the momentum of the impurity.

Let us assume an impurity with mass *M* moves through the system with velocity  $V = \dot{X}$ . Instead of looking at a moving impurity, one can also make a Galileian transform into a reference frame that moves with velocity -V in which the impurity stands still. Such a transformation creates currents in the fluids

$$j'_i = -n_i V$$

and shifts the chemical potential

$$\mu_i'=\mu_i+m_i\frac{V^2}{2},$$

with  $m_i$  the mass of the moved particles of the respective liquid and all primed quantities are after the transformation.

Importantly, we also find that

$$\frac{j_1}{n_1} = \frac{j_2}{n_2},$$

which means that the currents are not independent of each other.

The impurity effect can then be described as a shift in the grand canonical potential in terms of the energy of the impurity as well as a change in the potential of the liquids around it

$$\Omega_{d}^{'} = E_{d}^{'} - \mu_{1}^{'} N_{1} - \mu_{2}^{'} N_{2}.$$

The  $N_i$  have a negative sign, because they are taken out of the liquid.

The energy of the impurity is also affected by the shift

$$E_d' = E_d - P_d V + \frac{(m_1 N_1 + m_2 N_2) V^2}{2}$$

We can now relate the shift in thermodynamic potential to the Lagrangian of an impurity via  $L_d = -\Omega'_d$ ,

$$L_{d}(V,n) = -E_{d}^{'} + \left(\mu_{1}^{'}N_{1} + \mu_{2}^{'}N_{2}\right) = -\Omega_{d}^{'}(j^{'},\mu^{'}).$$

This is interesting, as on one side we have a Lagrangian and on the other a proper thermodynamic potential, i.e. a statistical quantity.

In the next step we vary the thermodynamic quantities  $j, \mu$  which allows us to identify the conjugate variables

$$d\Omega_{d}^{'} = \Psi_{1}dj_{1}^{'} + \Psi_{2}dj_{2}^{'} + N_{1}d\mu_{1}^{'} + N_{2}d\mu_{2}^{'}$$

with

$$\Psi_{i} = \partial_{j'_{i}} \Omega', N_{i} = \partial_{\mu'_{i}} \Omega'.$$

In equilibrium,  $\Psi_i$  and  $N_i$  are locked  $\Psi_i = \Psi_i(N_i)$ . However, for the kind of processes which we consider, the  $\Phi_i, N_i$  should be considered as dynamical variables. Legendre transforming the grandcanonical potential gives a quasi Hamiltonian

$$H_d\left(\Psi_{1,2}, N_{1,2}\right) = \Omega'_d - \sum_i \left(j'_i \Psi_i + \mu'_i N_i\right)$$
$$d\left(H_d\right) = -\sum_i \left(j'_i d\Psi_i + \mu'_i dN_i\right).$$

Following, this gives for the impurity Lagrangian

$$L_d(V, \Psi_{1,2}, N_{1,2}) = \frac{1}{2} \left( M - \sum_i m_i N_i \right) V^2 - V \left( \sum_i n_i \Psi_i \right) - \left( \sum_i \mu_i N_i \right) - H_d \left( \Psi_{1,2}, N_{1,2} \right).$$
(4.5)

This Lagrangian so far describes only the impurity that is in contact with its local environment, but not yet the coupling to the phonons, which we will derive later. For such a Lagrangian one can define the canonical momentum

$$P = \frac{\partial L}{\partial \dot{X}} = \left(M - \sum_{i} m_{i} n_{i}\right) V + \sum_{i} n_{i} \Psi_{i}$$

and the corresponding full Hamiltonian

$$H(P, \Psi, N) = PV - L$$
  
=  $\frac{1}{2} \frac{(P - \sum_{i} n_{i} \Psi_{i})^{2}}{M - \sum_{i} m_{i} N_{i}} + \sum_{i} \mu_{i} N_{i} + H_{d}(\Psi_{1,2}, N_{1,2}).$ 

The corresponding equations of motion are

 $\dot{P} = 0$ 

$$-\partial_{\Psi_i}H = n_iV - \partial_{\Psi_i}H_d = 0$$
$$-\partial_{N_i}H = -\mu_i - \frac{1}{2}m_iV^2 - \partial_{N_i}H_d = 0.$$

Also needed is the fact that  $j_1 = \frac{n_2}{n_1} j_2$ , which means that  $\partial_{j_1} = \frac{n_1}{n_2} \partial_{j_2}$  and translates to  $\Psi_1 = \frac{n_2}{n_1} \Psi_2$ .

At this point we have to make assumptions about the shape of  $E_d$ . For weak independent coupling between the impurity and the two liquids, the energy of the impurity can be approximated by the energy of depletonsolitons (see appendix 5.7) as

$$E_d = \frac{4}{3}c_1n_1\left(1 - \frac{V^2}{c_1^2}\right)^{3/2} + \frac{4}{3}c_2n_2\left(1 - \frac{V^2}{c_2^2}\right)^{3/2},$$

where  $c_i$  is the speed of sound of the *i*th liquid.

Also we do know the momentum of the depleton-impurity from microscopic considerations (see appendix 5.7)

$$P = -2n_1 \left( \frac{V}{c_1} \sqrt{1 - \frac{V^2}{c_1^2}} + \arcsin\left(\frac{V}{c_1}\right) \right) + -2n_2 \left(\frac{V}{c_2} \sqrt{1 - \frac{V^2}{c_2^2}} + \arcsin\left(\frac{V}{c_2}\right) \right).$$

These lead to the conditions

$$\frac{\partial P}{\partial n_i} = -2\arcsin\frac{V}{c_i}$$

and

$$\frac{\partial E}{\partial n_i} = 2c_i \left(1 - \frac{V^2}{c_i^2}\right)^{1/2}.$$

Lastly we can relate some of the partial derivatives to each other. By using that

$$\frac{\partial \mu_i}{\partial n_i} = \frac{m_i c_i^2}{n_i}$$

and that for the dilute system the energy per particle goes as  $\varepsilon = \varepsilon_i(n_i) + gn_1n_2$  we can replace *n* and *V* derivatives by  $\mu$  and *j* derivates. When we keep in mind that  $\Psi_i = \partial_{j_i}\Omega$  and  $N_i = \partial_{\mu_i}\Omega$  we obtain from the Hamiltonian equations a system of equations that allows us to solve the  $\Psi_i$  and  $N_i$  in terms of the impurity velocity *V*, the densities  $n_i$ , the speeds of sounds  $c_i$  and the interaction term *g*.

$$\frac{\partial L}{\partial V} - MV = n_1 \Psi_1 + n_2 \Psi_2 - m_1 V N_1 - m_2 V N_2 = P,$$
$$\frac{\partial L}{\partial n_1} = V \Psi_1 - \frac{m_1 c_1^2}{n_1} N_1 - g N_2 = \frac{\partial P}{\partial n_1} V - \frac{\partial E}{\partial n_1},$$
$$\frac{\partial L}{\partial n_2} = V \Psi_2 - \frac{m_2 c_2^2}{n_2} N_2 - g N_1 = \frac{\partial P}{\partial n_2} V - \frac{\partial E}{\partial n_2}.$$

The additional condition to close the system is that  $n_1\Psi_1 = n_2\Psi_2$ , which is a direct consequence from the fact that any equilibrium flow in one of the liquids must be accompanied by a flow in the other liquid. This set of equations can be inverted. Let us assume the case of g = 0. Then eliminating  $\Psi_1$  in favor of  $\Psi_2$  we obtain

$$\begin{pmatrix} \Psi_2 \\ N_1 \\ N_2 \end{pmatrix} = \begin{pmatrix} \kappa_1 \frac{n_1}{n_2} \Psi_{1,0} + \kappa_2 \Psi_{2,0} \\ \kappa_2 \frac{n_1 V}{m_1 c_1^2} \left( \frac{n_2}{n_1} \Psi_{2,0} - \Psi_{1,0} \right) + N_{1,0} \\ \kappa_1 \frac{n_1 V}{m_1 c_1^2} \left( \frac{n_1}{n_2} \Psi_{1,0} - \Psi_{2,0} \right) + N_{2,0} \end{pmatrix}$$

where

$$\Psi_{i,0} = -2 \arcsin \frac{V}{c_i}, \quad N_{i,0} = \frac{2n_i}{m_i c_i} \left(1 - \frac{V^2}{c_i^2}\right)^{1/2}$$

and

$$\kappa_{i} = \frac{\left(1 - \frac{V^{2}}{c_{i}^{2}}\right)}{\left(1 - \frac{V^{2}}{c_{1}^{2}}\right) + \left(1 - \frac{V^{2}}{c_{2}^{2}}\right)}.$$

This is reassuring, as these equations resemble the equation of a single liquid-impurity system. The phases are weighted superpositions of the original phases whereas the depletion clouds tend to change only a little.

When we reintroduce the *g*, the picture does not change that drastically. If we let  $E = \sqrt{m_1 c_1^2 m_2 c_2^2}$  and  $\chi_i = n_{\bar{i}}g/E$ ,  $\lambda_i = (gn_{\bar{i}} - m_i c_{\bar{i}}^2)$  and  $\eta_i = (gn_{\bar{i}} - m_i V^2)/E$ , where the bar denotes the opposite particle species, then we find for the new values

$$\Psi_{2} = \frac{1}{\left[1 - \frac{V^{2}}{c_{1}^{2}}\right] + \left[1 - \frac{V^{2}}{c_{2}^{2}}\right] - \chi_{1}\eta_{1} - \chi_{2}\eta_{2}} \left[ \begin{array}{c} \frac{n_{1}}{n_{2}}\kappa_{1}^{'}\Psi_{1,0} + \kappa_{2}^{'}\Psi_{2,0} + \\ + \chi_{2}\left(\lambda_{2}\frac{m_{1}VN_{1}}{n_{1}} + \lambda_{1}\frac{m_{2}VN_{2}}{n_{2}} - \eta_{2}\Psi_{1,0} - \eta_{1}\Psi_{2,0}\right) \end{array} \right], \quad (4.6)$$

where  $\kappa'_i = \left[1 - \frac{V^2}{c_i^2}\right]$ .

For the number occupations we have

$$N_{1} = \frac{1}{\left[1 - \frac{V^{2}}{c_{1}^{2}}\right] + \left[1 - \frac{V^{2}}{c_{2}^{2}}\right] - \chi_{1}\eta_{1} - \chi_{2}\eta_{2}} \begin{bmatrix} (\eta_{2} - \lambda_{2} + \chi_{2})(N_{\Psi_{2}} - N_{\Psi_{1}}) + (\lambda_{2}\frac{m_{2}V^{2}}{E} + (\lambda_{2} - \eta_{2})\frac{m_{1}c_{1}^{2}}{E})N_{1,0} \\ + (\lambda_{2}\frac{m_{2}V^{2}}{E} - (\eta_{2} + \chi_{1})\frac{m_{2}c_{2}^{2}}{E})N_{2,0} \end{bmatrix},$$

$$(4.7)$$

$$N_{2} = \frac{1}{\left[1 - \frac{V^{2}}{c_{1}^{2}}\right] + \left[1 - \frac{V^{2}}{c_{2}^{2}}\right] - \chi_{1}\eta_{1} - \chi_{2}\eta_{2}} \left[ \begin{array}{c} (\eta_{1} - \lambda_{1} + \chi_{1})\left(N_{\Psi_{1}} - N_{\psi_{2}}\right) + \left(\lambda_{1}\frac{m_{1}V^{2}}{E} + (\lambda_{1} - \eta_{1})\frac{m_{1}c_{1}^{2}}{E}\right)N_{1,0} \\ + \left(\lambda_{1}\frac{m_{1}V^{2}}{E} - (\eta_{1} + \chi_{2})\frac{m_{2}c_{2}^{2}}{E}\right)N_{2,0} \end{array} \right].$$

where  $N_{\Psi_i} = n_i V \Psi_i / E$ .

As expected, the interaction shifts the depletion and phase jumps. We have to keep in mind that the proper units are recovered when  $n \rightarrow \hbar n$ . The  $\eta, \lambda$  and  $\chi$  are dimensionless and correspond to energy ratios. The  $\chi_i$ are proportional to the potential energy felt by species *i* due to the other particles. The  $\lambda_i$  is that value corrected by the kinetic energy of the particle travelling at the speed of sound of the opposite species, and the  $\eta_i$  is that value, but corresponding to the speed of the impurity.

#### 4.2.2 The coupling of the impurity to phonons

So far we looked at the impurity as an isolated unit. To understand why the creation of an impurity may cause excitations of the Luttinger liquid, we have to understand how the coupling comes to happen. In the derivation we use only gauge and Galilean invariance to find that the coupling between the impurity and the phonons is necessary, as these arguments are very general and basically follow [121]. Finally we relate the coupling constants to thermodynamical quantities.

We remember that we identified the phononic fields with the density variations  $\rho(x) = \partial_x \theta(x)/\pi$  of the medium and the flow  $u(x) = \partial_x \phi(x)/m$  of the medium, such that  $n \to n + \rho(x)$  and  $\mu \to \mu - \dot{\phi} - mu^2/2$ . The phononic Lagrangian can be obtained by taking only the slow variations of the hydrodynamic Lagrangian den-

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sity  $\mathcal{L} = \mu n - e_0(n)$  [28] into account

$$\begin{split} L_{\rm ph} &= \int dx \left[ \mathscr{L}\left( n(x,t), \mu(x,t) \right) - \mathscr{L}\left( n, \mu \right) \right] \\ &= \int dx \left[ -\rho \dot{\mu} - \frac{m(n+\rho)u^2}{2} - \left( e_0\left( n+\rho \right) - e_0(n) - \mu \rho \right) \right], \end{split}$$

where  $e_0$  is the hydrodynamic energy functional of the liquid.

When the impurity is present, locally the supercurrent and the chemical potential are affected by the impurity

$$\mu' = \mu - \dot{\phi} - \frac{mu^2}{2} + \frac{m(V-u)^2}{2} = \mu(n) + \frac{mV^2}{2} - (\dot{\Phi} + V\partial_x \Phi)$$
$$j' = -(n+\rho)(V-u) = -nV - \frac{1}{\pi}(\dot{\theta} + V\partial_x \theta),$$

where it was used that the relative velocity between liquid and impurity is V - u. In the last step we used the exact continuity equation  $\dot{\theta}/\pi = -n(x)u = -(n+\rho)u$ . Also we have to keep in mind, that the phonon variables are locally evaluated at the impurity position X(t). We can now generalize the impurity Lagrangian 4.5 to take the phononic part into account and obtain the correct coupling. With the total time derivative

$$\frac{d}{dt} = \partial_t + \dot{X}\partial_x = \partial_t + V\partial_x$$

we get the phonon-impurity interaction

$$L_{\text{int}} = \frac{1}{\pi} \Psi \frac{d}{dt} \theta \left( X, t \right) + N \frac{d}{dt} \Phi \left( X, t \right).$$

This type of interaction can be transformed into the more common interaction term in (4.4). An easy way to see this is by using the chiral representation [113] where the phononic fields are written as right and left moving components  $\chi_{\pm}(x,t) = \chi_{\pm}(x \mp ct)$ , where *c* is the speed of sounds of the Luttinger liquid. We also know that the impurity has a classical trajectory  $\dot{X} = V$ , so that the total derivatives become

$$\frac{d}{dt}\phi, \frac{d}{dt}\theta \sim \frac{d}{dt}\chi_{\pm}(X,t) = (V \mp c) \partial_{X}\chi_{\pm}(X,t) \sim \partial_{X}\theta(X,t), \partial_{X}\phi(X,t).$$

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Such terms can be second-quantized into the form of the model, e.g.

$$V_{\theta} \partial_x \theta(X,t) = \int dx \partial_x \theta(x,t) \delta(x-X)$$
$$\rightarrow \int dx V_{\theta} \partial_x \theta(x,t) \sum_i \delta(x-X_i) = \int dx V_{\theta} \partial_x \theta(x,t) d^{\dagger} d$$

which allows to relate the  $N, \Psi$  of the impurity to the interaction constants with the liquid.

$$V_{\phi} = -\frac{N}{\sqrt{K}c}$$

$$V_{\theta} = \frac{\sqrt{K}\Psi}{\pi^{2}c}.$$
(4.8)

We can now use a similar derivation to find a physical interpretation of the coupling constants. Let us for now focus on the coupling of the form

$$H_{\rm int} = \int dx V_{\phi} \, \partial_x \phi \, d^{\dagger} d = \int dx m V_{\phi} u \, d^{\dagger} d.$$

Now let us assume that the field is flowing with velocity u in the lab frame and an impurity is created with momentum q in the comoving frame. The momentum in the lab frame will be  $p = q + m_d u$ , where  $m_d$  is the bare mass of the impurity. The energy of the impurity in the lab frame is  $\varepsilon (p = q + m_d u) = \varepsilon(q) + qu + m_d u^2/2$ , which follows from Galilean invariance [123]. Observing the system from the point of view of the lab frame, i.e. replacing  $q = p - m_d u$  we find

$$\varepsilon(p) = \varepsilon(p - m_d u) + (p - m_d u)u + m_d u^2/2 \approx \varepsilon(p) - m_d u \partial_p \varepsilon + pu - m_d \frac{u^2}{2} \approx \varepsilon(p) + (p - m_d \partial_p \varepsilon)u.$$

At the same time for small momenta we can assume the effective mass  $m^*$  for the impurity

$$\varepsilon(p) \approx \varepsilon_0 + \frac{p^2}{2m^*}.$$

We get thus for the coupling  $V_{\phi}$ 

$$V_{\phi} = \frac{p - m_d \partial_p \varepsilon}{m} = \frac{1 - \frac{m_d}{m^*}}{m} p = \frac{m^* - m_d}{m} v_d.$$

Thus the term  $V_{\phi} \sim \frac{\delta m_d}{m} v_d$ , where  $\delta m$  is the change in effective mass of the impurity.

A similar thing can be found for the term  $V_{\theta}$ . We see that it directly couples to the change in density, so with

$$\varepsilon_d(p,n+\rho) = \varepsilon_d(p,n) + \frac{\partial \varepsilon_d}{\partial n}\rho = \varepsilon_d(p,n) + \frac{\partial \varepsilon_d}{\partial n}\rho = \varepsilon_d(p,n) + \frac{\partial \varepsilon_d}{\partial n}\frac{\partial_x \theta}{\partial n}$$

or

$$V_{\theta} = \frac{1}{\pi} \frac{\partial \varepsilon_d}{\partial n}$$

#### 4.2.3 The Dynamical Structure Factor

As a reminder, we want to use our model (4.4) to find the dynamical structure factors

$$S_{b}(q,\omega) = \int dx dt e^{i(\omega t - qx)} \left\langle \rho_{b}(x,t) \rho_{b}(0,0) \right\rangle,$$
$$S_{f}(q,\omega) = \int dx dt e^{i(\omega t - qx)} \left\langle \rho_{f}(x,t) \rho_{f}(0,0) \right\rangle,$$

close to the edge of the spectrum. This means that all the available energy and momentum is deposited into the moving impurity and the low-lying Luttinger modes of the liquid. It is clear that the impurity carries almost all of the momentum, as the momentum and energy are in a linear relationship for the Luttinger liquid and therefore low energetic modes must only have little excess momentum. It is thus useful to project the relevant creation and annihilation operators onto the physically relevant subbands [24]

$$a(x) = a(x)|_{LL} + e^{ikx}d(x),$$
  
$$c(x) = c(x)|_{LL} + e^{ikx}d(x).$$

#### CHAPTER 4. BINARY ONE-DIMENSIONAL MIXTURES

Using Haldane's representation 4.2 for the Luttinger components

$$a^{\dagger}(x)\big|_{LL} = [n_b + \Pi_b]^{1/2} \left(\sum_{p} e^{i2p(\pi n_b x - \theta_b(x))} e^{-i\phi_b(x)}\right)$$
$$c^{\dagger}(x)\big|_{LL} = [n_i + \Pi_b]^{1/2} \left(\sum_{p} e^{i(2p+1)(\pi n_f x - \theta_f(x))} e^{-i\phi_f(x)}\right),$$

we can see that the fermions have no zero momentum contribution, but rather that their lowest momenta are the two Fermi points  $\pm \pi n_f$  in one dimension. It is common to only take the lowest lying *p* values. That however is not strictly necessary and we want to keep the option open for having contributions that are not of the lowest type. However we take into account that the prefactors  $[n_i + \Pi_i]^{1/2}$  fluctuates only on a small scale  $\sim \Pi_i/n_i \ll 1$  and we can approximate them as  $\approx n_i^{1/2}$ .

The density-density correlation can then, using momentum conservation and Haldane's representation (4.2), be rewritten as

$$\langle \rho_b(x,t) \rho_b(0,0) \rangle = \sum_p e^{iqx} \left\langle d_x^{\dagger} e^{i2p\theta_b(x)} e^{i\phi_B(x)} e^{-i2p\theta_b(0)} e^{-i\phi_b(0)} d_0 \right\rangle$$

$$+ \sum_p e^{iqx} \left\langle e^{-i2p\theta_b(x)} e^{-i\phi_B(x)} d_x d_0^{\dagger} e^{i2p\theta_b(0)} e^{i\phi_b(0)} \right\rangle,$$

$$(4.9)$$

where in the first sum the momenta  $q = -k - 2\pi p n_n$  and in the second sum  $q = 2\pi p n_b + k$ .

Equivalently for the fermions

$$\begin{split} \left\langle \rho_{f}(x,t) \rho_{f}(0,0) \right\rangle &= \sum_{p} \mathrm{e}^{iqx} \left\langle d_{x}^{\dagger} \mathrm{e}^{i(2p+1)\theta_{f}(x)} \mathrm{e}^{i\phi_{f}(x)} \mathrm{e}^{-i(2p+1)\theta_{f}(0)} \mathrm{e}^{-i\phi_{f}(0)} d_{0} \right\rangle \\ &+ \sum_{p} \mathrm{e}^{iqx} \left\langle \mathrm{e}^{-i(2p+1)\theta_{f}(x)} \mathrm{e}^{-i\phi_{f}(x)} d_{x} d_{0}^{\dagger} \mathrm{e}^{i(2p+1)\theta_{f}(0)} \mathrm{e}^{i\phi_{f}(0)} \right\rangle, \end{split}$$

with  $q = -k - (2p+1)\pi n_f$  in the first sum and  $q = (2p+1)\pi n_f + k$  in the second.

To evaluate the correlations we have to use the transformations (5.2) and (5.4) from the appendix to express the purely fermionic fields in terms of the diagonal polaronic fields. However, in the Hamiltonian there is still the interaction of the polaronic fields with the impurity

$$H_{\rm int} = \int dx \left[ V_{a,\phi} \partial_x \phi_a + V_{A,\Phi} \partial_x \phi_A + V_{a,\Pi} \Pi_a + V_{A,\Pi} \Pi_A \right] d^{\dagger} d.$$

Since the interaction Hamiltonian is not quartic, it can be gauged away by a transformation of the form [124]

$$U = \exp\left[i\int dx \sum_{j=a,A} \left(C_{j,\theta} \theta_j + C_{j,\phi} \phi_j\right) d^{\dagger} d(x)\right] = \exp\left[iS\right],$$

where the  $C_{j,\theta/\phi}$  are constants. We want the new Hamiltonian to be of the simple form

$$H_{\text{new}} = U^{\dagger} H_{\text{old}} U = H_a + H_A + H_d + \text{const.}$$

We can see that this works by using the canonical relationship  $[\phi(x), \partial_x \theta(x')] = i\pi \delta(x - x')$  and  $[d(x), d^{\dagger}(x')] = \delta(x - x')$ , because

$$\int_0^{x''} dx' \left[ \phi(x), \partial_x \theta(x') \right] = i\pi \int_0^{x''} \delta(x - x') dx' = i\pi \Theta \left( x'' - x' \right),$$

from which follows that  $[\theta(x), \partial_x \phi(x')] = i\pi \Theta(x' - x)$ , where  $\Theta(x)$  is the Heaviside function. Additionally we need that if [A, B] = c-number, then [A, f(B)] = [A, B] f'(B), given that f is sufficiently analytic.

Because the Hamiltonian is quadratic we have the finite expansion

$$H_{\text{new}} = U^{\dagger} H_{\text{old}} U = H_{\text{old}} - [iS, H_{\text{old}}] + \frac{1}{2} [iS, [iS, H_{\text{old}}]].$$

This expansion is sufficient if  $\frac{1}{2}[iS, [iS, H_{old}]]$  commutes with all other operators, since the next term would be the commutator of *iS* with a constant, which vanishes. So if we choose *iS* in such a way that  $-[iS, H_{old}] = -H_{int}$  then the interaction is indeed gone. We have to check that no new interaction terms are created during the transformation. Indeed, the basic commutators can be straightforwardly calculated. For the Luttinger Hamiltonian  $H_{LL} = \frac{v}{2\pi} \int dx \left[ (\partial_x \theta)^2 + (\partial_x \phi)^2 \right]$ , the impurity Hamiltonian  $H_d = \varepsilon_d \int dx d^{\dagger} d$  and  $H_{int} = \int dx \left( V_{\theta} \partial_x \theta + V_{\phi} \partial_x \phi \right)$ ,

 $iS = i \int dx \left( C_{\theta} \theta + C_{\phi} \phi \right) d^{\dagger} d$  gives

$$[iS, H_{LL}] = -v \int dx \left( C_{\theta} \partial_x \theta + C_{\phi} \partial_x \phi \right) d^{\dagger} d,$$
  

$$[iS, H_d] = 0$$
  

$$[iS, H_{int}] = -\pi \int dx \left( C_{\theta} V_{\phi} + C_{\phi} V_{\theta} \right) d^{\dagger} d$$
  

$$[iS, [iS, H]] = \frac{v\pi}{2} \int dx \left( d^{\dagger} d \right)^2 \left( C_{\theta}^2 + C_{\phi}^2 \right) = \text{const}$$

Thus choosing

$$C_{j, heta} = rac{V_{j,\phi}}{v_j}, \quad C_{j,\phi} = rac{V_{j, heta}}{\pi v_j},$$

allows us to diagonalize our Hamiltonian, where in the new Hamiltonian merely the dispersion relation of the impurity is shifted.

The transformation also has to be applied to our previous operators. While the Luttinger fields stay unaffected, the impurity operator is translated by an operator of the form  $e^{iS}$ ,  $S = \int dx C_x d^{\dagger} d(x)$ 

$$[iS, d_x] = iC_x d_x$$

and thus the expansion of  $U^{\dagger}dU$  does not terminate, but rather becomes

$$U^{\dagger}d(x)U = d(x)\left(\sum_{n=0}^{\infty} \frac{(-C_x)^n}{n!}\right) = d\mathrm{e}^{C_x}.$$

In our problem

$$d^{\dagger}(x) \rightarrow d^{\dagger}(x) \mathrm{e}^{i \sum_{j=a,A} \left( C_{j,\theta} \, \theta_j + C_{j,\phi} \, \phi_j \right)(x)}$$

We can gain an intuition for this. The creation or destruction of an impurity creates locally an excitation in the Luttinger liquid, expressed by the exponential cloud  $e^{i\sum_{j=a,A} (C_{j,\theta} \theta_j + C_{j,\phi} \phi_j)(x)}$ . Now the dynamical structure factors can be considerably simplified, as within the correlation factors the impurities can be separated out. At the same time we can rewrite everything in terms of the polaronic fields  $\phi_{a,A}$ ,  $\theta_{a,A}$ . One is left with

$$\begin{split} S_{b}(q,\omega) &= \\ \int dx \int dt \mathrm{e}^{i\omega t} \left( \left\langle \mathrm{e}^{i\left(2p\delta_{1}-C_{A,\theta}\right)\theta_{A}(x,t)} \mathrm{e}^{i\left(\varepsilon_{1}-C_{A,\theta}\right)\phi_{A}(x,t)} \mathrm{e}^{-i\left(2p\delta_{1}-C_{A,\theta}\right)\theta_{A}(0,0)} \mathrm{e}^{i\left(\varepsilon_{1}-C_{A,\Phi}\right)\phi_{A}(0,0)} \right\rangle \times \\ &\times \left\langle d^{\dagger}(x)d(0) \right\rangle \langle \ldots \rangle_{A \to a} \right), \end{split}$$

where the term  $\langle \dots \rangle_{A \to a}$  is similar to the first one, except that it contains the field  $\phi_a$ ,  $\theta_a$  and the corresponding prefactors. Here it did not matter, which of the two components of (4.9) were used, as they both contribute in the same way. The average  $\langle d^{\dagger}(x) d(0) \rangle = e^{-i\omega_q t} \delta(x - v_d t)$ . The remaining integral can be performed using standard methods [113] where the exponents created by the fields add up. At the edge of the spectra the dynamical structure factors show the characteristic behavior

$$S_{b,f}(\omega,q) \sim |\omega-\omega_q|^{2Z_{b,f}-1}$$

where  $\omega_d$  is the energy of the impurity and

$$Z_{b}(p) = \frac{1}{2} \left[ \left( 2p\delta_{1} - C_{A,\theta} \right)^{2} + \left( 2p\delta_{2} - C_{a,\theta} \right)^{2} + \left( \varepsilon_{1} - C_{A,\phi} \right)^{2} + \left( \varepsilon_{2} - C_{a,\phi} \right)^{2} \right],$$

$$Z_{f}(p) = \frac{1}{2} \left[ \left( 2p\beta_{1} + \beta_{1} - C_{A,\theta} \right)^{2} + \left( 2p\beta_{2} + \beta_{2} - C_{a,\theta} \right)^{2} + \left( \gamma_{1} - C_{A,\phi} \right)^{2} + \left( \gamma_{2} - C_{a,\phi} \right)^{2} \right],$$
(4.10)

and where the  $\alpha, \beta, \gamma, \delta$  come from the diagonalization of the Luttinger modes (5.2)(5.4). One can check that for non-interacting mixtures and non interacting impurities ( $C_{\theta,\phi} \rightarrow 0, v_A \rightarrow v_b$  and  $v_a \rightarrow v_f$ ) the free cases are recovered

$$Z_b = \frac{1}{2} \frac{1}{K_b}, \quad Z_f = \frac{1}{2} \left[ K_f + \frac{1}{K_f} \right].$$

We have to keep in mind, that these are the p = 0 cases. Because for weakly repulsive bosons  $K_b \gg 1$  the exponent in the structure factor can be negative. We have to keep in mind, that the p = 0 value in the bosonic case correspond to pure phase fluctuations, which do not exist for the fermions, as the Fermi momenta always

play a role there. One the other hand density fluctuations in the bosonic case lead for p = 1 to

$$Z_b = \frac{1}{2} \left[ 4K_b + \frac{1}{K_b} \right] \gg 1$$

which means that here the structure factor is strongly suppressed at the edges.

The *p* in the formulae 4.10 should be chosen to minimize the  $K_{b,f}$ , as that is the mode that has the longest range and thus dominates the small energy behaviour. Usually that is the p = 0 mode, but that is not necessarily a given if the other factors balance it. Remembering that  $C_{A/a,\theta} = \frac{\delta m}{m} \frac{v_d}{v}$  could take a wide range of values. In general such effects can happen when  $\left|\frac{\partial \varepsilon_d(k)}{\partial k}\right| < v_{f/b}$ . A similar observation has been made in [125].

If we neglect the interactions between the impurity and the liquids, i.e.  $C_{a/A} \equiv 0$ , and assume weak interliquid interactions such that  $v_A \approx v_b$  and  $v_a \approx v_f$ , the new exponents become

$$Z_b^{p=0} = \frac{1}{2} \left[ \frac{1}{K_b} \cos^2 \psi + \frac{1}{K_f} \sin^2 \psi \right]$$
$$Z_b^{p=1} = \frac{1}{2} \left[ \left( 4K_b + \frac{1}{K_b} \right) \cos^2 \psi + \left( 4K_f + \frac{1}{K_f} \right) \sin^2 \psi \right]$$
$$Z_f^{p=0} = \frac{1}{2} \left[ \left( K_f + \frac{1}{K_f} \right) \cos^2 \psi + \left( K_b + \frac{1}{K_b} \right) \sin^2 \psi \right].$$

First of all it is interesting to see, that both p = 0 cases generally lead to an increased suppression, because most commonly  $K_b \gg K_f$ . Especially for  $K_f$  the change can be very significant, as here the leading correction is  $K_b \sin^2 \psi$ , which even for small  $\psi$  can be significant enough to suppress the divergence completely.

How can one interpret these results? It is quite valuable to refer back to the earliest formulation of the problem, namely the X-ray Fermi edge singularity [119]. An electron from a low-lying valence band is excited into the conduction band of a metal. Mahan was the first to point out that the resulting deep hole and the fermions close to the Fermi edge can interact leading to logarithmic corrections to the polarisation bubble and power-law singularities at the absorption edges. It was however also seen, that by far not all metals did exhibit such divergencies. A second effect called the orthogonality catastrophe can lead to logarithmic corrections but with the opposite sign that can not only suppress the powerlaw divergence, but even the edge itself [126, 127]. The orthogonality catastrophe appears in many-particle systems, when suddenly the potential the particles experience changes. Though the overlap between single particle states is still close to unity, in many-particle

states the effect exponentiates and generally leads to a suppression of the singularity at the edge, unless the Mahan contribution is stronger. It seems that a similar mechanism happens also in one dimension. The terms containing the  $C_{A,a}$  are the Mahan terms, the rest can be described in terms of an orthogonality catastrophy, which for bosons can be seen in the exact solutions [20]. One can argue that the bosonic soliton impurities are a bigger distortion of the many-body wavefunction, leading to a stronger suppression when density fluctuations are involved. This view is supported by direct calculations [128].

#### 4.2.4 Summary of Results for 1D mixtures

We established that the edge-state singularity behaviour may persist in bosonic and fermionic mixtures, yet generally is suppressed compared to the non-interacting case. We calculated the depleton-impurity parameters when two interacting superfluids are present, see (4.6) and (4.7). These results depend on the insight that the two superfluid phase jumps must be coupled in equilibrium situations. These results are useful, as they are directly related to the coupling constants in between the fluids and the impurity (4.8). Further we calculated the dynamical structure factor for such a mixture. We included higher order terms in the Haldane representation which can become relevant when the impurity velocity becomes larger than the speed of sound of the Luttinger liquids. Such Cherenkov like effects were considered before in [121]. The coupling between the impurity and the polaronic cloud that is created locally around it creates a phase-shift in the operators, which in theory can at some points be cancelled by the higher order phase-shifts within the Haldane representation. This however would require considerable amounts of fine-tuning. In general the coupling to the additional Luttinger channel suppresses the divergence of the dynamical structure factor, unless cancelled by the before mentioned impurityliquid interactions. Adding even more weakly interacting components to the liquid would further increase the tendency of suppression. This effect would be most noticeably in the fermionic structure factor, where already small density-density interactions with the bosons can lead to a suppression due to the largeness of  $K_b$ . These findings should be experimentally accessible when multicomponent one-dimensional systems with tunable interactions are considered.

## **Chapter 5**

# Appendix

## 5.1 Bosonic Gaussian Integrals

We want to explain how bosonic gaussian integrals can be calculated. Given a matrix  $M_{ij}$  ( $N \times N$ ) whose N eigenvalues  $d_i$  have non-negative real parts, i.e.  $Red_i > 0$ , one can calculate general integrals of the form

$$Z[\eta,\eta^*] = \left(\frac{1}{\pi}\right)^N \int \prod_{k=1}^N d\left(\operatorname{Re} a_k\right) d\left(\operatorname{Im} a_k\right) \mathrm{e}^{-\sum_{ij}^N a_i^* M_{ij} a_j + \sum_j^N \left[a_j^* \eta_j + \eta_j^* a_j\right]}$$

To solve it, one assumes for the time being that M is Hermitian, which means its eigenvalues are real and the matrix can be written as  $M = U^{\dagger}DU$ , where U is a unitary transformation and D a diagonal matrix with real eigenvalues  $d_i$ . One can equivalently let the unitary transformation act on the  $\eta$  to obtain a new set of complex variables  $c_i = \sum_j U_{ij}a_j$ , which, however, are integrated over a purely real diagonal matrix

$$Z[\eta,\eta^*] = \left(\frac{1}{\pi}\right)^N \prod_{k=1}^N \int d(\operatorname{Re} c_k) d(\operatorname{Im} c_k) e^{-d_k |c_k|^2 + c_k^* J_k + J_k^* c_k} = \prod_{k=1}^N \frac{e^{J_k^* d_k^{-1} J_k}}{d_k},$$

where  $J_k = \sum_i U_{ij} \eta_j$ . The last step can be done by completing the square in the exponent, shifting the integration variables and integrating over the real and imaginary part respectively. Here it was also used that  $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$ .

#### CHAPTER 5. APPENDIX

Lastly we find

$$\prod_{k=1}^{N} \frac{e^{J_{k}^{*} d_{k}^{-1} J_{k}}}{d_{k}} = \frac{e^{\sum_{k} J_{k}^{*} d_{k}^{-1} J_{k}}}{\prod_{k} d_{k}} = \frac{e^{\vec{\eta}^{T} U^{\dagger} D^{-1} U \vec{\eta}}}{\det M} = \frac{e^{\vec{\eta}^{T} M^{-1} \vec{\eta}}}{\det M}.$$

Because the right hand side is analytic in M, we can analytically continue the result to matrices that are not Hermitean. We thus have that

$$Z[\eta,\eta^*] = \frac{\mathrm{e}^{\vec{\eta}M^{-1}\eta}}{\mathrm{det}M}.$$

The whole procedure is quite similar for real variable integration where

$$Z[\eta] = \int \prod_{k=1}^{N} \left(\frac{d c_k}{\sqrt{2\pi}}\right) \mathrm{e}^{-\frac{1}{2}\sum_{ij} c_i M_{ij} x_j + \sum_{j=1}^{N} c_j \eta_j} = \frac{\mathrm{e}^{\frac{1}{2}\sum_{ij}^{N} \eta_i \left(M^{-1}\right)_{ij} \eta_j}}{\sqrt{\mathrm{det}M}}.$$

Here M must be a complex symmetric function with non-negative real parts of its eigenvalue spectrum. In the proof, instead of an unitary transformation, an orthogonal transformation is used.

## 5.2 Summation over Matsubara frequencies

The following paragraphs are based on the exposition in the books of Mahan[119] and Bruus and Flensberg[30].

Sums of the form

$$S = \frac{1}{\beta} \sum_{i\omega_n} g(i\omega_n) e^{i\omega_n \tau}, \quad \omega_n = \frac{2n\pi}{\beta}$$

for  $\tau > 0$  are quite common and appear at several points in this thesis.

The trick is to rewrite the sum as a result of a complex integration, and each term in the sum as the result of a residue contribution. So we need a complex function that has poles at the values  $z = i\omega_n$  which happens to be

$$f_B(z) = \frac{1}{\mathrm{e}^{\beta z} - 1}.$$

This is the Bose function, which is responsible for the properties we are so interested in. The residual value of this function at its pole is

$$Res_{z=i\omega_n} \left[ f_b(z) \right] = \lim_{z \to i\omega_n} \frac{(z - i\omega_n)}{e^{\beta z} - 1} = \frac{1}{\beta}.$$


Figure 5.1: The contour stretches to infinity to enclose the whole complex plane, but without the poles on the imaginary axis the .

Keeping in mind that each residue is weighted with an additional  $2\pi i$  in the application of the residue theorem, it becomes clear the the sum *S* can be written as an integral of the form

$$S = \frac{1}{\beta} \sum_{i\omega_n} g(i\omega_n) e^{i\omega_n \tau} = \int_C \frac{dz}{2\pi i} f_B(z)g(z)e^{z\tau}.$$

The contour C itself only is located around the poles around  $i\omega_n$ , but not around other residues of g(z) itself.

How to continue further naturally depends on the specific form g(z) takes. Two cases are prevalent. In the first case, g(z) has a number of simple residues, i.e.

$$g(z) = \prod_k \frac{1}{z - z_k}.$$

Then we can choose a contour  $C_{tot}$  (see figure 5.1) that covers the entire complex plane. The important insight is that the outer contour (the radius) does not contribute to the integrale in the limit as  $f_B(z)e^{\tau z}$  goes to zero provided  $\tau > 0$  and  $z = Re^{i\phi}$  with  $R \to \infty$ . Then the countour integral can be decomposed into the part stemming from our original sum, i.e. the residues along the y-axis, and the remaining residues that are scattered along the complex plane and stem from the poles  $z_k$ . Thus



Figure 5.2: The contour now not only excludes the poles, but also the branch cut (dark bar) and could in principle be distorted to exclude the branch only.

$$\int_{C_t} \frac{dz}{2\pi i} f_B(z)g(z)e^{\tau z} = 0$$
  
=  $S + \sum_k Res_{z=z_k} [g(z)] f_B(z_k)e^{z_k\tau}.$ 

So

$$S = -\sum_{k} \operatorname{Res}_{z=z_{k}} \left[g(z)\right] f_{B}(z_{k}) \mathrm{e}^{z_{k}\tau}.$$

For completeness we should also look at the case where the function g(z), rather than having simple poles, has a branch cut say along the negative x - axis, x < -a (see figure 5.2).

As before, the complex plane can be enclosed by a contour that by itself carries no weight, but the terms arising from the residues of g(z) are replaced by contour integrals along the branch cut. We need to keep in mind that the mathematical direction of contour integration demands, that the lower branch is transversed in the negative direction. As the function is not well defined on the branch cut itself, one rather shifts the complex variable by a small imaginary amount along the upper branch  $z = Re(z) + i\eta$  and the lower branch by a small negative imaginary amount  $z = Re(z) - i\eta$ . Replacing the integration variable Re(z) by  $\varepsilon$ , we arrive at the

solution for the case when g(z) has a branch cut along the real axis

$$S = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon f_B(\varepsilon) \left[ g\left(\varepsilon + i\eta\right) - g\left(\varepsilon - i\eta\right) \right] \mathrm{e}^{\varepsilon \tau},$$

where necessarily the parts of the real axis without a branch cut does not contribute, as  $[g(\varepsilon + i\eta) - g(\varepsilon - i\eta)] \rightarrow 0$ . This sum can of course be extended for the case where additional single poles appear for g(z) on the complex plane.

At this point we should also mention the other important case, namely where the Matsubara sum stretches over the frequencies  $\omega_n = (2n+1)\pi/\beta$ . This case becomes necessary when studying fermions, the other great class of particles in nature. The same derivation still holds, only that the Bose function has to be replaced by a function which has poles at the new set of frequencies. This function is the Fermi function

$$f_F(z)=\frac{1}{\mathrm{e}^{\beta z}+1},$$

and has very different properties compared with the Bose function.

### 5.3 Estimation of relaxation times

From the generalized Gross-Pitaevskii equation (2.13) we can see, that the time evolution of the growth or decay of the order parameter  $\Phi$  is controlled by

$$\frac{1}{\tau_0} \approx \frac{g^2}{(2\pi)^2 \hbar} \int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 \delta\left(\mathbf{k}_1, \mathbf{k}_2 + \mathbf{k}_3\right)$$
$$\times \delta\left(\varepsilon_1 - \varepsilon_2 - \varepsilon_3\right) \left(1 + f_1^0\right) f_2^0 f_3^0.$$

which is proportional to the collision term that changes the number of particles in the condensate and the thermal cloud, while conserving the overall particle number. It was also assumed that  $\mathbf{v}_s = 0$ . If the distribution f is a bose distribution, then the collision term in between the thermal particles vanishes and these are in thermal equilibrium. Because we want to look at thermal fluctuations, this is a decent approximation. We are thus to

assume the equilibrium distribution

$$f(\varepsilon_i) = \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1},$$

where  $\mu$  is a small parameter. We define all (almost) constant factors from the Harttree-Fock potential into the chemical potential such that the energy functions becomes

$$\varepsilon_i = \frac{\hbar^2 \left| \mathbf{k}_i^2 \right|}{2m},$$

which is also valid, as we are at a high temperature (close to critical temperature in fact), where the Bogoliubov spectrum can be replaced by a free particle spectrum. The first integration leads to the replacement of  $\mathbf{k}_1 = \mathbf{k}_2 + \mathbf{k}_3$ .

The  $\varepsilon_1$  term becomes then

$$\varepsilon_1 = \frac{\hbar^2 |\mathbf{k}_1|^2}{2m} = \frac{\hbar^2}{2m} |\mathbf{k}_2 + \mathbf{k}_3|^2 = \frac{\hbar^2}{2m} \left(k_2^2 + k_3^2 + k_2 k_3 \cos \theta\right),$$

where  $\theta$  is the angle between the two vectors and the  $k_i$  the absolute values of the momenta. The  $\mathbf{k}_2$  integration is changed to

$$\int d^3\mathbf{k}_2 = 2\pi \int_0^\infty k_2^2 dk_2 \int_{-1}^1 d\left(\cos\theta\right).$$

Next, one integrates over  $\cos \theta$  while keeping in mind that

$$\delta(\varepsilon_1 - \varepsilon_2 - \varepsilon_3) = \delta\left(\frac{\hbar^2}{2m}k_2k_3\cos\theta\right)$$
$$= \frac{2m}{\hbar^2k_2k_3}\delta(\cos\theta).$$

The result is

$$\frac{1}{\tau_0} = \frac{4g^2m}{\hbar^4} \int_0^\infty \int_0^\infty k_2 k_3 \left(1 + f_1\right) f_2 f_3 \, dk_2 dk_3.$$

We want to approximate the last integral to see that  $\tau_0 \not\rightarrow \infty$ , as this would mean that the dynamics freeze out.

Substituting  $x = \beta \hbar^2 k_2^2 / 2m$  and  $y = \beta \hbar^2 k_3^2 / 2m$  leads to

$$\frac{1}{\tau_0} = \frac{4g^2m^3}{\beta^2\hbar^7} \int_0^\infty \int_0^\infty \frac{dxdy}{\left(e^{x-\beta\mu} - 1\right)\left(e^{y-\beta\mu} - 1\right)} \left(1 + \frac{1}{e^{x+y-\beta\mu} - 1}\right).$$

Lastly we approximate

$$\begin{split} \int_0^\infty & \int_0^\infty \frac{dx \, dy}{\left(\mathrm{e}^{x-\beta\mu}-1\right) \left(\mathrm{e}^{y-\beta\mu}-1\right)} \left(1+\frac{1}{\mathrm{e}^{x+y-\beta\mu}-1}\right) > \int_0^\infty \int_0^\infty \frac{dx \, dy}{\left(\mathrm{e}^{x-\beta\mu}-1\right) \left(\mathrm{e}^{y-\beta\mu}-1\right)} \\ &= \left(\int_0^\infty \frac{dx}{\left(\mathrm{e}^{x-\beta\mu}-1\right)}\right)^2. \end{split}$$

Let us approximate the asymptotic behaviour of the integrals by rewriting

$$I \equiv \int_0^\infty \frac{dx}{\left(\mathrm{e}^{x-\beta\mu}-1\right)} = \int_0^\infty \mathrm{e}^{-h(x,t)} dx,$$

where  $t = -1/\beta\mu$  is a large parameter and

$$h(x) = \log\left(\mathrm{e}^{x}\mathrm{e}^{1/t} - 1\right).$$

Let us expand the function h(x,t) around small x, as this is indeed the part of the integral with the strongest contribution. Then

$$\begin{split} h(x,t) &= \log\left(e^{x}e^{1/t} - 1\right) \\ &= -t + \log\left(e^{x} - e^{-1/t}\right) \\ &= -t + \log\left(\left(1 - e^{-1/t}\right) + x + \frac{x^{2}}{2} + O(x^{3})\right). \\ &= -t + \log\left(1 - e^{-1/t}\right) + \log\left(1 + \left(1 - e^{-1/t}\right)^{-1}x + \left(1 - e^{-1/t}\right)^{-1}\frac{x^{2}}{2} + O(x^{3})\right) \end{split}$$

Next we rescale  $x \to y = (1 - e^{-1/t})x$ , a transformation which in the higher limits for  $t \to \infty$  gets rid of all terms of higher order than *x*. Whereas the prefactor gets rid of the first log lerm

$$I = \int_0^\infty e^t e^{-1 - (1 - e^{-1/t})^{-1} x - (1 - e^{-1/t})^{-1} x^2/2 + \dots} \frac{dx}{(1 - e^{-1/t})}$$
$$= e^{-1 + t} \int_0^\infty dy e^{-y - (1 - e^{-1/t})y^2/2 - \dots}$$
$$\lim_{t \to \infty} e^{t - 1} \int_0^\infty dy e^{-y} = e^{t - 1}$$

This means we can approximate

$$\frac{1}{\tau_0} > \frac{4g^2m^3}{\beta^2\hbar^7} \mathrm{e}^{t-1},$$

which proves that the dynamics do not freeze out and equilibrium fluctuational effects can be observed for experimental times  $t > \tau_0 \rightarrow 0$ .

## **5.4** Discussion of the Polylogarithm at $\alpha = 2$

For the interesting case  $\alpha = 2$  one can rather straightforwardly perform the calculation directly

$$\operatorname{Li}_{2}\left(\mathrm{e}^{-z}\right) = \sum_{n=1}^{\infty} \frac{\mathrm{e}^{-zn}}{n^{2}} = \frac{\pi^{2}}{6} - \sum_{n=1}^{\infty} \frac{1 - \mathrm{e}^{-zn}}{n^{2}}$$
$$= \frac{\pi^{2}}{6} - \sum_{n=1}^{\infty} \int_{0}^{z} \frac{\mathrm{e}^{-xn}}{n} dx = \frac{\pi^{2}}{6} - \int_{0}^{z} dx \sum_{n} \frac{\mathrm{e}^{-xn}}{n}$$
$$= \frac{\pi^{2}}{6} + \int_{0}^{z} dx \log\left(1 - \mathrm{e}^{-x}\right).$$

Since  $x \le z \ll 1$  one can expand

$$\log \left[1 - e^{-x}\right] = \log \sum_{n=1}^{\infty} (-1)^{n+1} = \log x \sum_{n=0}^{\infty} \frac{x^n}{(n+1)!} (-1)^n$$
$$= \log x + \log \sum_{n=0}^{\infty} \frac{x^n}{(n+1)!} (-1)^n.$$

Integrating over *x* 

$$\int_0^z dx \left[ \log x + \log \sum_{n=0}^\infty \frac{x^n}{(n+1)!} \left( -1 \right)^n \right] \approx \int_0^\infty dx \log x + \sum_{n=1}^\infty \int_0^z dx \frac{x^n}{(n+1)!} \left( -1 \right)^n$$
$$= z (\log z - 1) + \sum_{n=1}^\infty \frac{z^{n+1}}{n(n+1)} \left( -1 \right)^n.$$

Thus

$$\operatorname{Li}_{2}\left(e^{-z}\right) = \frac{\pi^{2}}{6} + z\log z - z + \sum_{n=1}^{\infty} \frac{z^{n+1}}{n(n+1)!} (-1)^{n}$$

and already the leading order correction contains the logarithm.

## 5.5 Short introduction to Grassmann fields

Grassmann fields are in a sense the extension of the coherent state formalism to anticommuting (fermionic) creation/annihiliation operators. Because the operators anticommute, we have that  $\hat{c}_i \hat{c}_j = -\hat{c}_j \hat{c}_i$ , especially  $\hat{c}_i^2 = 0$ .

A coherent state  $|\eta\rangle$  is then defined similarly

$$\hat{c}_i |\eta\rangle = \eta |\eta\rangle$$
.

Naturally these  $\eta$  cannot be complex numbers as in the bosonic case, since

$$\hat{c}_{i}\hat{c}_{j}\left|\eta_{i}
ight
angle\left|\eta_{j}
ight
angle=\eta_{i}\eta_{j}\left|\eta_{i}
ight
angle\left|\eta_{j}
ight
angle$$

$$=-\hat{c}_{j}\hat{c}_{i}\left|\eta_{i}
ight
angle\left|\eta_{j}
ight
angle=-\eta_{j}\eta_{i}\left|\eta_{i}
ight
angle\left|\eta_{j}
ight
angle$$

and especially  $\eta_i^2 = 0$ .

An algebra can be defined in which allows for addition and multiplication. Given a set of fermionic states  $|1\rangle |2\rangle \dots |N\rangle$ , which by virtue of the fact that  $(\hat{c}_i^{\dagger})^2 = 0$  can only be occupied by a single particle or not at all,

a general vector in that space can be written as

$$c_0+\sum_{i=0}^N c_{i_1,\ldots,i_n}\eta_{i_1}\eta_{i_2}\ldots\eta_{i_n},$$

where all the *c*s are complex numbers and in every product of  $\eta$ s, each  $\eta_i$  can appear at most once. One can define differentiation and integration with respect to the  $\eta_i$ 

$$\partial_{\eta_i}\eta_j = \delta_{ij},$$
  
 $\int d\eta_i = 0,$   
 $\int d\eta_i \eta_i = 1.$ 

There is no need to consider integration boundaries and integrals of functions become particularily simple, as these functions are defined by their Taylor expansion to first order for which the above defined rules apply.

The coherent state can then be written as

$$|\eta\rangle = \mathrm{e}^{-\sum_i c_i \eta_i \hat{c}_i^{\dagger}} |0\rangle,$$

where  $|0\rangle$  is the vacuum state and the  $c_i$  are either 0 or 1, depending of whether the state is occupied or not. As for the bosonic case, one may introduce conjugate fields  $\eta^*$ , but these are simply new Grassmann fields without relation to the original field  $\eta$ . For our case important, the Gaussian integration

$$\int d\eta^* d\eta \mathrm{e}^{-\eta^*\lambda\eta} = \lambda,$$

where  $\lambda$  is a complex number. For a matrix **A** we have the generalized Gaussian integration

$$\int \left(\prod_{i} d\eta_{i}^{*} d\eta_{i}\right) e^{-\eta^{*} \mathbf{A} \eta} = \det \mathbf{A}$$
(5.1)

which differs from the important bosonic case where the Gaussian integral would give det  $A^{-1}$ . Along with the

completeness relation

$$\int d(\eta^*,\eta) e^{-\sum_i \eta_i^* \eta} |\eta\rangle \langle \eta| = I,$$

it becomes clear that a coherent state picture with imaginary time integration, as in the bosonic case, can be straightforwardly extended, with the difference that the fields themselves are Grassmannian fields  $\psi$  and that the trace operation in the definition leads to the boundary condition  $\psi(0) = -\psi(\beta)$ , which translates into Matsubara frequencies

$$\omega_n = (2n+1)\beta^{-1}, \quad n \in \mathbb{N}.$$

## 5.6 Diagonalization of two interacting Luttinger liquids

The goal is to diagonalize the Hamiltonian

$$H_{\text{tot}} = \frac{v_b}{2} \int dx \left[ \frac{K_b}{2} \left( \partial_x \phi_b \right)^2 + \frac{\pi}{K_b} \Pi_b^2 \right] + \frac{v_f}{2} \int dx \left[ \frac{K_f}{2} \left( \partial_x \phi_f \right)^2 + \frac{\pi}{K_f} \Pi_f^2 \right] + \frac{g\pi}{2\sqrt{K_b K_f}} \int dx \Pi_b \Pi_f.$$

We will substitute the bosonic and fermionic fields with the new fields  $\phi_{a/A}, \Pi_{a/A}$ 

$$\phi_b = \delta_1 \Pi_A + \delta_2 \Pi_a, \phi_b = \varepsilon_1 \phi_A + \varepsilon_2 \phi_a,$$
  
$$\phi_f = \beta_1 \Pi_A + \beta_2 \Pi_a, \phi_f = \gamma_1 \phi_A + \gamma_2 \phi_a.$$

Substituting the modes A and a we have

$$\begin{split} H_{\text{tot}} &= \int dx \left[ \frac{v_b K_b}{2\pi} \varepsilon_1^2 \left( \partial_x \phi_A \right)^2 + \frac{v_b K_b}{2\pi} \varepsilon_2^2 \left( \partial_x \phi_a \right)^2 + \frac{v_b K_b}{\pi} \varepsilon_1 \varepsilon_2 \partial_x \phi_A \partial_x \phi_a + \frac{v_b \pi}{2K_b} \delta_1^2 \Pi_A^2 + \frac{v_b \pi}{2K_b} \delta_2^2 \Pi_a^2 + \frac{v_b \pi}{K_b} \delta_1 \delta_2 \Pi_A \Pi_a \right] \\ &+ \int dx \left[ \frac{v_f K_f}{2\pi} \gamma_1^2 \left( \partial_x \phi_A \right)^2 + \frac{v_f K_f}{2\pi} \gamma_2^2 \left( \partial_x \phi_a \right)^2 + \frac{v_f K_f}{\pi} \gamma_1 \gamma_2 \partial_x \phi_A \partial_x \phi_a + \frac{v_f \pi}{2K_f} \beta_1^2 \Pi_A^2 + \frac{v_f \pi}{2K_f} \beta_2^2 \Pi_a^2 + \frac{v_f \pi}{K_f} \beta_1 \beta_2 \Pi_A \Pi_a \right] \\ &+ \int dx \frac{g\pi}{2\sqrt{K_b K_f}} \left( \beta_1 \delta_1 \Pi_A^2 + \beta_2 \delta_2 \Pi_a^2 + \left( \beta_1 \delta_2 + \beta_2 \delta_1 \right) \Pi_A \Pi_a \right) \\ &= \int dx \left[ \frac{v_b K_b}{2\pi} \varepsilon_1^2 + \frac{v_f K_f}{2\pi} \gamma_1^2 \right] \left( \partial_x \phi_A \right)^2 + \left[ \frac{v_b \pi}{2K_b} \delta_1^2 + \frac{v_f \pi}{2K_f} \beta_1^2 + \frac{g\pi}{2\sqrt{K_b K_f}} \beta_1 \delta_1 \right] \Pi_A^2 \\ &+ \int dx \left[ \frac{v_b K_b}{2\pi} \varepsilon_2^2 + \frac{v_f K_f}{2\pi} \gamma_1^2 \right] \left( \partial_x \phi_a \right)^2 + \left[ \frac{v_b \pi}{2K_b} \delta_2^2 + \frac{v_f \pi}{2K_f} \beta_2^2 + \frac{g\pi}{2\sqrt{K_b K_f}} \beta_2 \delta_2 \right] \Pi_a^2 \\ &+ \int dx \left[ \frac{v_b K_b}{\pi} \varepsilon_1 \varepsilon_2 + \frac{v_f K_f}{2\pi} \gamma_1 \gamma_2 \right] \partial_x \phi_A \partial_x \phi_a + \left[ \frac{v_b \pi}{K_b} \delta_1 \delta_2 + \frac{v_f \pi}{K_f} \beta_1 \beta_2 + \frac{g\pi}{2\sqrt{K_b K_f}} \left( \beta_1 \delta_2 + \beta_2 \delta_1 \right) \right] \Pi_A \Pi_a. \end{split}$$

Eliminating the mixed terms gives the constraints

$$\left[\frac{v_b K_b}{\pi}\varepsilon_1\varepsilon_2 + \frac{v_f K_f}{\pi}\gamma_1\gamma_2\right] = 0, \left[\frac{v_b \pi}{K_b}\delta_1\delta_2 + \frac{v_f \pi}{K_f}\beta_1\beta_2 + \frac{g\pi}{2\sqrt{K_b K_f}}\left(\beta_1\delta_2 + \beta_2\delta_1\right)\right] = 0$$

Additionally we want the fields to behave like appropriate Luttinger liquids, i.e.  $\left[\Pi_{a/A}(x), \Phi_{a/A}(x')\right] = i\delta(x - x')$ and  $\left[\Pi_a, \Pi_A\right] = [\phi_a, \phi_A] = [\Pi_A, \phi_a] = [\Pi_a, \phi_A] = 0$ . This gives

$$(\delta_1 \varepsilon_1 + \delta_2 \varepsilon_2) = 1$$
  
 $(\beta_1 \gamma_1 + \beta_2 \gamma_2) = 1$ 

In addition we still need to enforce that  $[\Pi_b, \phi_f] = [\Pi_f, \phi_b] = 0$ . This leads to

$$eta_1 eta_1 + eta_2 eta_2 = 0$$
  
 $\delta_1 \gamma_1 + \delta_2 \gamma_2 = 0.$ 

This suggests that the amplitudes of  $(\delta, \varepsilon)$  and  $(\beta, \gamma)$  cancel out and that together with the first condition the system can be described by a single mixing angle  $\psi$ . Additionally the parity of  $\varepsilon_1 \varepsilon_2$  should be the opposite of  $\gamma_1 \gamma_2$ . The ansatz to make would be

$$\varepsilon_{1} = -C_{1} \frac{1}{\sqrt{v_{b}K_{b}}} \cos \psi \qquad \varepsilon_{2} = C_{2} \frac{1}{\sqrt{v_{b}K_{b}}} \sin \psi$$

$$\gamma_{1} = C_{1} \frac{1}{\sqrt{v_{f}K_{f}}} \sin \psi \qquad \gamma_{2} = C_{2} \frac{1}{\sqrt{v_{f}K_{f}}} \cos \psi$$

$$\delta_{1} = -\frac{1}{C_{1}} \sqrt{v_{b}K_{b}} \cos \psi \qquad \delta_{2} = \frac{1}{C_{2}} \sqrt{v_{b}K_{b}} \sin \psi$$

$$\beta_{1} = \frac{1}{C_{1}} \sqrt{v_{f}K_{f}} \sin \psi \qquad \beta_{2} = \frac{1}{C_{2}} \sqrt{v_{f}K_{f}} \cos \psi$$
(5.2)

Using that  $\cos\psi\sin\psi = \frac{\sin 2\psi}{2}$  and  $\cos^2\psi - \sin^2\psi = \cos 2\psi$  one is lead by using the second constraint that

$$\tan 2\psi = g \frac{\sqrt{v_f v_b}}{\left(v_f^2 - v_b^2\right)}.$$
(5.3)

In addition we can subsitute those values into the non-vanishing prefactors

$$\begin{bmatrix} \frac{v_b K_b}{2\pi} \varepsilon_1^2 + \frac{v_f K_f}{2\pi} \gamma_1^2 \end{bmatrix} = \frac{1}{2\pi} \left[ C_1^2 \cos^2 \psi + C_2^2 \sin^2 \psi \right] = \frac{C_1^2}{2\pi} \\ \begin{bmatrix} \frac{v_b \pi}{2K_b} \delta_1^2 + \frac{v_f \pi}{2K_f} \beta_1^2 + \frac{g\pi}{2\sqrt{K_b K_f}} \beta_1 \delta_1 \end{bmatrix} = \frac{\pi}{2C_1^2} \left[ v_b^2 \cos^2 \psi + v_f^2 \sin^2 \psi + g\sqrt{v_b v_f} \sin \psi \cos \psi \right] \\ \begin{bmatrix} \frac{v_b K_b}{2\pi} \varepsilon_2^2 + \frac{v_f K_f}{2\pi} \gamma_2^2 \end{bmatrix} = \frac{C_2^2}{2\pi} \\ \begin{bmatrix} \frac{v_b \pi}{2K_b} \delta_2^2 + \frac{v_f \pi}{2K_f} \beta_2^2 + \frac{g\pi}{2\sqrt{K_b K_f}} \beta_2 \delta_2 \end{bmatrix} = \frac{\pi}{2C_2^2} \left[ v_b^2 \sin^2 \psi + v_f^2 \cos^2 \psi + g\sqrt{v_b v_f} \sin \psi \cos \psi \right].$$

From this it follows that

$$v_A^2 = \left[ v_b^2 \cos^2 \psi + v_f^2 \sin^2 \psi + g \sqrt{v_b v_f} \sin \psi \cos \psi \right]$$
$$v_a^2 = \left[ v_b^2 \sin^2 \psi + v_f^2 \cos^2 \psi + g \sqrt{v_b v_f} \sin \psi \cos \psi \right].$$

We can use that  $\cos^2(\arctan(x)/2) = \frac{\sqrt{1+x^2+1}}{2\sqrt{1+x^2}} = \frac{1}{2} + \frac{1}{2}\frac{1}{\sqrt{1+x^2}}$  and  $\sin^2(\arctan(x)/2) = \frac{\sqrt{1+x^2}-1}{2\sqrt{1+x^2}} = \frac{1}{2} - \frac{1}{2}\frac{1}{\sqrt{1+x^2}}$  and  $\cos(\arctan(x)/2)\sin(\arctan(x)/2) = \frac{x}{2\sqrt{1+x^2}}$ 

$$v_{a/A}^2 = \frac{1}{2} \left( v_b^2 + v_f^2 \right) + \frac{1}{2} \frac{v_b^2 - v_f^2 + g \sqrt{v_b v_f x}}{\sqrt{1 + x^2}},$$

where  $x = g \frac{\sqrt{v_f v_b}}{\left(v_f^2 - v_b^2\right)}$ . Then

$$v_{a/A}^2 = \frac{1}{2} \left( v_b^2 + v_f^2 \right) \pm \frac{1}{2} \sqrt{\left( v_f^2 - v_b^2 \right)^2 + g^2 v_f v_b}.$$

Additionally one has the factors  $C_{1/2}$ . A particularily useful choice is such that  $K_{a,A} = 1$ . We have that

$$K_A = \pi \sqrt{\frac{\left[\frac{v_b K_b}{2\pi} \varepsilon_1^2 + \frac{v_f K_f}{2\pi} \gamma_1^2\right]}{\left[\frac{v_b \pi}{2K_b} \delta_1^2 + \frac{v_f \pi}{2K_f} \beta_1^2\right]}} = \frac{C_1^2}{v_A}$$
$$K_a = \frac{C_2^2}{v_a}.$$

From this it follows that  $C_1 = \sqrt{v_A}$  and  $C_2 = \sqrt{v_a}$  is a convenient choice. So one finally obtains

$$\begin{aligned} \varepsilon_{1} &= -\sqrt{\frac{v_{A}}{v_{b}K_{b}}}\cos\psi \quad \varepsilon_{2} = \sqrt{\frac{v_{a}}{v_{b}K_{b}}}\sin\psi \\ \gamma_{1} &= \sqrt{\frac{v_{A}}{v_{f}K_{f}}}\sin\psi \quad \gamma_{2} = \sqrt{\frac{v_{a}}{v_{f}K_{f}}}\cos\psi \\ \delta_{1} &= -\sqrt{\frac{v_{b}K_{b}}{v_{A}}}\cos\psi \quad \delta_{2} = \sqrt{\frac{v_{b}K_{b}}{v_{a}}}\sin\psi \\ \beta_{1} &= \sqrt{\frac{v_{f}K_{f}}{v_{A}}}\sin\psi \quad \beta_{2} = \sqrt{\frac{v_{f}K_{f}}{v_{a}}}\cos\psi. \end{aligned}$$
(5.4)

## 5.7 Solitonic dispersion relation

The Gross-Pitaevskii equation allows for special solutions that are moving with constant speed in time. Such a solution is called soliton and is in the case of a gray solition represented by a dip in the particle density and a phase jump of the macroscopic wave-function across the dip [50]. It is therefore a good model for an impurity, as the fluid has to create a hole in which the impurity sits and generally a phase jump is expected across the impurity.

So we are looking for solutions of the time-dependent GP equation that move with velocity V, i.e.  $\Phi =$ 

 $\Phi(x - Vt)$ . One can rescale all lengths by the healing length  $\xi$  to have a dimensionless ansatz

$$\Phi = \sqrt{n}f(y)\mathrm{e}^{-i\mu t/\hbar},$$

where  $y = (x - Vt) / \xi$ .

This gives

$$\sqrt{2}i\frac{V}{c}\frac{df}{dy} = \frac{d^2f}{dy^2} + f\left(1 - |f|^2\right).$$

Further we demand that the impurity is localized, meaning that far away from the dip, the condensate is flat

$$|f| \to 1, \quad \frac{df}{dy} \to 0.$$

A solution that fulfills these conditions is [129]

$$\Phi(x-Vt) = \sqrt{n} \left( i \frac{V}{c} + \sqrt{1 - \frac{V^2}{c^2}} \tanh\left(\frac{x-Vt}{\sqrt{2}}\sqrt{1 - \frac{V^2}{c^2}}\right) \right),$$

which is the non-stationary generalization of the boxed-potential boundary solution.

The energy of such an isolated solution is finite and given by

$$E_d = \int_{-\infty}^{\infty} \left[ \frac{\hbar^2}{2m} \left| \frac{d\Phi}{dx} \right|^2 + \frac{g}{2} \left( |\Phi|^2 - n \right) \right],$$

which is the energy difference with respect to the ground state solution. The result is

$$E_d = \frac{4}{3}\hbar cn \left(1 - \frac{V^2}{c^2}\right)^{3/2}.$$

Because increasing the velocity reduces the energy, one can argue that the soliton has something like a negative mass, which is in accordance with the observation of the dip and the depletion of particles out of the condensate through the impurity.

The canonical momentum associated with the soliton can be found by using the relationship  $V = \partial E_d / \partial p_c$ to give

$$p_{c} = \int_{0}^{E_{d}} \frac{d(E)}{V} = \int_{0}^{E_{d}} \frac{\partial(E)}{\partial V} \frac{dV}{V} =$$
$$= -2\hbar n \left( \frac{V}{c} \sqrt{1 - \frac{V^{2}}{c^{2}}} + \arcsin\left(\frac{V}{c}\right) \right),$$

which is however not equivalent to the physical momentum.

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