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The Hallmarks of Superfluidity in Exotic Phases of Bose Gases Self-bound Droplets, Mixed Bubbles and Supersolids

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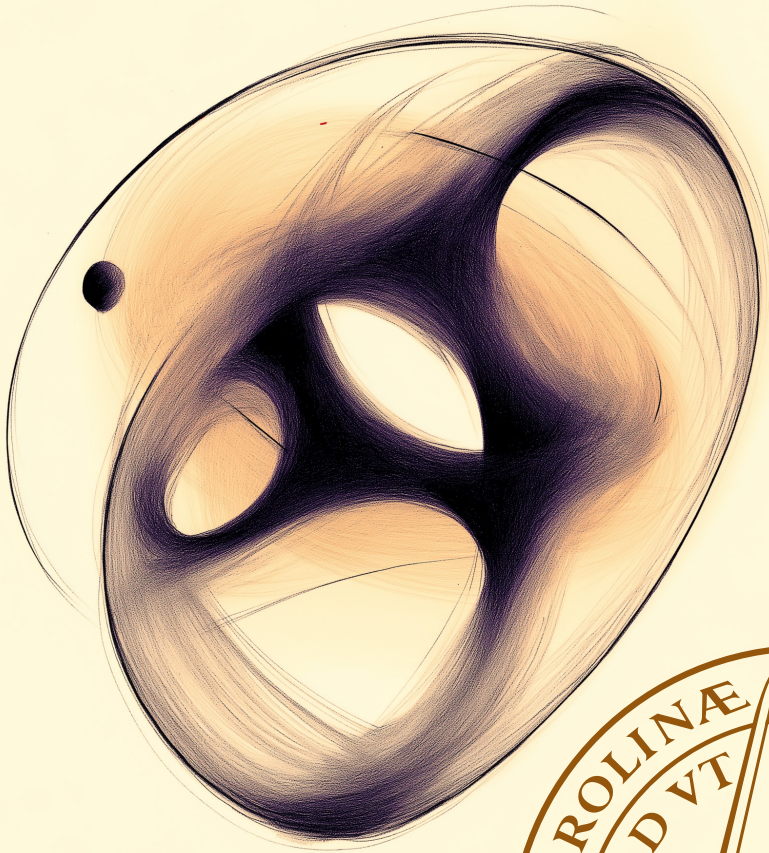
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The Hallmarks of Superfluidity in Exotic Phases of Bose Gases

Self-bound Droplets, Mixed Bubbles and Supersolids

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DEPARTMENT OF PHYSICS | FACULTY OF ENGINEERING | LUND UNIVERSITY



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Self-bound Droplets, Mixed Bubbles and Supersolids

by Philipp Stürmer



LUND
UNIVERSITY

Thesis for the degree of Doctor of Philosophy in Physics

Thesis advisors: Prof. Stephanie M. Reimann

Faculty opponent: Dr. Dmitry Petrov

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Title and subtitle The Hallmarks of Superfluidity in Exotic Phases of Bose Gases Self-bound Droplets, Mixed Bubbles and Supersolids			
Abstract <p>This thesis investigates superfluidity in exotic phases of ultracold bosonic gases, namely self-bound droplets, mixed bubbles, and dipolar supersolids. We investigated these systems analytically and numerically using an extended Gross-Pitaevskii and Bogoliubov-de Gennes formalism. The dissertation offers six chapters, providing the necessary derivations to build the required background and understanding for the six papers this thesis comprises of:</p> <p>In Paper I, we show that two-dimensional self-bound droplets in a bosonic mixture can support multiply singly-quantized vortices and give a protocol to create self-bound meta-stable persistent currents carrying vorticity.</p> <p>Paper II studies the ground state properties of two-dimensional droplets via a super-Gaussian variational ansatz, showing excellent agreement with numerical solutions. Furthermore, we study whether the breathing mode is a feasible excitation in these droplets with and without vorticity.</p> <p>In Paper III, we numerically demonstrate the existence of mixed bubbles near phase separation in a one-dimensional torus. These mixed bubbles coincide with a Higgs-Amplitude mode in the excitation spectrum. Additionally, we show that metastable persistent currents can occur, and the associated avoided level-crossing opens intriguing prospects for atomtronic concepts.</p> <p>Paper IV investigates a dynamic stirring process in a toroidal dipolar supersolid with a weak link. The weak link couples two angular modes, allowing phase slips to occur under rotation. These phase slips induce a dynamic self-organizational process of continuous melting and re-freezing of crystal sites in the supersolid.</p> <p>In Paper V, we demonstrate the existence of one-dimensional self-bound droplets in the few-body regime using exact diagonalization and compare these results to mean-field solutions. Across the transition from superfluid to self-bound droplet, we find the few-body precursor of a Higgs-Amplitude mode and observe a change in the rotational dispersion relation from negative curvature to parabolic.</p> <p>Lastly, Paper VI investigates the decoupling of first sound, second sound, and Higgs-Amplitude mode across the superfluid-supersolid transition in a toroidal dipolar supersolid. These modes emerge from their elementary excitations, and we propose experimental protocols to probe these sound and amplitude modes selectively.</p>			
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Supersolids

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A doctoral thesis at a university in Sweden takes either the form of a single, cohesive research study (monograph) or a summary of research papers (compilation thesis), which the licentiate student has written alone or together with one or several other author(s).

In the latter case the thesis consists of two parts. An introductory text puts the research work into context and summarizes the main points of the papers. Then, the research publications themselves are reproduced, together with a description of the individual contributions of the authors. The research papers may either have been already published or are manuscripts at various stages (in press, submitted, or in draft).

Cover illustration front: AI-generated ballpoint drawing of the three vortex state in Fig 4.2 using Midjourney.

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MADE IN SWEDEN 

*Above all, do not lose your desire to walk.
Everyday, I walk myself into a state of well-being and walk away from every illness.
I have walked myself into my best thoughts,
and I know of no thought so burdensome that one cannot walk away from it.
But by sitting still, and the more one sits still, the closer one comes to feeling ill.
Thus if one just keeps on walking, everything will be all right.
- Søren Kierkegaard*

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List of publications

This thesis is based on the following publications, referred to by their Roman numerals:

I Rotating Binary Bose-Einstein Condensates and Vortex Clusters in Quantum Droplets

M. Nilsson Tengstrand, **P. Stürmer**, E. Ö. Karabulut, and S. M. Reimann
Physical Review Letters, **123**, 160405 (2019)

Contributions: I contributed to the conceptualization of the project, did some of the simulations, and helped write the first draft.

II Breathing mode in two-dimensional binary self-bound Bose-gas droplets

P. Stürmer, M. Nilsson Tengstrand, R. Sachdeva, and S. M. Reimann
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Contributions: I contributed to the conceptualization of the project, did all the analytical calculations, wrote some of the code, did the simulations and wrote the first draft.

III Mixed bubbles in a one-dimensional Bose-Bose mixture

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Contributions: I contributed to the conceptualization of the project, wrote some of the Gross-Pitaevskii code, wrote the Bogoliubov de-Gennes code, did the simulations, did the analytical calculations, and wrote the first draft.

IV Toroidal dipolar supersolid with a rotating weak link

M. Nilsson Tengstrand, **P. Stürmer**, J. Ribbing, and S. M. Reimann
Phys. Rev. A, **107**, 063316, (2023)

Contributions: I contributed to the conceptualization of the project, wrote some of the code, did some of the simulations and wrote parts of the first draft.

V **Superfluid-droplet crossover in a binary boson mixture on a ring: Exact diagonalization solutions for few-particle systems in one dimension**

L. Chergui, J. Bengtsson, J. Bjerlin, P. Stürmer, G. M. Kavoulakis, and S. M. Reimann

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Contributions: I contributed to discussions of the project, wrote parts of the Gross-Pitaevskii code, did some of the simulations and wrote parts of the first draft.

VI **Decoupled sound and amplitude modes in trapped dipolar supersolids**

J. Hertkorn, P. Stürmer, K. Mukherjee, K. S. H. Ng, P. Uerlings, F. Hellstern, L. Lavoine, S. M. Reimann, T. Pfau, and R. Klemt

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Contributions: I contributed to the conceptualization of the project, wrote parts of the Gross-Pitaevskii code, did some of the simulations and wrote parts of the first draft.

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Popular Science Summary

A regular gas or liquid consists of atoms or molecules all moving in arbitrary directions. If we cool it down, the particles' movement slows down until it becomes tightly constrained and turns solid. In the quest to cool everything to absolute zero - the lowest possible temperature - during the early 20th century, we managed to cool and solidify almost any element but Helium. Somehow, Helium resisted the urge to solidify and just remained liquid. As the temperature decreased, it suddenly stopped boiling, remained utterly still, and started creeping out of its container. What was going on?

This strange behavior was due to the unique quantum properties of Helium. At extremely low temperatures, the Helium atoms entered a bizarre state of matter known today as a superfluid. The superfluid can flow without any viscosity (describing how much friction atoms within a fluid experience), allowing it to creep up the sides of its container. The lack of viscosity would mean that a superfluid would never stop moving once set to motion, like stirring a coffee that would never stop spinning. Not only this - the coffee would also move in odd ways if we stirred it faster. The vortex (swirl) in the center would not get bigger but split up in discrete intervals as we stir faster and form smaller vortices until tiny swirls cover the coffee's surface. These two phenomena, persistent flow and quantized vortices, are prominent hallmarks of superfluidity.

As time progressed, scientists found a connection between superfluidity and another state of matter, a so-called Bose-Einstein condensate. In such a condensate, the different coffee particles lose all sense of identity and behave as one big matter-wave. The smoking gun for the connection between superfluidity and Bose-Einstein condensation? The occurrence of superfluidity in Helium appeared at roughly the same temperature as was predicted for Bose-Einstein condensation.

While there is still ongoing research on the properties of superfluid Helium, another contender emerged where researchers use alkaline or even lanthanide atoms and cool them via lasers down to a billionth of a degree above absolute zero. Luckily, these atoms are also very agreeable, and we can convince them to interact less or more strongly, with some even acting as small magnets over a long distance instead of just colliding with each other.

This malleability leads to more and more exotic phases, with the most recent discovery supported by so-called quantum fluctuations. If the Bose-Einstein condensate is coffee in your cup with all the properties of a superfluid, quantum fluctuations would then be a proto-coffee (a coffee yet to be made with water and ground beans) around your cup. The collisions between particles in the (coffee) condensate can kick them out of the condensate and into the proto-coffee and vice-versa. Usually, this effect

is too small to influence the coffee, and we can ignore it. But if the interactions are tuned enough, the proto-coffee shows its effect and can lead to a self-bound Bose gas - a large droplet of coffee that doesn't need a cup. The question remains: how much of the superfluidity remains in this coffee droplet?

If the coffee, however, is magnetic, a so-called supersolid might occur. Here, the coffee is not only superfluid but also shows signs of being solid, with lumps of coffee crystallizing into a periodic and predictable pattern. But how could a solid behave like a superfluid, and how does one bring these concepts together?

This thesis and the papers therein add to the body of research attempting to answer these questions with a particular focus on the hallmarks of superfluidity via numerical studies in the mean-field regime.

Chapter I

Introduction

This thesis concerns frictionless flow - superfluidity - and how it manifests in exotic phases of weakly interacting Bose gases. When a bosonic gas or liquid's temperature decreases below some critical value, it can transition into a superfluid state. This phase transition connects deeply to the quantum particle statistics of the system and allows the superfluid to flow without dissipation. The connection between superfluidity and Bose statistics follows two separate roads in history¹, challenging many of the most famous physicists of the 20th century and heavily influencing the development and understanding of modern condensed matter physics along the way.

The first of these roads started 100 years ago when Satyendra Bose considered Planck's derivation of black-body radiation [5]. Planck's model introduced the quantization of energy [6], paving the way for modern quantum mechanics. In his work, Bose introduced indistinguishable particles and how to count their states. Applying these concepts to Planck's work, he managed to recover Planck's law, but crucially without making any of the classical assumptions [5]. However, Bose struggled with getting his work published and contacted Einstein, with whom he had prior correspondence, for help [1, 3]. The idea of indistinguishable particles heralded quantum statistics and the split of all particles into two fundamental classes - today known as Bosons and Fermions.

One week after Einstein received Bose's paper, he extended Bose's work from photons to a monoatomic ideal gas with conserved particle numbers [2]. Einstein found that by lowering the temperature, the states of the ideal gas would become saturated until a specific critical temperature, after which atoms would start accumulating in a single

¹For comprehensive historical reviews of superfluidity and Bose-Einstein condensation, see Refs. [1–4].

quantum state - they would condense [7–9]. This was the first paper that made use of de Broglie’s particle-wave duality [10], and Einstein argued that if particles are waves, they should follow the same (Bose) statistics as photons². After Einstein’s prediction, not much happened with his idea due to the criticism that such a phase transition could not occur in a finite system [3]. This changed when both historical roads met in 1938.

The second historical road concerns superfluid Helium. By the end of the 19th century, an increasing interest in low-temperature physics had led to the successful liquefaction of most major gases, except Helium [12]. This changed in 1908 when Kamerlingh Onnes succeeded in this endeavor at the University of Leiden [12, 13]. Only in 1932, when cooling liquid Helium down further, it was observed that it suddenly stopped boiling and became completely calm, indicating a second phase transition [14]. This phase transition shows a λ -shaped singularity in the specific heat [15], today referred to as the λ -point, and Helium above and below the transition point as Helium I and II, respectively.

In 1938, Nature published two hallmark papers back-to-back on liquid Helium, both concerning the first observations of superfluidity. In the first, Kapitza investigated the flow through a thin slit between two highly-polished disks [16]. Above the λ -point, there was no flow through the slit, while below, the flow occurred so rapidly that Kapitza could only propose an upper bound on the viscosity. The second paper, by Allen and Misener [17, 18], described similar experiments through thin capillaries with varying diameters. Similarly, the flow sped up significantly below the λ -point and was independent of applied pressure and capillary diameter. In analogy with superconductivity, Kapitza dubbed this effect superfluidity [16].

At this point, there was little theoretical understanding of the effects, and quantum mechanics was still in its infancy. The first up to the task was London, who had heard of the above experiments by Kapitza and Allen & Misener a few months before their respective papers [19]. Before turning to superfluidity, London had developed a theory of superconductivity based on a macroscopic wavefunction [20], an idea that he would carry over to superfluidity.

By late 1937, Einstein’s seminal work on quantum condensation had gotten a reputation as purely academic without getting any further attention [2, 3]. Nevertheless, it sparked a debate between Einstein, Ehrenfest, and Ehrenfest’s graduate student Uhlenbeck at a statistical physics conference [19]. By the end of the discussion, Uhlenbeck had withdrawn his criticism of Bose-Einstein condensation in finite-size systems. London also attended the conference and overheard this discussion, previously unaware of Einstein’s papers on Bose-Einstein condensation [19]. As London knew

²Later, Schroedinger heard of de Broglie’s idea for the first time through Einstein’s paper [1, 11].

that ^4He is bosonic, he immediately connected the recent superfluidity experiments to Bose-Einstein condensation. He promptly published two papers [21, 22], noting that the transition temperature to a condensed state reasonably estimates the λ -point. These papers mark the historical convergence between superfluidity and Bose-Einstein condensation.

Shortly after this paper, London started collaborating with Tisza, who similarly struggled with the political climate developing in Europe [19]. Quickly into their collaboration and after a sleepless night [19], Tisza proposed a so-called two-fluid hydrodynamic model [23] to explain various experimental results of superfluid ^4He . One component of this model would be a Bose-condensed part, describing the superfluid with zero viscosity, while the non-condensed part carries all viscosity. Notably, in this description, both components have an independent velocity field. While this idea was initially deeply upsetting for London [19], Tisza could explain all prior hydrodynamic results for the first time [23].

A significant drawback of London and Tisza's model was that it rested on the idea of a non-interacting ideal Bose gas without interactions [21, 22]. ^4He molecules, however, are strongly interacting. This discrepancy drew Landau's attention, who had just been released from political prison with the help of his friend Kapitza [4]. In 1941, Landau published his seminal paper on superfluid ^4He [24, 25]. Here, he introduced the idea that one can describe the superfluid through weakly interacting quasi-particles and their collective modes, such as sound and entropy waves. With this excitation spectrum of quasi-particles, Landau could do quantitative calculations and explain the thermodynamic and hydrodynamic properties of superfluid Helium [24, 25]. Landau, however, categorically rejected the connection between superfluidity and an ideal Bose gas as proposed by London and Tisza [24, 25].

The first formal work that combined both theoretical ideas was done in 1947 by Bogoliubov [26], whose work we will follow in most of Ch. 3. Applying the method of second quantization, he derived the excitation spectrum of a weakly interacting Bose gas. He showed that it can support superfluidity under the same argument Landau brought forth [26]. As such, he first showed that Bose-Einstein condensation and superfluidity are deeply connected. Bogoliubov's work effectively kick-started an extensive theory of superfluidity and weakly interacting Bose gases, which is the theoretical ground for this thesis.

The next breakthrough occurred as late as 1995, when, for the first time, Bose-Einstein condensation occurred in an experiment using ultra-cold gases of alkali atoms [27, 28]. By now, these experimental set-ups have become highly tunable, with many combinations of alkali [29] and lanthanide [30–34] atoms possible, where one can almost freely tune the interaction strength between the atoms via Feshbach resonances [35–

41]. With this tunability comes the ability to create systems that would otherwise not exist or are difficult to realize, allowing for a perfect playground in fundamental research. One of these systems comes from a proposal in 2015 [42], where the interaction between two different components would make the gas unstable. However, by including a higher-order term in the mathematical description that originates from the interaction of atoms outside the condensed state with the condensate itself, one can re-stabilize this system so that it may exist without an external trapping potential. This system subsequently occurred in a one-component dipolar system of lanthanide atoms [43, 44] and a two-component mixture as initially proposed in [45, 46].

Another of these systems comes as a so-called supersolid, somehow combining a superfluid’s zero viscosity with a crystalline solid’s rigid structure. Proposed in the late 1960s [47, 48] and long hunted for [49], the formalism mentioned above of atoms outside of the condensed state interacting with the condensate itself led to the observation of a supersolid in the same dipolar lanthanide system as for the one-component self-bound droplet [50–52].

This thesis describes the mechanisms involved in forming the self-bound and dipolar supersolid systems described above and how to probe their superfluid properties. The goal for this first introductory part of this thesis is simple: What would be the most helpful document for myself if I were back at the beginning of my PhD studies to understand the research papers included in this thesis? As such, we start by describing Bose-Einstein condensation, first following Bose’s and Einstein’s work in Ch. 2, before generalizing it to interacting systems. Ch. 3 calculates the effect of atoms outside the condensed state on the condensed ground state by following Bogoliubov’s seminal paper [26] and its extension for two components [53], before describing self-bound droplet formation [42, 54]. We formally introduce the concept of superfluidity in Ch. 4 for one and two superfluid components before turning to supersolidity in Ch. 5. After giving a concluding outlook in Ch. 6, we include the full texts of the papers that comprise this thesis’s original research.

Chapter 2

Bose-Einstein Condensation

'From a certain temperature on, the molecules 'condense' without attractive forces, that is, they accumulate at zero velocity. The theory is pretty, but is there also some truth in it?'
- Einstein to Ehrenfest, 1924 [2]

We start this thesis by considering the origin and definition of a Bose-Einstein condensate - a state of matter where below a critical temperature T_c a macroscopic fraction of particles occupy the same quantum state. Initially, in Sec. 2.1, we will briefly look at the historical development starting from Planck's law of black-body radiation [6], leading to Bose's introduction of quantum statistics [5] and Einstein's generalization from photons to massive non-interacting particles [7–9]. In the final parts in Sec. 2.2, we follow Onsager and Penrose's generalization [55, 56] and give three different definitions of Bose-Einstein condensation with interacting particles before introducing the Bogoliubov approximation [26], which most of Ch. 3 builds on.

2.1 Planck, Bose & Einstein

The Bose-Einstein condensate originates from the equally named quantum statistics bosonic particles obey. Bose developed these as an alternative explanation of Planck's black-body radiation law that does not rely on any classical assumptions [5]. In Planck's original derivation¹ [6], he modeled the black body as having walls consisting of harmonic oscillators that eventually reach thermal equilibrium if the temperature T is held constant by continuously emitting and absorbing radiation. In this thermal equilibrium, the spectral shape of the radiation then solely depends on the black

¹For a detailed derivation with a strong historical narrative of Planck, Bose and Einstein see Ref. [1].

body's temperature and is independent of shape or material. After some calculation [1, 6] he recovered the energy density $u(\nu)$ per frequency interval $d\nu$

$$u(\nu)d\nu = \frac{8\pi\nu^2}{c^3} \bar{E} d\nu, \quad (2.1)$$

where c is the speed of light, ν the frequency and \bar{E} the average harmonic oscillator energy. If one then inserts according to Boltzmann $\bar{E} = k_B T$, where k_B is the Boltzmann constant, one recovers the Rayleigh-Jeans law $u(\nu) = 8\pi\nu^2 k_B T / c^3$, which experiences the ultraviolet catastrophe $\int_0^\infty u(\nu) d\nu \rightarrow \infty$ [1]. Intrigued by the universality of black-body radiation, Planck looked towards finding a more suitable average energy and divided the energy associated with a certain frequency into a part in the oscillators and a part in the medium [6]. As the black body approaches thermal equilibrium, it will assume the most probable partition between these two parts that maximizes entropy. The probability of finding a certain amount of energy in the oscillators is proportional to the number of ways to divide this energy between the oscillators. This is similar to how, in a set of two dice, the most likely outcome is seven, as the largest number of combinations of the two dice gives seven. The problem now lies that if this energy is infinitely divisible, there will be an infinite amount of variations possible. Planck recognized this and proposed that the harmonic oscillators have quantized energy $E_n = nh\nu$, where n is an integer, and h is some constant originating from experimental data. One can then write the average energy $\bar{E} = \sum_{n=0}^\infty E_n p(n)$, where

$$p(n) = \frac{\exp(-\beta E_n)}{\sum_{n=0}^\infty \exp(-\beta E_n)}, \quad (2.2)$$

is the Boltzmann distribution for a system in thermodynamic equilibrium with $\beta = 1/(k_B T)$ the inverse temperature. Inserting $E_n = nh\nu$ one then quickly finds

$$u(\nu) = \frac{8\pi\nu^2}{c} \frac{h\nu}{\exp(\beta h\nu) - 1}, \quad (2.3)$$

which is Planck's radiation law and $(\exp(\beta h\nu) - 1)^{-1}$ the Bose-Einstein distribution.

In 1924 Bose proposed an alternative derivation [1, 5] where he calculated the phase space volume in the interval $d\nu$ for a photon with momentum $h\nu/c$ as $\int d\mathbf{r} d\mathbf{p} = 8\pi h^3 \nu^2 V d\nu / c^3$. If one divides this volume into cells of size h^3 , one finds $8\pi\nu^2 d\nu / c^3$ of these cells in the frequency interval $d\nu$. Similarly to Planck, the question then turns

to counting the different ways of distributing N photons over the cells, which Bose assumed to be indistinguishable. The number of distinct orderings of the cells g_i with n_i particles is then

$$t_i = \frac{(n_i + g_i - 1)!}{n_i!(g_i - 1)!} \approx \frac{(n_i + g_i)!}{n_i!g_i!}, \quad (2.4)$$

where we have made the last step for a large number of cells $g_i \gg 1$. As before, in the thermodynamic equilibrium, the system follows the most probable distribution, such that we want to maximize [1, 5]

$$t = \prod_i t_i = \prod_i \frac{(n_i + g_i)!}{n_i!g_i!}, \quad (2.5)$$

with the constraint that there are N_s particles with frequency ν_s and a total energy $E = \sum_s N_s h\nu_s$. Maximizing Eq. (2.5) under these constraints, one finds that

$$N_s = \frac{8\pi\nu_s^2}{c^3} d\nu_s \frac{1}{\exp(\beta h\nu) - 1}, \quad (2.6)$$

which is equivalent to Planck's result [1, 5].

Bose struggled to publish this result but contacted Einstein for help [1, 3]. Previously, Bose had translated Einstein's theory of relativity and Einstein agreed and recognized the value in Bose's work [1, 3]. Einstein also extended it to massive non-interacting particles by introducing particle number conservation, which was not given in Bose's derivation as photons are continuously emitted and absorbed [5, 7–9]. The average occupation number of bosons in a state j with energy E_j and chemical potential μ at a temperature then becomes

$$\langle \hat{N}_j \rangle = \frac{1}{\exp(\beta(E_j - \mu)) - 1}, \quad (2.7)$$

with the total particle number $N = \sum_j \langle \hat{N}_j \rangle$. The lowest state E_0 grows larger in population at a given T faster with μ than any other $\langle \hat{N}_{j \neq 0} \rangle$. As μ approaches E_0 with increasing N , the groundstate becomes macroscopically occupied, and $\langle \hat{N}_0 \rangle$ becomes of order N (in the following, we write $\sim \mathcal{O}(N)$) [57]. We refer to $\langle n_0 \rangle / N$ as the condensate fraction, which depends on T in the case of large N , with a critical

temperature T_c marking when the ground state becomes macroscopically occupied. We can estimate T_c by requiring that the de-Broglie wavelength

$$\lambda_T = \sqrt{\frac{2\pi\hbar^2}{Mk_B T}} \quad (2.8)$$

which describes the spatial extent of an individual particle's wavefunction, becomes comparable to the interparticle spacing $d = n^{-1/3}$ and gives

$$k_B T_c \approx \frac{2\pi\hbar^2 n^{2/3}}{M}, \quad (2.9)$$

below which the ground state is macroscopically occupied².

2.2 Bose-Einstein Condensation in Interacting Systems

We can generalize Einstein's theory of the non-interacting Bose gas [5, 7–9] to a macroscopic number of particles occupying a single-particle state for an interacting system. While this is accurate enough in words, we want to put this into mathematical language and go through three definitions of Bose-Einstein Condensation that all emerge from this description.

We may investigate such a macroscopic occupation via the reduced single-particle density matrix $n_1(\mathbf{r}, \mathbf{r}') = \langle \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}') \rangle$, where $\hat{\Psi}^\dagger$ and $\hat{\Psi}$ are second quantized bosonic field operators and $n_1(\mathbf{r}, \mathbf{r}')$ measures the correlations³ between particles at position \mathbf{r}' and \mathbf{r} in an interacting system. The density matrix is hermitian and, as such, can be diagonalized with real eigenvalues λ_i and their respective eigenfunctions χ_i :

$$n_1(\mathbf{r}, \mathbf{r}') = \sum_i \lambda_i \chi_i^*(\mathbf{r}) \chi_i(\mathbf{r}'). \quad (2.10)$$

This expression fulfills the above generalization of a Bose-Einstein condensate if only one of the eigenvalues λ_i becomes $\sim \mathcal{O}(N)$, where N is the number of particles,

²For a homogeneous Bose gas in a box, an exact calculation gives $T_c = \zeta(3/2)^{-2/3} 2\pi\hbar^2 n^{2/3} / M$, where ζ is the Riemann-Zeta function [58, 59].

³One could also see this as the immediate response of the system when inserting a particle at position \mathbf{r} and removing another at \mathbf{r}' .

and the remaining λ_i remain $\sim \mathcal{O}(1)$. If only one of the eigenvalues is $\sim \mathcal{O}(N)$, it commonly refers to a “simple” Bose-Einstein condensate, which describes the systems investigated in this thesis. If however multiple eigenvalues are $\sim \mathcal{O}(N)$, one has a “fragmented” condensate [60, 61]. By extracting one of the eigenvalues for a simple condensate, we arrive at the description first formalized by Onsager and Penrose [56],

$$n_1(\mathbf{r}, \mathbf{r}') = \lambda_0 \chi_0^*(\mathbf{r}) \chi_0(\mathbf{r}') + \sum_{i \neq 0} \lambda_i \chi_i^*(\mathbf{r}) \chi_i(\mathbf{r}'). \quad (2.11)$$

Now, let us assume that our system is in the thermodynamic limit where both the particle number N and volume $V \rightarrow \infty$, but the density $n = N/V = \text{const.}$, an approximation we will frequently use throughout this thesis. We consider non-uniform densities in Ch. 3.2. Due to the systems’ translational invariance, we can transform the bosonic field operators into \mathbf{k} -space. Then $n_1(\mathbf{r}, \mathbf{r}') = V^{-1} \sum_{\mathbf{k}} \exp(-i\mathbf{k}(\mathbf{r} - \mathbf{r}')/\hbar) \langle \hat{\Psi}_{\mathbf{k}}^\dagger \hat{\Psi}_{\mathbf{k}} \rangle$, where $\langle \hat{\Psi}_{\mathbf{k}}^\dagger \hat{\Psi}_{\mathbf{k}} \rangle = \langle \hat{N}_{\mathbf{k}} \rangle$ is the average momentum occupation number according to Bose-Einstein statistics. In this case, the eigenfunctions χ_i also become plane waves, such that if we turn the sum over \mathbf{k} into an integral⁴ over D-dimensions in the thermodynamic limit, n_1 becomes

$$n_1(\mathbf{r}, \mathbf{r}') = \frac{\langle \hat{\Psi}_0^\dagger \hat{\Psi}_0 \rangle}{V} + \int \frac{d\mathbf{k}}{(2\pi)^D} e^{-i\mathbf{k}(\mathbf{r} - \mathbf{r}')/\hbar} \frac{1}{e^{\beta(E_{\mathbf{k}} - \mu)} - 1}, \quad (2.12)$$

where $\beta = 1/(k_B T)$ is the inverse temperature, $E_{\mathbf{k}}$ the systems energy spectrum and $\mu < E_{\mathbf{k}}$ the chemical potential. We now focus on the first term in Eq. (2.12) for simplicity and immediately see that in the case of a condensed system, there will still be some correlation, even if $|\mathbf{r} - \mathbf{r}'| \rightarrow \infty$. The correlation maximizes for a fully condensed system and introduces the concept of “Off-diagonal long-range order” [62]. Some caution about off-diagonal long-range order in a realistic system confined in an external trapping potential is warranted. In this case, the system does not extend to infinity, so the concept of $|\mathbf{r} - \mathbf{r}'| \rightarrow \infty$ becomes meaningless, and off-diagonal long-range order is not a sufficient definition of a Bose-Einstein condensate.

Lastly, due to the macroscopic state occupation, we can motivate a similar separation for the field operator

$$\hat{\Psi}(\mathbf{r}, t) = \hat{\psi}(\mathbf{r}, t) + \hat{\vartheta}(\mathbf{r}, t), \quad (2.13)$$

⁴For finite size systems with periodic boundary conditions \mathbf{k} is quantized as $\mathbf{k} = 2\pi n\hbar/l$ due to the finite volume V .

where $\hat{\psi}$ describes the condensed part and $\hat{\vartheta}$ is a fluctuation operator accounting for the remaining states. In the case of an infinite, uniform system in the thermodynamic limit, we can expand $\hat{\Psi}$ as before in single-particle plane waves, such that

$$\hat{\Psi}(\mathbf{r}, t) = \frac{\hat{a}_0}{\sqrt{V}} + \sum_{\mathbf{k} \neq 0} \hat{a}_{\mathbf{k}} \frac{e^{i\mathbf{k}\mathbf{r}/\hbar}}{\sqrt{V}}. \quad (2.14)$$

The transformation into single-particle plane waves is canonical, such that the operators $\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}}^\dagger$ fulfill bosonic commutation relations, too. The number operator in the momentum operator representation $\hat{N}_{\mathbf{k}} = \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}$ then gives the number of particles with momentum \mathbf{k} . Due to the canonical transformation we then get [63, 64]

$$\lim_{V \rightarrow \infty} \frac{1}{V} [\hat{a}_0, \hat{a}_0^\dagger] = \lim_{V \rightarrow \infty} \frac{1}{V} \rightarrow 0. \quad (2.15)$$

For an infinite system, where $V \rightarrow \infty$, the non-commutativity vanishes and \hat{a}_0 and \hat{a}_0^\dagger become complex numbers $\hat{a}_0 \rightarrow a_0 = \sqrt{N_0} e^{i\phi}$ with some phase value ϕ , resulting in the transformation to a classical field

$$\hat{\psi}(\mathbf{r}, t) \rightarrow \psi(\mathbf{r}, t). \quad (2.16)$$

Eq. (2.16) is the so-called Bogoliubov approximation [26] and means that the condensate can be described effectively as a coherent (classical) state. Correspondingly, we will, in the remainder of this thesis, write $\hat{a}_0^{(\dagger)} \rightarrow a_0^{(*)}$ where the (\dagger) and $(*)$ indicate that we, in general, refer to both annihilation and creation operators or complex conjugated pairs.

Alternatively, to arrive at the same result as in Eq. (2.15), we can split the total particle number operator \hat{N} with $\langle \hat{N} \rangle = N$ into $\hat{N} = \hat{N}_0 + \sum_{\mathbf{k} \neq 0} \hat{N}_{\mathbf{k}}$, where $\hat{N}_0 = \hat{a}_0^\dagger \hat{a}_0$ is the number operator for the condensed state. If $\langle \hat{N}_0 \rangle$ is of order $\mathcal{O}(\langle \hat{N} \rangle)$ and $N \gg 1$ then the non-commutivity also vanishes [65].

In the following chapters, we rely heavily on the Bogoliubov approximation [26] in deriving the equation of state for the condensed ground state and the contribution of the fluctuation operator $\hat{\vartheta}$ within the infinite system framework. Only after setting up the basic scaffolding will we investigate when we can use the approximation of an infinite and uniform system for a real, experimental system in a trap.

Chapter 3

The weakly interacting Bose gas

'It is useful to note that N. N. Bogoliubov has succeeded recently, by an ingenious application of second quantization, in determining the general form of the energy spectrum of a Bose-Einstein gas with a weak interaction between the particles.'

- Landau, 1949 [66]

The theory of weakly interacting Bose gases traces back to Bogoliubov's seminal paper in 1947 [26]. Here, he laid the foundation of these systems by introducing quasi-particles to explain superfluidity in terms of the quasi-particle collective excitations. Continuing on this foundation, Gross [67] and Pitaevskii [68] independently derived a non-linear Schrödinger equation describing the ground state and time-evolution of the bosonic macroscopic wavefunction that we today call the Gross-Pitaevskii equation.

The quasi-particle treatment introduced by Bogoliubov [26] together with the Gross-Pitaevskii equation [67, 68] presents the main theoretical foundation of this thesis. We start this chapter by considering an infinite and uniform Bose gas in Sec. 3.1 to introduce the Bogoliubov treatment in a simple environment. This results in the ground state properties and the effects of non-condensed particles on the ground state. After this, we extend this treatment to a non-uniform Bose gas within the so-called local density approximation in Sec. 3.2 before considering specific one-component (Sec. 3.3) and two-component (Sec. 3.4) systems. Lastly, in Sec. 3.5, we consider the formation of self-bound droplets in contact and dipolar interacting systems and the formation of mixed bubbles in two-component contact interacting systems.

3.1 The Uniform Bose Gas

Let us first consider a general system of bosons at zero temperature, where the bosons only interact via one-body potential and two-body interaction, described by the second-quantized Hamiltonian

$$\hat{H} = \int d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{h}_0(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \quad (3.1)$$

$$+ \frac{1}{2} \iint d\mathbf{r}' d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}', t) \hat{\Psi}^\dagger(\mathbf{r}, t) \Phi(\mathbf{r}' - \mathbf{r}) \hat{\Psi}(\mathbf{r}', t) \hat{\Psi}(\mathbf{r}, t), \quad (3.2)$$

where $\hat{h}_0(\mathbf{r}, t) = -\hbar^2 \nabla^2 / (2m) + V_{\text{ext}}(\mathbf{r}, t)$ is the one-body potential with an external field V_{ext} and Φ is a (for-now) arbitrary two-body interaction potential.

In general, this is a difficult problem to solve exactly, so it becomes necessary to apply some approximations. Under certain conditions, one may put the interaction functional towards infinity, leading to the so-called fermionization of bosons and the Tonks-Girardeau regime in one dimension [69–71]. The usual approach that we will follow here is to assume that most particles are in the condensed ground state as described in the previous chapter and that the interaction potential is small, thus entering a weakly-interacting regime [26, 64].

We now apply another simplification that will allow us to obtain the system's ground state properties analytically. Assuming that our system is infinite and uniform, we set $V_{\text{ext}}(\mathbf{r}) = 0$. Thus, the system is translational invariant, and we can write the bosonic field operators as $\hat{\Psi}^{(\dagger)}(\mathbf{r}) = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{(\dagger)} \psi_{\mathbf{k}}^{(*)}(\mathbf{r})$ with the single-particle wavefunctions as plane waves

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} \exp\left(i \frac{\mathbf{k} \cdot \mathbf{r}}{\hbar}\right). \quad (3.3)$$

Utilizing these transformations, we can write the stationary (grand canonical) Hamiltonian \hat{H}_{gc} in momentum creation and annihilation operators as

$$\begin{aligned} \hat{H}_{\text{gc}} = \hat{H} - \mu \hat{N} &= \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) \\ &+ \frac{1}{2V} \sum_{\mathbf{k}_1 \mathbf{k}_2, \mathbf{q}} \hat{a}_{\mathbf{k}_1 - \mathbf{q}}^\dagger \hat{a}_{\mathbf{k}_2 + \mathbf{q}}^\dagger \hat{a}_{\mathbf{k}_2} \hat{a}_{\mathbf{k}_1} \Phi(\mathbf{q}), \end{aligned} \quad (3.4)$$

where the index gc indicates that we work with the grand canonical Hamiltonian. Additionally, in Eq. (3.4), we have assumed that the interaction potential is radially symmetric, such that we can write

$$\Phi(|\mathbf{r} - \mathbf{r}'|) = \frac{1}{V} \sum_{\mathbf{k}} \Phi(\mathbf{k}) \exp\left(-i \frac{\mathbf{k}(\mathbf{r} - \mathbf{r}')}{\hbar}\right). \quad (3.5)$$

Let us investigate the ground state properties if the system is fully condensed and every particle is in the $\mathbf{k} = 0$ state. In this case, we get the ground state energy $E_{\text{gc},0}$ as

$$E_{\text{gc},0} = \frac{N_0^2}{2V} \Phi(0) - \mu N_0 \quad (3.6)$$

to zeroth-order. The chemical potential determines the equation of state by $\partial E_{\text{gc},0} / \partial N_0 = 0$ and gives

$$\mu = \Phi(0) \frac{N_0}{V}. \quad (3.7)$$

Now applying the Bogoliubov approximation from Eq. (2.16) and keeping terms up to second order in creation and annihilation operators $\hat{a}_{\mathbf{k}}^{(\dagger)}$ while maintaining linear momentum conservation, the remaining second-order Hamiltonian $\hat{H}_{\text{gc},2}$ is then given by

$$\begin{aligned} \hat{H}_{\text{gc},2} = & \sum_{\mathbf{k} \neq 0} \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} \left[\frac{\hbar^2 k^2}{2m} - \mu + \frac{N_0}{V} (\Phi(0) + \Phi(\mathbf{k})) \right] \\ & + \frac{1}{2V} \sum_{\mathbf{k} \neq 0} \Phi(\mathbf{k}) \left[a_0^{*2} \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} + a_0^2 \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{-\mathbf{k}}^{\dagger} \right]. \end{aligned} \quad (3.8)$$

In the first line, the interacting terms represent a particle's Hartree-Fock mean field produced by interactions with its surrounding particles. The $\Phi(0)$ Hartree term describes a particle in the state \mathbf{k} interacting with the N_0 atoms in the condensed state. In contrast, the $\Phi(\mathbf{k})$ Fock term describes the scattering process of a particle in the \mathbf{k} state into the condensed state and a condensed particle into the \mathbf{k} state. The terms in the second line represent the scattering of two particles in the condensed state into the $\pm \mathbf{k}$ states and vice-versa.

In Sec. 2.2 we mentioned that a_0 and a_0^\dagger represent complex numbers and can be written as $a_0^{(*)} = \sqrt{N_0}e^{\pm i\phi}$. We now want to absorb the phase factor $e^{\pm i\phi}$ into the remaining $\hat{a}_{\mathbf{k}}^{(\dagger)}$ and replace μ with Eq. (3.7). Then we can write $a_0^{(*)}/\sqrt{V} = \sqrt{N_0/V} = \sqrt{n_0}$, where n_0 is the ground state density. The second order Hamiltonian $\hat{H}_{\text{gc},2}$ then becomes

$$\begin{aligned} \hat{H}_{\text{gc},2} = \sum_{\mathbf{k} \neq 0} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \left[\frac{\hbar^2 k^2}{2m} + n_0 \Phi(\mathbf{k}) \right] \\ + \frac{n_0}{2} \sum_{\mathbf{k} \neq 0} \Phi(\mathbf{k}) \left[\hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} + \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger \right]. \end{aligned} \quad (3.9)$$

Eq. (3.9) contains off-diagonal elements in creation and annihilation operators, which we want to remove by diagonalization. In the process, we will obtain the quantum fluctuation's \hat{v} effect on the ground state. As the following procedure is general to any quadratic bosonic Hamiltonian, let us generalize Eq. (3.9) to

$$\hat{H}_{\text{gc},2} = \sum_{\mathbf{k} \neq 0} T_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k} \neq 0} \left[U_{\mathbf{k}} \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} + U_{\mathbf{k}}^* \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger \right], \quad (3.10)$$

where in our case $T_{\mathbf{k}} = \hbar^2 k^2 / 2m + n_0 \Phi(\mathbf{k})$ and $U_{\mathbf{k}} = n_0 \Phi(\mathbf{k})$. $\hat{H}_{\text{gc},2}$ is hermitian and can thus be diagonalized by unitary transformations, which we define as [26, 64]

$$\begin{aligned} \hat{a}_{\mathbf{k}} &= u_{\mathbf{k}}^* \hat{\alpha}_{\mathbf{k}} - v_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}^\dagger, \\ \hat{a}_{\mathbf{k}}^\dagger &= u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^\dagger - v_{\mathbf{k}}^* \hat{\alpha}_{-\mathbf{k}}. \end{aligned} \quad (3.11)$$

These transformations are commonly referred to as Bogoliubov transformations [26, 64], where $\hat{\alpha}_{\mathbf{k}}$ and $\hat{\alpha}_{\mathbf{k}}^\dagger$ are quasi-particle operators of the diagonalized Hamiltonian. The quasi-particle amplitudes $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are uniquely determined by requiring

$$\hat{H}'_{\text{gc},2} = \sum_{\mathbf{k} \neq 0} E_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + K_{\mathbf{k}} \hat{1}, \quad (3.12a)$$

$$|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1, \quad (3.12b)$$

where the first line is the diagonalized Hamiltonian of free bosonic quasi-particles $\hat{\alpha}_{\mathbf{k}}$, plus some operator-independent zero-point energy $K_{\mathbf{k}}$, and the second line ensures

that the transformations in Eq. (3.11) are canonical. One commonly writes the amplitudes $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ in terms of hyperbolic functions \sinh and \cosh . This method, however, becomes quite cumbersome for any but the simplest systems. Here, we focus on the equations of motion instead. The quasi-particle Hamiltonian $\hat{H}'_{\text{gc},2}$ and $\hat{H}_{\text{gc},2}$ describe the same system. As such, the equation of motion in the Heisenberg picture is invariant of the chosen representation. We thus calculate $[\hat{\alpha}_{\mathbf{k}}, \hat{H}_{\text{gc},2}]$ and $[\hat{\alpha}_{\mathbf{k}}, \hat{H}'_{\text{gc},2}]$ and compare coefficients¹ for $\hat{a}_{\mathbf{k}}$ and $\hat{a}_{-\mathbf{k}}^\dagger$. This results in the following linear system²

$$\begin{bmatrix} T_{\mathbf{k}} & -U_{\mathbf{k}} \\ U_{\mathbf{k}}^* & -T_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{bmatrix} = E_{+\mathbf{k}} \begin{bmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{bmatrix} \quad (3.13)$$

where we have additionally assumed $U_{\mathbf{k}} = U_{-\mathbf{k}}$ and $U_{\mathbf{k}}^* = U_{-\mathbf{k}}^*$. $E_{+\mathbf{k}}$ is then the solution to the linear system as

$$E_{+\mathbf{k}} = \sqrt{T_{\mathbf{k}}^2 - |U_{\mathbf{k}}|^2}, \quad (3.14)$$

or for our system

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} (\epsilon_{\mathbf{k}} + 2n_0\Phi(\mathbf{k}))}, \quad (3.15)$$

which is the Bogoliubov excitation spectrum generalized for arbitrary radially symmetric interactions [26] and $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ is the free particle spectrum.

Lastly, we are interested in determining $K_{\mathbf{k}}$, for which we introduce the vacuum state $|0\rangle$ with $\hat{a}_{\mathbf{k}} |0\rangle = 0$. Then $\langle 0 | \hat{H}_{\text{gc},2} | 0 \rangle = 0$, which must also hold for $\hat{H}'_{\text{gc},2}$:

$$\langle 0 | \hat{H}'_{\text{gc},2} | 0 \rangle = \sum_{\mathbf{k} \neq 0} E_{\mathbf{k}} |v_{\mathbf{k}}|^2 + K_{\mathbf{k}} \stackrel{!}{=} 0. \quad (3.16)$$

We can obtain $|v_{\mathbf{k}}|^2$ by multiplying the first line in Eq. (3.13) with $u_{\mathbf{k}}^*$, complex conjugating the second line before multiplying it with $v_{\mathbf{k}}$ and lastly utilizing Eq. (3.12b), which gives

¹We can obtain the same result formally by placing the resulting equations between $\langle 1 | \dots | 0 \rangle$ and $\langle 0 | \dots | 1 \rangle$ pairs.

²In the representations given in the main text, both $\hat{H}_{\text{gc},2}$ and $\hat{H}'_{\text{gc},2}$ sum over all $\mathbf{k} \neq 0$. However, the Bogoliubov transformations in Eq. (3.11) explicitly depend on the direction of \mathbf{k} . It is, therefore, necessary to restrict the sum to $\mathbf{k} > 0$ and include an additional term for $-\mathbf{k}$ to ensure correctness.

$$|v_{\mathbf{k}}|^2 = \frac{1}{2} \left(\frac{T_{\mathbf{k}}}{E_{\mathbf{k}}} - 1 \right) \quad (3.17)$$

and thus

$$\begin{aligned} K &= \frac{1}{2} \sum_{\mathbf{k} \neq 0} (E_{\mathbf{k}} - T_{\mathbf{k}}) \\ &= \frac{1}{2} \sum_{\mathbf{k} \neq 0} \left(\sqrt{\epsilon_{\mathbf{k}} (\epsilon_{\mathbf{k}} + 2n_0 \Phi(\mathbf{k}))} - \epsilon_{\mathbf{k}} - n_0 \Phi(\mathbf{k}) \right). \end{aligned} \quad (3.18)$$

K represents the zero-point contribution of the quantum fluctuation term $\hat{\mathcal{V}}$ to the ground state energy E_0 . For a three-dimensional one-component Bose gas with contact interaction, this is commonly called the Lee-Huang-Yang (LHY) correction [72, 73] or Bogoliubov vacuum energy, which we will calculate in Sec. 3.3.

In the thermodynamic limit, where we can replace the \mathbf{k} -sum with an integral over momentum-space in D dimensions, the equation of state Eq. (3.7) then becomes

$$\begin{aligned} \mu &= \Phi(0)n_0 + \\ &\frac{1}{2} \frac{\partial}{\partial n_0} \int \frac{d^D \mathbf{k}}{(2\pi)^D} \left(\sqrt{\epsilon_{\mathbf{k}} (\epsilon_{\mathbf{k}} + 2n_0 \Phi(\mathbf{k}))} - \epsilon_{\mathbf{k}} - n_0 \Phi(\mathbf{k}) \right), \end{aligned} \quad (3.19)$$

where we used the Bogoliubov vacuum energy in Eq. (3.18) as a correction to the ground state energy.

Before considering real physical systems and their different external potentials V_{ext} in modern experimental setups, let us do some mathematical housekeeping and deal with the ramifications of the used approximations. So far, we have been deliberately vague about 'weak' interactions and that 'most' particles are in the condensed ground state. Now, we want to put some quantitative labels on these statements. If the majority of particles are condensed, it implies that $\sum_{\mathbf{k} \neq 0} \langle \hat{N}_{\mathbf{k}} \rangle = \sum_{\mathbf{k} \neq 0} \langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle = N - N_0 \ll N$ and as such

$$\frac{N - N_0}{N} = \frac{\sum_{\mathbf{k} \neq 0} \langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle}{N} \ll 1. \quad (3.20)$$

The sum can be obtained by utilizing the Bogoliubov transformations in Eq. (3.11) and via the mean quasi-particle occupation number $\langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle = (\exp(\beta(E_{\mathbf{k}} - \mu)) - 1)^{-1}$, and thus for $T = 0$ K

$$\begin{aligned}
\frac{N - N_0}{N} &= \frac{1}{2N} \sum_{\mathbf{k} \neq 0} \left(\frac{T_{\mathbf{k}}}{E_{\mathbf{k}}} - 1 \right) \\
&= \frac{1}{2N} \sum_{\mathbf{k} \neq 0} \left(\frac{\epsilon_{\mathbf{k}} + n_0 \Phi(\mathbf{k})}{\sqrt{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}} + 2n_0 \Phi(\mathbf{k}))}} - 1 \right) \ll 1.
\end{aligned} \tag{3.21}$$

Surprisingly, the resulting depletion of the condensate is finite despite $T = 0$ K and results from Eq. (3.12b), which enforces bosonic commutation relations and is thus a genuine quantum effect.

As a result of the approximation up to second-order in $\hat{H}_{\text{gc},2}$, it describes a system of free bosonic quasi-particles, where particle numbers are not conserved ($[\hat{H}_{\text{gc},2}, \hat{N}_{\mathbf{k}}] \neq 0$). We could, however, remedy this by including a weak interaction between quasi-particles by including third-order terms as well, allowing the quasi-particles to reach statistical equilibrium [26]. As such, quasi-particles are continuously destroyed and created, so we must decide whether to focus on the total particle number N or the ground state particle number N_0 . As the condensate depletion in Eq. (3.21) is assumed to be small, one can safely replace N_0 with N post hoc³.

Most of the papers in this thesis investigate a system under rotation. We now want to see how to introduce this rotation into a system. We can write the rotation operator as $\hat{R}(t) = \exp(-i\theta(t)\hat{L}_z/\hbar)$, where $\hat{R}(t)$ rotates a state $|\hat{\Psi}(t)\rangle$ by an angle $\theta(t)$ around the z -axis, such that $|\hat{\Psi}'(t)\rangle = \hat{R}(t)|\hat{\Psi}(t)\rangle$. We can then calculate the time evolution of the state $|\hat{\Psi}(t)\rangle$ as

$$\begin{aligned}
i\hbar\partial_t |\hat{\Psi}'(t)\rangle &= i\hbar\partial_t \left(\hat{R}(t) |\hat{\Psi}(t)\rangle \right) \\
&= \left(i\hbar(\partial_t \hat{R}(t))\hat{R}^\dagger(t) + \hat{R}(t)\hat{H}(t)\hat{R}^\dagger(t) \right) |\hat{\Psi}'(t)\rangle
\end{aligned} \tag{3.22}$$

Here, the second term describes the transformation into the co-rotating frame. Assuming that $\theta(t)$ changes as $\theta(t) = -\int_{t_0}^t dt' \Omega(t')$, where t_0 is the initial time and $\Omega(t)$ is the rotation's instantaneous angular velocity, the time derivative becomes $\partial_t \hat{R}(t) = i\Omega(t)\hat{L}_z\hat{R}(t)/\hbar$. If all the operators in $\hat{H}(t)$ rotate at the same constant Ω , the problem becomes time-independent and we can amend the one-particle potential by writing $\hat{h}_0 \rightarrow \hat{h}_0 - \Omega\hat{L}_z$ [74].

³Alternatively, insert $N_0 = N - \langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle$ in the resulting energy expression while discarding all $\langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle^2 \ll 1$.

3.2 The Local Density Approximation

De Gennes first generalized the above process in the context of superconductors [75] to a spatially modulated system. We now want to follow this procedure and allow the bosonic field operators to become position-dependent $\hat{\Psi} \rightarrow \hat{\Psi}(\mathbf{r})$, either due to interactions or due to an external trapping potential $V_{\text{ext}}(\mathbf{r})$. As we will see, the above derivation still holds if we assume that at every \mathbf{r} , there is a locally uniform system surrounding it. First, we begin by the usual separation into ground and excited state $\hat{\Psi}(\mathbf{r}) = \psi(\mathbf{r}) + \hat{\vartheta}(\mathbf{r})$, inserting it into Eq. (3.2) directly and keeping terms in $\hat{\vartheta}(\mathbf{r})$ up to second order. We can then write the resulting (grand canonical) Hamiltonian as

$$\hat{H}_{\text{gc}}(\mathbf{r}) = \hat{H}_{\text{gc},0}(\mathbf{r}) + \hat{H}_{\text{gc},1}(\mathbf{r}) + \hat{H}_{\text{gc},2}(\mathbf{r}) + \mathcal{O}(\hat{\vartheta}^3(\mathbf{r})), \quad (3.23)$$

where the index gives the order in $\hat{\vartheta}^{(\dagger)}(\mathbf{r})$ and $\mathcal{O}(\hat{\vartheta}^3(\mathbf{r}))$ represents the discarded higher-order terms. The terms themselves then become

$$\begin{aligned} \hat{H}_{\text{gc},0}(\mathbf{r}) &= \int d\mathbf{r} \psi^*(\mathbf{r}) \hat{h}_0(\mathbf{r}) \psi(\mathbf{r}) \\ &+ \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' n_0(\mathbf{r}) n_0(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}'), \end{aligned} \quad (3.24a)$$

$$\begin{aligned} \hat{H}_{\text{gc},1}(\mathbf{r}) &= \int d\mathbf{r} \psi^*(\mathbf{r}) \hat{h}_0(\mathbf{r}) \hat{\vartheta}(\mathbf{r}) \\ &+ \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' \Phi(\mathbf{r} - \mathbf{r}') \left[n_0(\mathbf{r}') \psi^*(\mathbf{r}) \hat{\vartheta}(\mathbf{r}) \right. \\ &\quad \left. + n_0(\mathbf{r}) \psi^*(\mathbf{r}') \hat{\vartheta}(\mathbf{r}') \right] + \text{h.c.}, \end{aligned} \quad (3.24b)$$

$$\begin{aligned} \hat{H}_{\text{gc},2}(\mathbf{r}) &= \int d\mathbf{r} \hat{\vartheta}^\dagger(\mathbf{r}) \hat{h}_0(\mathbf{r}) \hat{\vartheta}(\mathbf{r}) \\ &+ \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' \Phi(\mathbf{r} - \mathbf{r}') \left[n_0(\mathbf{r}) \hat{\vartheta}^\dagger(\mathbf{r}') \hat{\vartheta}(\mathbf{r}') \right. \\ &\quad + n_0(\mathbf{r}') \hat{\vartheta}^\dagger(\mathbf{r}) \hat{\vartheta}(\mathbf{r}) + \psi^*(\mathbf{r}) \psi(\mathbf{r}') \hat{\vartheta}^\dagger(\mathbf{r}') \hat{\vartheta}(\mathbf{r}) \\ &\quad + \psi^*(\mathbf{r}') \psi(\mathbf{r}) \hat{\vartheta}^\dagger(\mathbf{r}) \hat{\vartheta}(\mathbf{r}') \\ &\quad \left. + \psi^*(\mathbf{r}) \psi^*(\mathbf{r}') \hat{\vartheta}(\mathbf{r}') \hat{\vartheta}(\mathbf{r}) + \psi(\mathbf{r}) \psi(\mathbf{r}') \hat{\vartheta}^\dagger(\mathbf{r}') \hat{\vartheta}^\dagger(\mathbf{r}) \right]. \end{aligned} \quad (3.24c)$$

where $|\psi(\mathbf{r})|^2 = n_0(\mathbf{r})$. As before, we only want to maintain terms of second-order in $\hat{\vartheta}^{(\dagger)}(\mathbf{r})$, so we set $\hat{H}_{\text{gc},1} = 0$. We can remove $\hat{H}_{\text{gc},1}$ by enforcing

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + \int d\mathbf{r}' n_0(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') - \mu \right) \psi(\mathbf{r}) = 0, \quad (3.25)$$

which describes the equation of state for $\hat{H}_{\text{gc},0}$ and assumes that $\Phi(\mathbf{r} - \mathbf{r}')$ is radially symmetric. Eq. (3.25) also constitutes the so-called time-independent Gross-Pitaevskii equation and is the main numerical tool used in this thesis. The time-dependent Gross-Pitaevskii equation results from Eq. (3.25) by using $\exp(-i\mu t/\hbar)$ [74] and was first independently derived by Gross [67] and Pitaevskii [68] in the study of vortices in weakly interacting Bose gases⁴. The second-order terms in $\hat{H}_{\text{gc},2}$ are sorted by their Hartree, Fock, and pair-exchange contributions in the first, second, and third lines, respectively, and as before, correspond to interactions in and out of the condensate from the remaining quantum field.

Instead of representing the fluctuation operator in single-particle plane waves and then introducing the unitary Bogoliubov transformations, we now perform both at the same time but with arbitrary single-particle wavefunctions instead:

$$\hat{\vartheta}(\mathbf{r}) = \sum_{\nu \neq 0} \left[u_{\nu}^*(\mathbf{r}) \hat{\alpha}_{\nu} - v_{\nu}(\mathbf{r}) \hat{\alpha}_{\nu}^{\dagger} \right], \quad (3.26)$$

where $\hat{\alpha}_{\nu}$ and $\hat{\alpha}_{\nu}^{\dagger}$ are again bosonic operators, which satisfy the generalized canonical relation

$$\begin{aligned} \int d\mathbf{r} [u_{\nu}^*(\mathbf{r}) u_{\nu'}(\mathbf{r}) - v_{\nu}^*(\mathbf{r}) v_{\nu'}(\mathbf{r})] &= \delta_{\nu\nu'}, \\ \int d\mathbf{r} [u_{\nu}^*(\mathbf{r}) v_{\nu'}(\mathbf{r}) - v_{\nu}^*(\mathbf{r}) u_{\nu'}(\mathbf{r})] &= 0. \end{aligned} \quad (3.27)$$

As before, we can write a diagonalized Hamiltonian in the new operators

$$\hat{H}'_{\text{gc},2} = \sum_{\nu \neq 0} E_{\nu} \hat{\alpha}_{\nu}^{\dagger} \hat{\alpha}_{\nu} + K_{\mathbf{k}} \hat{\mathbb{1}}, \quad (3.28)$$

⁴Alternatively, one can calculate the Heisenberg equation of motion for the field operator $\partial_t \hat{\Psi}(\mathbf{r}, t) = [\hat{H}, \hat{\Psi}(\mathbf{r}, t)]i/\hbar$ and then apply the Bogoliubov approximation, where one ignores quantum fluctuations [57, 59].

and calculate the Heisenberg equation of motions via $[\hat{\vartheta}(\mathbf{r}), \hat{H}_{\text{gc},2}]$ and $[\hat{\vartheta}(\mathbf{r}), \hat{H}'_{\text{gc},2}]$ to establish a set of equations, which diagonalizes $\hat{H}_{\text{gc},2}$:

$$\begin{aligned} (E_\nu(\mathbf{r}) - \hat{h}_0(\mathbf{r})) u_\nu(\mathbf{r}) &= \int d\mathbf{r}' \Phi(\mathbf{r} - \mathbf{r}') \\ &\quad \left[(n_0(\mathbf{r}') + \psi^*(\mathbf{r}')\psi(\mathbf{r})) u_\nu(\mathbf{r}) - \psi(\mathbf{r}')\psi(\mathbf{r}) v_\nu(\mathbf{r}') \right], \\ (E_\nu(\mathbf{r}) - \hat{h}_0(\mathbf{r})) v_\nu(\mathbf{r}) &= - \int d\mathbf{r}' \Phi(\mathbf{r} - \mathbf{r}') \\ &\quad \left[(n_0(\mathbf{r}') + \psi^*(\mathbf{r}')\psi(\mathbf{r})) v_\nu(\mathbf{r}) - \psi(\mathbf{r}')\psi(\mathbf{r}) u_\nu(\mathbf{r}') \right]. \end{aligned} \quad (3.29)$$

These equations constitute the so-called Bogoliubov-de Gennes [75] equations. They are, in the current integral form, difficult to solve as they require knowledge of the ground state wavefunction $\psi(\mathbf{r})$ as well as the quasi-particle amplitudes $u_\nu(\mathbf{r})$ and $v_\nu(\mathbf{r})$ at every position. We can remedy this by assuming that the Bose gas is slowly varying in space so that it can be roughly described by plane waves, which leads to the following transformations [76–78]:

$$\begin{aligned} u_\nu(\mathbf{r}) &\rightarrow u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}/\hbar}, \\ E_\nu(\mathbf{r}) &\rightarrow E_{\mathbf{k}}(\mathbf{r}), \\ \sum_\nu &\rightarrow \sum_{\mathbf{k} \neq 0}. \end{aligned} \quad (3.30)$$

The left side of Eq. (3.29) then becomes

$$\begin{aligned} (E_{\mathbf{k}}(\mathbf{r}) - \hat{h}_0(\mathbf{r})) u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}/\hbar} &= \\ \left(E_{\mathbf{k}}(\mathbf{r}) - \frac{\hbar^2 k^2}{2m} - V_{\text{ext}}(\mathbf{r}) + \mu(\mathbf{r}) \right) u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}/\hbar}. \end{aligned} \quad (3.31)$$

For the right side of Eq. (3.29) we can represent each term in the integral as $\Phi(\mathbf{r} - \mathbf{r}') X(\mathbf{r}, \mathbf{r}') q_{\mathbf{k}}(\mathbf{r}, \mathbf{r}') \exp(i\mathbf{k}\mathbf{r}'/\hbar)$, where $X(\mathbf{r}, \mathbf{r}')$ represents the factors containing $\psi(\mathbf{r})$ and $q_{\mathbf{k}}(\mathbf{r}, \mathbf{r}') \exp(i\mathbf{k}\mathbf{r}'/\hbar)$ the different quasi-particle amplitudes. Expanding $X(\mathbf{r}, \mathbf{r}') q_{\mathbf{k}}(\mathbf{r}, \mathbf{r}')$ in \mathbf{r}' around \mathbf{r} up to first order and Fourier transforming $\Phi(\mathbf{r} - \mathbf{r}')$ gives

$$\Phi(\mathbf{k}) X(\mathbf{r}) q_{\mathbf{k}}(\mathbf{r}) - i [\nabla_{\mathbf{k}} \Phi(\mathbf{k})] \nabla_{\mathbf{r}} [X(\mathbf{r}) q_{\mathbf{k}}(\mathbf{r})] + \dots \quad (3.32)$$

We can insert only the zeroth-order term if the first-order term is much smaller, leading to the validity criterion to use the so-called local density approximation

$$\frac{[\nabla_{\mathbf{k}}\Phi(\mathbf{k})] \nabla_{\mathbf{r}} [X(\mathbf{r})q_{\mathbf{k}}(\mathbf{r})]}{\Phi(\mathbf{k})X(\mathbf{r})q_{\mathbf{k}}(\mathbf{r})} \ll 1. \quad (3.33)$$

In this case, the Bogoliubov de-Gennes equations⁵ become

$$\begin{bmatrix} \frac{\hbar^2 k^2}{2m} + \Phi(\mathbf{k})n_0(\mathbf{r}) & -\Phi(\mathbf{k})\psi^2(\mathbf{r}) \\ \Phi(\mathbf{k})\psi^{*2}(\mathbf{r}) & -\frac{\hbar^2 k^2}{2m} - \Phi(\mathbf{k})n_0(\mathbf{r}) \end{bmatrix} \begin{bmatrix} u_{\mathbf{k}}(\mathbf{r}) \\ v_{\mathbf{k}}(\mathbf{r}) \end{bmatrix} = E_{+\mathbf{k}}(\mathbf{r}) \begin{bmatrix} u_{\mathbf{k}}(\mathbf{r}) \\ v_{\mathbf{k}}(\mathbf{r}) \end{bmatrix} \quad (3.34)$$

which represents the same eigenvalue problem as in Eq. (3.13) but with $\psi \rightarrow \psi(\mathbf{r})$ and $q_{\mathbf{k}} \rightarrow q_{\mathbf{k}}(\mathbf{r})$. This means that we can treat any spatially modulated system in which the interaction is symmetric under position exchange, locally as an infinite, uniform system as long as the criterion in Eq. (3.33) is valid. We can then still use our previously developed procedure of the uniform, infinite Bose gas in future chapters and transform any global quantity to a local one post hoc.

3.3 One-Component Systems

So far, we have omitted any specifics of the interaction potential Φ besides that it needs to be symmetric under position exchange. While many different interaction types are possible in modern experimental setups, such as short-range only, short-range and long-range interactions such as dipolar [86] or Rydberg [87, 88] interactions, or contact interactions of a soft-core type, in this thesis, we are interested in only two kinds of interactions: short-range (so-called 'contact') and dipolar long-range. In the weakly interacting limit, short-range interactions can be classified by a single number a_s , the s-wave scattering length if the actual interaction potential drops off faster than $|r|^3$ (in the case of a three-dimensional system), which allows us to introduce the pseudopotential [72, 73, 89]

$$\Phi_{\text{pseudo}}(\mathbf{r}) = \frac{4\pi\hbar^2 a_s}{m} \delta(\mathbf{r}). \quad (3.35)$$

⁵The same set of equations can also be used to calculate the collective excitations under small perturbations of an existing ground state [44, 57, 59, 79–85]. We use this technique in Papers III and VI.

Note that if the system only interacts via short-range interaction, then the integral parts in Eq. (3.29) vanish due to the $\delta(\mathbf{r})$, resulting in the standard Bogoliubov-de Gennes equations.

The second type of interaction is long-range dipolar, where the two-body interaction potential between two parallel dipoles becomes [90–92]

$$\Phi_{\text{dd}}(\mathbf{r}) = \frac{C_{\text{dd}}}{4\pi|\mathbf{r}|^3} (1 - 3 \cos^2 \theta), \quad (3.36)$$

where θ is the angle between the dipole's polarization direction and \mathbf{r} making it anisotropic. The dipolar interaction strength C_{dd} is either $\mu_0\mu_{\text{dd}}^2$ for magnetic dipoles or $d_{\text{dd}}^2/\epsilon_0$ for electric dipoles. Here, μ_0 is the vacuum permeability, μ_{dd} the magnetic dipole moment, d_{dd} the electric dipole moment, and ϵ_0 the vacuum permittivity. The dipolar two-body potential $\Phi_{\text{dd}}(\mathbf{r})$ goes to zero with $|\mathbf{r}|^3$ and has higher-order contributions besides the s-wave scattering lengths, which makes it long-range. For a one-component system that exhibits both short-range and long-range dipolar interactions, the total two-body interaction potential becomes

$$\Phi(\mathbf{r}) = \frac{4\pi\hbar^2 a_s}{m} \delta(\mathbf{r}) + \frac{C_{\text{dd}}}{4\pi|\mathbf{r}|^3} (1 - 3 \cos^2 \theta), \quad (3.37)$$

which has the Fourier transform [93]

$$\Phi(\mathbf{k}) = \frac{4\pi\hbar^2 a_s}{m} + \frac{C_{\text{dd}}}{3} (3 \cos^2 \alpha - 1). \quad (3.38)$$

Here α is the angle between \mathbf{k} and the dipole polarization. The ground state energy contribution of the two-body interaction is then given by

$$E_{\text{gc},0} = \frac{1}{2} n_0^2 \Phi(|\mathbf{k}|=0) = n_0^2 \frac{2\pi\hbar^2 a_s}{m} [1 + \epsilon_{\text{dd}} (3 \cos^2 \alpha - 1)]. \quad (3.39)$$

When using $\Phi(\mathbf{k})$ in K to get the quantum fluctuation contribution to the ground state energy, we transform the discrete sum over \mathbf{k} into a continuous integral in the thermodynamic limit

$$K = \frac{V}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left[E_{\mathbf{k}} - \frac{\hbar^2 k^2}{2m} - n_0 \Phi(\mathbf{k}) \right]. \quad (3.40)$$

However, we integrate with $\mathbf{k} \rightarrow \infty$, which violates the weakly interacting limit for high momenta. As such, the integral diverges in the ultraviolet, and we calculate the scattering amplitude at low momenta up to second order in the Born-approximation [89]:

$$\begin{aligned} K &= \frac{V}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left[E_{\mathbf{k}} - \frac{\hbar^2 k^2}{2m} - n_0 \Phi(\mathbf{k}) + \frac{\Phi(\mathbf{k})}{k^2} \frac{2mn_0^2}{\hbar^2} \right] \\ &= \frac{V\hbar^2}{m} \frac{128}{15} \sqrt{a_s^5 n_0^5 \pi} \mathcal{Q}_5(\epsilon_{\text{dd}}). \end{aligned} \quad (3.41)$$

Here $\mathcal{Q}_l(\epsilon_{\text{dd}})$ comes from the polar-angle part of the momentum integration defined as

$$\mathcal{Q}_l(x) = \int_0^1 du [1 + x(3u^2 - 1)]^{l/2}. \quad (3.42)$$

The time-independent Gross-Pitaevskii equation in the local density approximation then becomes

$$\begin{aligned} \left(\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) - \mu + gn_0(\mathbf{r}) + \int d\mathbf{r}' n_0(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \right. \\ \left. + \frac{128}{3} \frac{\hbar^2 \sqrt{a_s^5 \pi}}{m} \mathcal{Q}_5(\epsilon_{\text{dd}}) n_0^{3/2} \right) \psi(\mathbf{r}) = 0. \end{aligned} \quad (3.43)$$

Note that while the mean-field level dipolar term is anisotropic, the beyond mean-field correction in the local density approximation is not. This isotropy is due to the expansion in Eq. (3.33) and following inclusion of only the zeroth order term in the local density approximation, which only becomes anisotropic in the first term due to $\nabla_{\mathbf{k}} \Phi(\mathbf{k})$.

Additionally, $\mathcal{Q}_l(x)$ acquires an imaginary part when $x > 1$, which leads to a phonon instability in the system's phase resulting from the modes in Eq. (3.15) becoming imaginary for low \mathbf{k} when ϵ_{dd} becomes large. For systems considered in this thesis, we use $\epsilon_{\text{dd}} > 1$. However, as the imaginary part is small, we discard it for the systems considered here [94–98].

An additional benefit of keeping ϵ_{dd} small is that we may expand it to polynomial order around $\epsilon_{\text{dd}} = 0$ [96, 99]

$$\mathcal{Q}_5(\epsilon_{\text{dd}}) = 1 + \frac{3}{2}\epsilon_{\text{dd}}^2 + \frac{1}{7}\epsilon_{\text{dd}}^3 - \frac{3}{56}\epsilon_{\text{dd}}^4 + \mathcal{O}(\epsilon_{\text{dd}}^5). \quad (3.44)$$

The expansion of $\mathcal{Q}_5(\epsilon_{\text{dd}})$ simplifies numerical implementation as well as analytical variational calculations, where one commonly keeps terms up to the second order, which permits only small deviations from the full expression.

Lastly, let us look at the depletion density in Eq. (3.21). For the contact and dipolar interaction, it is then equal to

$$\frac{N - N_0}{N} = \frac{3}{8\sqrt{\pi}} \sqrt{a_s^3 n} \mathcal{Q}_3(\epsilon_{\text{dd}}) \ll 1. \quad (3.45)$$

The depletion includes \mathcal{Q}_3 while the ground state energy has $l = 5$. This implies that quantum fluctuations have a much stronger effect on ground state energy than condensate depletion. In the depletion, $\sqrt{a_s^3 n}$ emerges as the leading parameter to determine whether the system is weakly interacting. One usually refers to $\sqrt{a_s^3 n}$ as the diluteness parameter. We can apply the theory presented here if the system is weakly interacting (i.e., if Eq. (3.45) holds).

3.4 Two-Component Systems

We continue with systems that consist of two distinct Bose gases in the statistical sense and derive the ground state energy contribution of the quantum fluctuations in the most general case for spinless bosons⁶. As such, each species i comes equipped with its total particle number N_i , mass m_i , and interactions between species i and j occur via the two-body interaction potential $\Phi_{ij}(\mathbf{r} - \mathbf{r}')$. The resulting second quantized (grand-canonical) Hamiltonian then reads

$$\begin{aligned} \hat{H}_{\text{gc}} = & \sum_i \int d\mathbf{r} \hat{\Psi}_i^\dagger(\mathbf{r}) (\hat{h}_{0,i} - \mu_i) \hat{\Psi}_i(\mathbf{r}) \\ & + \frac{1}{2} \sum_{ij} \iint d\mathbf{r} d\mathbf{r}' \hat{\Psi}_i^\dagger(\mathbf{r}) \hat{\Psi}_j^\dagger(\mathbf{r}') \Phi_{ij}(\mathbf{r} - \mathbf{r}') \hat{\Psi}_j(\mathbf{r}') \hat{\Psi}_i(\mathbf{r}), \end{aligned} \quad (3.46)$$

where we have assumed that the same external trap in $\hat{h}_{0,i}$ acts on both species in the same way. Utilizing the local density approximation, i.e., assuming it is safe to

⁶Most often only systems of equal masses such as different hyperfine states are considered in the literature, simplifying the following calculation considerably.

represent the system as uniform as long as it is slowly varying in space, we again write the second quantized field operators in single-particle plane waves, which transforms the system into \mathbf{k} -space:

$$\begin{aligned}\hat{H}_{\text{gc}} = & \sum_i \sum_{\mathbf{k}} \left(\frac{\hbar^2 k^2}{2m_i} - \mu_i \right) \hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},i} \\ & + \frac{1}{2V} \sum_{i,j} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}} \hat{a}_{\mathbf{k}_1 - \mathbf{q},i}^\dagger \hat{a}_{\mathbf{k}_2 + \mathbf{q},j}^\dagger \Phi_{ij}(\mathbf{q}) \hat{a}_{\mathbf{k}_2,j} \hat{a}_{\mathbf{k}_1,i}.\end{aligned}\quad (3.47)$$

As before, we separate the system into a condensed $\mathbf{k} = 0$ and non-condensed $\mathbf{k} \neq 0$ part and only keep terms up to second order in creation and annihilation operators $\hat{a}_{\mathbf{k},i}^{(\dagger)}$

$$\begin{aligned}E_{\text{gc},0} = & \frac{1}{2V} (\Phi_{11}(0)N_{0,1}^2 + \Phi_{22}(0)N_{0,2}^2 + 2\Phi_{12}(0)N_{0,1}N_{0,2}) \\ & - \mu_1 N_{0,1} - \mu_2 N_{0,2},\end{aligned}\quad (3.48a)$$

$$\begin{aligned}\hat{H}_{\text{gc},2} = & \sum_i \sum_{\mathbf{k} \neq 0} \hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},i} \left(\frac{\hbar^2 k_i^2}{2m_i} - \mu_i \right) \\ & + \frac{1}{2V} \sum_i \sum_{\mathbf{k} \neq 0} \left[2\Phi_{ii}(0)N_{0,i} \hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},i} \right. \\ & \quad \left. + \Phi_{ii}(\mathbf{k})N_{0,i} \left(2\hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},i} + \hat{a}_{-\mathbf{k},i} \hat{a}_{\mathbf{k},i} + \hat{a}_{-\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},i}^\dagger \right) \right] \\ & + \frac{1}{2V} \sum_{i \neq j} \sum_{\mathbf{k} \neq 0} \left[2\Phi_{12}(0)N_{0,i} \hat{a}_{\mathbf{k},j}^\dagger \hat{a}_{\mathbf{k},j} \right. \\ & \quad + \Phi_{12}(\mathbf{k})\sqrt{N_{0,i}N_{0,j}} \left(\hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},j} + \hat{a}_{\mathbf{k},j}^\dagger \hat{a}_{\mathbf{k},i} \right. \\ & \quad \left. \left. + \hat{a}_{-\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},j}^\dagger + \hat{a}_{-\mathbf{k},i} \hat{a}_{\mathbf{k},j} \right) \right]\end{aligned}\quad (3.48b)$$

Following Eq. (3.48a), the equation of state for component i is then

$$\mu_i = \Phi_{ii}(0)n_{0,i} + \Phi_{12}(0)n_{0,j}.\quad (3.49)$$

We can generalize the second-order term in Eq. (3.48b) to a generic quadratic Hamiltonian by setting

$$\begin{aligned}
T_{\mathbf{k},i} &= \frac{\hbar^2 k^2}{2m_i} - \mu_i + \Phi_{ii}(0)n_{0,i} + \Phi_{ii}(\mathbf{k})n_{0,i} + \Phi_{12}(0)n_{0,j}, \\
U_{\mathbf{k},i} &= \Phi_{ii}(\mathbf{k})n_{0,i}, \\
C_{\mathbf{k}} &= \Phi_{12}(\mathbf{k})\sqrt{n_{0,1}n_{0,2}},
\end{aligned} \tag{3.50}$$

resulting in the generalized Hamiltonian [64]

$$\begin{aligned}
\hat{H}_{\text{gc},2} &= \sum_i \sum_{\mathbf{k} \neq 0} T_{\mathbf{k},i} \hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},i} + \frac{U_{\mathbf{k},i}}{2} \left(\hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{-\mathbf{k},i}^\dagger + \hat{a}_{\mathbf{k},i} \hat{a}_{-\mathbf{k},i} \right) \\
&+ C_{\mathbf{k}} \left(\hat{a}_{\mathbf{k},1}^\dagger \hat{a}_{-\mathbf{k},2}^\dagger + \hat{a}_{\mathbf{k},1}^\dagger \hat{a}_{\mathbf{k},2} + \hat{a}_{\mathbf{k},1} \hat{a}_{\mathbf{k},2}^\dagger + \hat{a}_{-\mathbf{k},1} \hat{a}_{-\mathbf{k},2} \right).
\end{aligned} \tag{3.51}$$

Here, the first line represents two separate non-interacting single-component systems that can be diagonalized individually, and the second line the interaction between the two systems. Again, we want to bring this into a diagonalized form

$$\hat{H}'_{\text{gc},2} = \sum_{\mathbf{k} \neq 0} E_{\mathbf{k},\alpha} \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + E_{\mathbf{k},\beta} \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} + K_{\mathbf{k}} \hat{\mathbb{1}}, \tag{3.52}$$

where $\hat{\alpha}_{\mathbf{k}}$ and $\hat{\beta}_{\mathbf{k}}$ are the new quasi-particle operators resulting from the Bogoliubov transformations

$$\begin{aligned}
\hat{\alpha}_{\mathbf{k}} &= \sum_i (u_{\mathbf{k},i}^* \hat{a}_{\mathbf{k},i} - v_{\mathbf{k},i} \hat{a}_{-\mathbf{k},i}^\dagger), \\
\hat{\beta}_{\mathbf{k}} &= \sum_i (m_{\mathbf{k},i}^* \hat{a}_{\mathbf{k},i} - n_{\mathbf{k},i} \hat{a}_{-\mathbf{k},i}^\dagger).
\end{aligned} \tag{3.53}$$

For the two-component case, the canonical relations become

$$\begin{aligned}
\sum_i (u_{\mathbf{k},i,\alpha}^* u_{\mathbf{k},i,\beta} - v_{\mathbf{k},i,\alpha} v_{\mathbf{k},i,\beta}^*) &= \delta_{\alpha,\beta}, \\
\sum_\alpha (u_{\mathbf{k},i,\alpha}^* u_{\mathbf{k},j,\alpha} - v_{\mathbf{k},i,\alpha} v_{\mathbf{k},j,\alpha}^*) &= \delta_{i,j}, \\
\sum_i (u_{\mathbf{k},i,\alpha}^* v_{\mathbf{k},i,\beta} - v_{\mathbf{k},i,\alpha}^* u_{\mathbf{k},i,\beta}) &= 0, \\
\sum_\alpha (u_{\mathbf{k},i,\alpha}^* v_{\mathbf{k},j,\alpha} - v_{\mathbf{k},i,\alpha}^* u_{\mathbf{k},j,\alpha}) &= 0.
\end{aligned} \tag{3.54}$$

Here the i, j -index refers to the different components in \hat{H}_{gc} and the α, β -index to the different components in \hat{H}'_{gc} . For example $u_{\mathbf{k},1,\alpha} \equiv u_{\mathbf{k},1}$, $u_{\mathbf{k},1,\beta} \equiv m_{\mathbf{k},1}$, $v_{\mathbf{k},2,\beta} \equiv n_{\mathbf{k},2}$ and so on.

We again calculate the Heisenberg equation of motions for the two different Hamiltonians $[\hat{\alpha}_{\mathbf{k}}, \hat{H}_{\text{gc},2}]$ and $[\hat{\alpha}_{\mathbf{k}}, \hat{H}'_{\text{gc},2}]$ and compare coefficients before the operator terms. Here, we must be careful to compare only operators of the correct valued $\pm \mathbf{k}$, meaning we restrict the sum over \mathbf{k} to $\mathbf{k} > 0$, acquiring separate terms for $+\mathbf{k}$ and $-\mathbf{k}$. We then obtain the following linear system

$$\begin{bmatrix} T_{\mathbf{k},1} & U_{\mathbf{k},1} & C_{\mathbf{k}} & C_{\mathbf{k}} \\ -U_{\mathbf{k},1} & -T_{\mathbf{k},1} & -C_{\mathbf{k}} & -C_{\mathbf{k}} \\ C_{\mathbf{k}} & C_{\mathbf{k}} & T_{\mathbf{k},2} & U_{\mathbf{k},2} \\ -C_{\mathbf{k}} & -C_{\mathbf{k}} & -U_{\mathbf{k},2} & -T_{\mathbf{k},2} \end{bmatrix} \begin{bmatrix} u_{\mathbf{k},1} \\ v_{\mathbf{k},1} \\ u_{\mathbf{k},2} \\ v_{\mathbf{k},2} \end{bmatrix} = E_{\mathbf{k},\alpha} \begin{bmatrix} u_{\mathbf{k},1} \\ v_{\mathbf{k},1} \\ u_{\mathbf{k},2} \\ v_{\mathbf{k},2} \end{bmatrix}, \tag{3.55}$$

where $T_{\mathbf{k},i}$, $U_{\mathbf{k},i}$ and $C_{\mathbf{k}}$ are direction independent of \mathbf{k} and are real. Additionally, there is an analogous system for $E_{\mathbf{k},\beta}$. The eigenvalues $E_{\mathbf{k},\alpha}$ are then solutions to

$$\begin{aligned}
&[E_{\mathbf{k},1}^2 - E_{+\mathbf{k},\alpha}^2] [E_{\mathbf{k},2}^2 - E_{+\mathbf{k},\alpha}^2] \\
&- 4C_{\mathbf{k}}^2(T_{\mathbf{k},1} - U_{\mathbf{k},1})(T_{\mathbf{k},2} - U_{\mathbf{k},2}) = 0,
\end{aligned} \tag{3.56}$$

where we have written $E_{\mathbf{k},i}^2 = T_{\mathbf{k},i}^2 - U_{\mathbf{k},i}^2$ as the single species Bogoliubov spectrum in Eq. (3.15). Solving the eigenvalue problem gives

$$\begin{aligned}
E_{\mathbf{k},\alpha(\beta)} &= \left(\frac{E_{\mathbf{k},1}^2 + E_{\mathbf{k},2}^2}{2} \right. \\
&\quad \left. \pm \sqrt{\frac{(E_{\mathbf{k},1}^2 - E_{\mathbf{k},2}^2)^2}{4} + 4C_{\mathbf{k}}^2(T_{\mathbf{k},1} - U_{\mathbf{k},1})(T_{\mathbf{k},2} - U_{\mathbf{k},2})} \right)^{1/2},
\end{aligned} \tag{3.57}$$

where the $\hat{\alpha}_{\mathbf{k}}$ quasi-particles have the "+"-branch and $\hat{\beta}_{\mathbf{k}}$ quasi-particles the "-"-branch. We can calculate the ground state energy contribution from quantum fluctuations K as before by knowing that there are no quantum fluctuations in the vacuum state, such that $\langle 0 | \hat{H}_{\text{gc},2} | 0 \rangle = 0$:

$$K = -E_{\mathbf{k},\alpha}(|v_{\mathbf{k},1}|^2 + |v_{\mathbf{k},2}|^2) - E_{\mathbf{k},\beta}(|n_{\mathbf{k},1}|^2 + |n_{\mathbf{k},2}|^2). \quad (3.58)$$

Rewriting Eq. (3.55) we can calculate the quasi-particle amplitudes via

$$\begin{aligned} u_{\mathbf{k},1}(T_{\mathbf{k},1} - E_{\mathbf{k},\alpha}) + U_{\mathbf{k},1}v_{\mathbf{k},1} + (u_{\mathbf{k},2} + v_{\mathbf{k},2})C_{\mathbf{k}} &= 0, \\ v_{\mathbf{k},1}(T_{\mathbf{k},1} + E_{\mathbf{k},\alpha}) + U_{\mathbf{k},1}u_{\mathbf{k},1} + (u_{\mathbf{k},2} + v_{\mathbf{k},2})C_{\mathbf{k}} &= 0, \\ u_{\mathbf{k},2}(T_{\mathbf{k},2} - E_{\mathbf{k},\alpha}) + U_{\mathbf{k},2}v_{\mathbf{k},2} + (u_{\mathbf{k},1} + v_{\mathbf{k},1})C_{\mathbf{k}} &= 0, \\ v_{\mathbf{k},2}(T_{\mathbf{k},2} + E_{\mathbf{k},\alpha}) + U_{\mathbf{k},2}u_{\mathbf{k},2} + (u_{\mathbf{k},1} + v_{\mathbf{k},1})C_{\mathbf{k}} &= 0. \end{aligned} \quad (3.59)$$

From here, we can get the amplitudes in three steps. First, we show that the quasi-particle amplitudes are real. Secondly, we get an expression that relates $u_{\mathbf{k},i}$ and $v_{\mathbf{k},i}$; lastly, we use the canonical condition in Eq (3.54) to get an expression relating all four amplitudes. To show that the amplitudes are real, we multiply the first line by $u_{\mathbf{k},1}^*$ and complex conjugate the second before multiplying by $v_{\mathbf{k},1}$. After repeating the same in reverse order for the same lines, we add each pair to get the $C_{\mathbf{k}}$ -terms and recognize

$$\begin{aligned} u_{\mathbf{k},2}u_{\mathbf{k},1}^* + v_{\mathbf{k},2}u_{\mathbf{k},1}^* + u_{\mathbf{k},2}^*v_{\mathbf{k},1} + v_{\mathbf{k},2}^*v_{\mathbf{k},1} \\ = u_{\mathbf{k},2}^*u_{\mathbf{k},1} + v_{\mathbf{k},2}^*u_{\mathbf{k},1} + u_{\mathbf{k},2}v_{\mathbf{k},1}^* + v_{\mathbf{k},2}v_{\mathbf{k},1}^*, \end{aligned} \quad (3.60)$$

which can only be valid if the amplitudes are real. From subtracting the first and second (third and fourth) lines in Eq. (3.59), we get $u_{\mathbf{k},i} = k_{\mathbf{k},i}v_{\mathbf{k},i}$ with

$$k_{\mathbf{k},i} = \frac{T_{\mathbf{k},i} - U_{\mathbf{k},i} + E_{\mathbf{k},\alpha}}{T_{\mathbf{k},i} - U_{\mathbf{k},i} - E_{\mathbf{k},\alpha}}. \quad (3.61)$$

Lastly, we repeat the first steps when we showed that all amplitudes are real and accumulate terms in a way that we have two equations with equal prefactors for the $C_{\mathbf{k}}$ -terms, which gives us $|v_{\mathbf{k},1}|^2 \Lambda_{\mathbf{k}} = |v_{\mathbf{k},2}|^2$ with

$$\Lambda_{\mathbf{k}} = \frac{k_{\mathbf{k},1}^2(T_{\mathbf{k},1} - E_{\mathbf{k},\alpha}) + 2U_{\mathbf{k},1}k_{\mathbf{k},1} + T_{\mathbf{k},1} + E_{\mathbf{k},\alpha}}{k_{\mathbf{k},2}^2(T_{\mathbf{k},2} - E_{\mathbf{k},\alpha}) + 2U_{\mathbf{k},2}k_{\mathbf{k},2} + T_{\mathbf{k},2} + E_{\mathbf{k},\alpha}}. \quad (3.62)$$

Using the canonical relations in Eq. (3.54), we then find that

$$|v_{\mathbf{k},1}|^2 = [(k_{\mathbf{k},1}^2 - 1) + (k_{\mathbf{k},2}^2 - 1)\Lambda_{\mathbf{k}}]^{-1}, \quad (3.63)$$

such that,

$$|v_{\mathbf{k},1}|^2 + |v_{\mathbf{k},2}|^2 = \frac{1 + \Lambda_{\mathbf{k}}}{(k_{\mathbf{k},1}^2 - 1) + (k_{\mathbf{k},2}^2 - 1)\Lambda_{\mathbf{k}}}. \quad (3.64)$$

We notice that in these expression $C_{\mathbf{k}}$ occurs only implicitly in $E_{\mathbf{k},\alpha(\beta)}$, which allows us to simplify the quasi-particle energies to

$$E_{\mathbf{k},\alpha(\beta)} = \left(\frac{E_{\mathbf{k},1}^2 + E_{\mathbf{k},2}^2}{2} \pm \mathcal{R} \right)^{1/2}, \quad (3.65)$$

where \mathcal{R} stands for the remaining term in Eq. (3.57). Using this, and after some manipulation of Eq. (3.64), we finally arrive at

$$K_{\mathbf{k}} = \frac{1}{2} (E_{\mathbf{k},\alpha} + E_{\mathbf{k},\beta} - T_{\mathbf{k},1} - T_{\mathbf{k},2}). \quad (3.66)$$

This expression is valid for any interaction as long as it is radially symmetric and symmetric under component exchange. We could generalize this expression to even more components; however, this thesis only looks at short-range interacting two-component systems where the local density approximation is valid. In the systems considered here, the interaction strengths g_{ii} are positive, and in the following, we further assume

$$\frac{g_{12}^2}{g_{11}g_{22}} = 1 + \mathcal{O} \left(\frac{\sum_{\mathbf{k}} \langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle + \langle \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} \rangle}{N} \right), \quad (3.67)$$

where the last term gives the order of the relative depletion $(N - N_0)/N$. In contact-interacting systems $E_{\mathbf{k},\alpha(\beta)}$ then becomes

$$E_{\mathbf{k},\alpha,\beta} = \left(\frac{E_{\mathbf{k},1}^2 + E_{\mathbf{k},2}^2}{2} \right) \pm \sqrt{\frac{(E_{\mathbf{k},1}^2 - E_{\mathbf{k},2}^2)^2}{4} + 4\epsilon_{\mathbf{k},1}\epsilon_{\mathbf{k},2}g_{12}^2n_{0,1}n_{0,2}} \quad (3.68)$$

and the fluctuation correction to the ground state becomes [42, 53]

$$K = V \int \frac{d^D \mathbf{k}}{2(2\pi)^D} \left[E_{\mathbf{k},\alpha} + E_{\mathbf{k},\beta} - \frac{\hbar^2 k^2}{2m_1} - g_{11}n_1 - \frac{\hbar^2 k^2}{2m_2} - g_{22}n_2 \right]. \quad (3.69)$$

Note that the $E_{\mathbf{k},\beta}$ -branch may acquire an imaginary part for small \mathbf{k} if the interaction strengths are chosen inappropriately such that $g_{12}^2 > g_{11}g_{22}$. However, this branch also vanishes in the leading order of condition Eq. (3.67), so we can safely ignore it when working in this regime⁷. Removing this term is analogous to removing the imaginary part in the dipolar case of Eq. (3.41). Lastly, we look at the quantum depletion of the condensate, specific for each component,

$$\frac{N_i - N_{0,i}}{N_i} = \frac{\sum_{\mathbf{k} \neq 0} \langle \hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},i} \rangle}{N} = \frac{\sum_{\mathbf{k} \neq 0} (|v_{\mathbf{k},i}|^2 + |n_{\mathbf{k},i}|^2)}{N} \ll 1, \quad (3.70)$$

which we will evaluate separately for different spatial dimensions in the next section.

Above, we derived the Bogoliubov vacuum energy for two components following Refs. [42, 53, 64] for a depletion small enough to be weakly interacting. While we specialized in the contact-interacting case, the derivation is valid as long as $\Phi(\mathbf{r} - \mathbf{r}')$ is radially symmetric. We now continue with a brief overview of the specific shape of the Bogoliubov vacuum energy and condensate depletion in different dimensions [42, 53, 54] before considering systems where the usually negligible effects become important.

3.4.1 Binary Bose Mixtures in Three Dimensions

As before, we express the interaction strengths in three dimensions via the s-wave scattering length a_s , which requires using the second-order Born approximation [89] to get rid of the ultraviolet divergence for high \mathbf{k} in a weakly interacting approximation

⁷There is, however, an approach to remedy this instability by treating the attraction between the two components as a BEC-BCS cross-over and introducing a bosonic pairing term [100].

$$g_{ij} \rightarrow g_{ij} \left[1 + \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{\sqrt{m_i m_j} g_{ij}}{\hbar^2 k^2} \right], \quad (3.71)$$

where $g_{ij} = 4\pi\hbar^2 a_{s,ij} / \sqrt{m_i m_j}$ is the contact interaction strength as before. The Bogoliubov vacuum energy density $E_B = K/V$ in the most general case is then, after integration of Eq. (3.69) [42, 53, 101],

$$E_B = \frac{8}{15\pi^2} \left(\frac{m_1}{\hbar^2} \right)^{3/2} (g_{11} n_1)^{5/2} f^{(3d)} \left(\frac{m_2}{m_1}, \frac{g_{12}^2}{g_{11} g_{22}}, \frac{g_{22} n_2}{g_{11} n_1} \right), \quad (3.72)$$

where

$$f^{(3D)}(z, u, x) = \frac{15}{32} \int_0^\infty dk k^2 \left[\frac{1}{\sqrt{2}} \sum_{\pm} g_{\pm}(z, u, x) - \frac{1+z}{2z} k^2 - 1 - x + \left(1 + x^2 z + \frac{4xzu}{1+z} \right) \frac{1}{k^2} \right], \quad (3.73)$$

with

$$g_{\pm}(z, u, x) = \left(k^2 + \frac{xk^2}{z} + \frac{k^4}{4} + \frac{k^4}{4z^2} \pm \sqrt{\left(k^2 - \frac{xk^2}{z} + \frac{k^4}{4} - \frac{k^4}{4z^2} \right)^2 + \frac{4z u k^4}{z}} \right)^{1/2}. \quad (3.74)$$

This integral generally has no closed solution but results in a combination of elementary and elliptic functions⁸. However, in the case of equal masses $m_1 = m_2 = m$ we can write

$$g_{\pm}(1, u, x) = k \left(\left(1 + x + \frac{k^2}{2} \right) \pm \sqrt{(1 - x^2 + 4xu)} \right)^{1/2}$$

$$f^{(3D)}(1, u, x) = \frac{15}{32} \int_0^\infty dk k^2 \left[\frac{1}{\sqrt{2}} \sum_{\pm} g_{\pm}(1, u, x) - k^2 - 1 - x + (1 + x^2 + 2xu) \frac{1}{k^2} \right], \quad (3.75)$$

⁸See Supplemental Material of Ref. [101].

which solves to

$$E_B = \frac{8}{15\pi^2} \frac{m^4}{\hbar^3} \sum_{\pm} c_{\pm}^5, \quad (3.76)$$

with the Bogoliubov sound modes c_{\pm} given by [42, 53, 101]

$$c_{\pm}^2 = \frac{g_{11}n_1 + g_{22}n_2 \pm \sqrt{(g_{11}n_1 - g_{22}n_2)^2 + 4g_{12}^2n_1n_2}}{2m}. \quad (3.77)$$

As noted before, the c_- -branch vanishes in the for us relevant regime when $g_{12}^2 = g_{11}g_{22}$ and turns imaginary when exceeding that limit. The time-independent Gross-Pitaevskii equation then becomes

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g_{ii}n_i(\mathbf{r}) + g_{12}n_j(\mathbf{r}) + \frac{4}{3\pi^2} \frac{m^{3/2}g_{ii}}{\hbar^3} (g_{11}n_1 + g_{22}n_2)^{3/2} \right] \psi_i(\mathbf{r}) = \mu \psi_i(\mathbf{r}) \quad (3.78)$$

and the depletion in Eq. (3.70) for component i in this case becomes

$$\begin{aligned} \frac{N_i - N_{0,i}}{N_i} &= \frac{\sum_{\mathbf{k} \neq 0} (|v_{\mathbf{k},i}|^2 + |n_{\mathbf{k},i}|^2)}{N_i} \\ &= \frac{8}{3\sqrt{\pi}} a_{ii} \sqrt{a_{11}n_1 + a_{22}n_2} \ll 1 \end{aligned} \quad (3.79)$$

which reduces to Eq. (3.45) in the case for $g_{11} \sim g_{22}$, $n_1 \sim n_2$ and $\epsilon_{\text{dd}} = 0$.

As noted above, the \mathbf{k} integral has no closed solution in the $m_1 \neq m_2$ case. However, Eq. (3.72) is still numerically solvable for certain parameters. One can then use the resulting data to find a fit and obtain an approximate function. At the time of writing this thesis, an approximate expression for different masses only exists in the three-dimensional case [102],

$$E_B \approx \frac{8m_1^{3/2}(g_{11}n_1)^{5/2}}{15\pi^2\hbar^3} \left[1 + \left(\frac{m_1}{m_2} \right)^{3/5} \frac{g_{22}n_2}{g_{11}n_1} \right]^{5/2}. \quad (3.80)$$

3.4.2 Binary Bose Mixtures in Two Dimensions

When considering low-dimensional systems with $D < 3$, we must determine whether the system only appears lower-dimensional in a geometric sense or is truly lower-dimensional. In the first case, the ratio of the reduced axis (for example, the z -direction in a two-dimensional system) to the perpendicular one is small as $l_z/l_\perp \ll 1$, while collisions in the reduced axis between particles may still occur. We then refer to the system as quasi-lower dimensional. In a genuinely lower-dimensional system, this direction freezes out, and no interactions are allowed anymore with $l_z < a_s$ [57, 59]. This argument is equivalent to requiring that the energy of the confining potential is far larger than any other energy in the system, including thermal energy and the chemical potential, such that $\hbar\omega_z > \mu$ [57, 103, 104].

We start with a genuine two-dimensional system, where the short-range interaction coupling constant in two dimensions is [54]

$$g_{ij}^{(2D)} = \frac{4\pi\hbar^2}{\sqrt{m_i m_j}} \frac{1}{\ln \epsilon_{ij}/\kappa^2}, \quad (3.81)$$

with $\epsilon_{ij} = 4 \exp(-2\gamma)/a_{ij}^2$ and κ is a momentum cut-off as the two-dimensional scattering integral diverges for large momenta. For conciseness, all g_{ij} and a_{ij} in this section are to be understood as their two-dimensional version $g_{ij}^{(2D)}$ and $a_{ij}^{(2D)}$. In a system axially confined by a harmonic oscillator with oscillator length a_z , the two-dimensional scattering length a_{ij} becomes [105]

$$a_{ij} = a_z \left(2\sqrt{\frac{\pi}{B}} e^{-\gamma} \right) \exp \left(-\sqrt{\frac{\pi}{2}} \frac{a_z}{a_{ij}} \right), \quad (3.82)$$

where γ is Euler's constant and $B \approx 0.91$.

In two dimensions, the integral for the Bogoliubov vacuum energy E_B with equal masses $m_1 = m_2 = m$ then becomes [54, 101]

$$E_B^{(2D)} = \frac{1}{4\pi} \frac{m}{\hbar^2} (g_{11} n_1)^2 f^{(2D)} \left(1, \frac{g_{12}}{g_{11} g_{22}}, \frac{g_{22} n_2}{g_{11} n_1}, \frac{\kappa}{\sqrt{m_1 g_{11} n_1}} \right), \quad (3.83)$$

$$f^{(2D)}(1, u, x, \kappa) = \frac{1}{\sqrt{2}} \int_0^\kappa dk k \left[\sum_{\pm} g_{\pm}(1, u, x) - k^2 - 1 - x \right],$$

which integrates to

$$E_B^{(2D)} = \frac{1}{8\pi} \frac{m^3}{\hbar^2} \sum_{\pm} c_{\pm}^4 \ln \left(\frac{m^2 c_{\pm} \sqrt{e}}{\hbar^2 \kappa^2} \right). \quad (3.84)$$

While we can show that the system's energy is independent of the cut-off κ by $\partial(E_0 + E_B)/\partial\kappa^2 = 0$, we want to remove the cut-off dependence explicitly. For that we choose a new set of coupling constants \tilde{g}_{ij} with

$$\tilde{g}_{ij} = \frac{4\pi\hbar^2}{\sqrt{m_i m_j}} \ln \left(\frac{\epsilon_{ij}}{\Delta} \right), \quad (3.85)$$

where we choose Δ such that $\tilde{g}_{12} = \sqrt{\tilde{g}_{11}\tilde{g}_{22}}$. The scattering amplitudes \tilde{g}_{ij} and g_{ij} are related via the Born series expansion [54]

$$g_{ij} = \tilde{g}_{ij} \left[1 + \tilde{g}_{ij} \ln \left(\frac{\kappa^2}{\Delta} \right) \frac{\sqrt{m_i m_j}}{4\pi\hbar^2} \right] + \mathcal{O}(\tilde{g}_{ij}^3). \quad (3.86)$$

If κ^2 is larger but not exponentially larger than Δ , the two expressions are equivalent, and we can use both interchangeably. Otherwise we can insert it into Eq. (3.84) and keep terms in \tilde{g}_{ij} up to second order to get for $m_1 = m_2 = m$,

$$E_B = \frac{1}{8\pi} \frac{m}{\hbar^2} (\tilde{g}_{11}n_1 + \tilde{g}_{22}n_2)^2 \ln \left(\frac{m\sqrt{e}}{\hbar^2\Delta} (\tilde{g}_{11}n_1 + \tilde{g}_{22}n_2) \right). \quad (3.87)$$

The time-independent Gross-Pitaevskii equation for component i is then

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g_{ii}n_i(\mathbf{r}) + g_{12}n_j(\mathbf{r}) \right. \\ \left. + \frac{m}{4\pi\hbar^2} g_{ii} \left(\sum_i g_{ii}n_i \right) \ln \left(\frac{me}{\hbar^2\Delta} \left(\sum_i g_{ii}n_i \right) \right) \right] \psi_i(\mathbf{r}) = \mu \psi_i(\mathbf{r}), \quad (3.88)$$

which we use in Papers I and II. Lastly, we are interested when our approximations hold for a two-dimensional system such that it is weakly interacting, i.e.

$$\frac{N_i - N_{0,i}}{N_i} = \frac{\sum_{\mathbf{k} \neq 0} (|v_{\mathbf{k},i}|^2 + |n_{\mathbf{k},i}|^2)}{N_i} = \frac{g_{ii}m}{4\pi\hbar^2} \ll 1. \quad (3.89)$$

This means that the relative number of particles in the non-condensed states is independent of the density and only depends on the interaction coupling constant and the system's mass.

3.4.3 Binary Bose Mixtures in One Dimension

If a system is strongly confined in two orthogonal directions by a harmonic potential such that $l_{\perp} < a_s$, the system is one-dimensional with its scattering amplitude [106]

$$g_{ij}^{(1D)} = -\frac{2\hbar^2}{\sqrt{m_i m_j} a_{ij}^{(1D)}} \quad (3.90)$$

where $a_{ij}^{(1D)} = -a_{\perp}^2/a_{ij}$ is the one-dimensional scattering length. As in the previous section, all g_{ij} and a_{ij} are to be understood as their one-dimensional version $g_{ij}^{(1D)}$ and $a_{ij}^{(1D)}$. The Bogoliubov vacuum energy E_B for equal masses $m_1 = m_2 = m$ then becomes [54, 101]

$$E_D^{(1D)} = \frac{1}{2\pi} \frac{m}{\hbar^2} (g_{11} n_1)^{3/2} f^{(1D)} \left(1, \frac{g_{12}^2}{g_{11} g_{22}}, \frac{g_{22} n_2}{g_{11} n_1} \right) \quad (3.91)$$

$$f^{(1D)}(1, u, x) = \frac{1}{\sqrt{2}} \int_0^{\infty} dk \left[\sum_{\pm} g_{\pm}(1, u, x) - k^2 - 1 - x \right],$$

which integrates to

$$E_B = -\frac{2}{3\pi} \frac{m^2}{\hbar} \sum_{\pm} c_{\pm}^3. \quad (3.92)$$

Note that the energy has a minus sign compared to the three-dimensional case in Eq. (3.76), affecting the self-bound droplet and mixed bubble systems investigated in the next section. The time-independent Gross-Pitaevskii equation for component i in the local density approximation then becomes

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g_{ii} n_i(\mathbf{r}) + g_{12} n_j(\mathbf{r}) - \frac{m^{1/2} g_{ii}}{\pi \hbar} (g_{11} n_1 + g_{22} n_2)^{1/2} \right] \psi_i(\mathbf{r}) = \mu \psi_i(\mathbf{r}) \quad (3.93)$$

which we use in Papers III and V. Lastly, let us calculate the depletion. Here, the integral diverges to infinity for small \mathbf{k} , meaning that there technically is no Bose-Einstein condensation possible as all particles would be outside of the ground state.

Nevertheless, the Bogoliubov theory presented here accurately describes the energy of a weakly interacting one-dimensional Bose gas despite assuming a condensate [107, 108]. We can, however, introduce a lower momentum cut-off κ for the depletion integral, where we send $\kappa \rightarrow 1/\xi_{\pm}$ after integration, where $1/\xi_{\pm} = \sqrt{4c_{\pm}^2 m^2/\hbar^2}$ is the characteristic momentum-scale⁹. The depletion then becomes to zeroth-order

$$\frac{N_i - N_{0,i}}{N_i} = \frac{\sum_{\mathbf{k} \neq 0} (|v_{\mathbf{k},i}|^2 + |n_{\mathbf{k},i}|^2)}{N_i} \approx \frac{1.13}{16\sqrt{2}} \frac{\sqrt{m}}{\hbar\pi} \frac{g_{ii}}{\sqrt{g_{11}n_1 + g_{22}n_2}} \ll 1, \quad (3.94)$$

where the prefactor 1.13 approximates $\sqrt{2}(4 + \log(4/(2 - \sqrt{2})^2)) - 8$. As the depletion only depends on $\sqrt{g/n}$ in the case of $g_{11} \sim g_{22}$ and $n_1 \sim n_2$, a one-dimensional system becomes weakly interacting for high densities, contrary to the three-dimensional case.

3.5 On Droplets & Bubbles

Let us now look closer at the energy and stability of a uniform, three-dimensional, two-component system. Starting with the mean-field interaction term $E_0 = \sum_{ij} = g_{ij}n_i n_j/2$ we find that the system is mechanically stable as long as $g_{12}^2 < g_{11}g_{22}$. It undergoes phase separation [109] for $g_{12} > \sqrt{g_{11}g_{22}}$, meaning that the components will avoid occupying the same spatial region; or collapse for $g_{12} < -\sqrt{g_{11}g_{22}}$. Here, the collapse shows as a feedback process where the strongly attractive g_{12} increases the density in the center. This increase, in turn, increases the total attraction further, until in the Gross-Pitaevskii formalism, all atoms collapse onto a single point¹⁰. Suppose we were to plot the energy in the n_1 - n_2 -plane. We can then determine the eigenvectors in the n_1 - n_2 -plane by writing E_0 as $\sum_{\pm} \lambda_{\pm} n_{\pm}$, with n_{\pm} as [42, 101]

$$\begin{aligned} n_+ &= \frac{\alpha^{-1/2}n_1 + \alpha^{1/2}n_2}{\sqrt{\alpha + \alpha^{-1}}}, \\ n_- &= \frac{-\alpha^{1/2}n_1 + \alpha^{-1/2}n_2}{\sqrt{\alpha + \alpha^{-1}}}. \end{aligned} \quad (3.95)$$

⁹We will discuss the origin of this in Sec. 4.3.

¹⁰This is the regime where the Bogoliubov approximation used in this thesis loses its validity and three-body processes start taking over [110–113].

Here $\alpha = \sqrt{g_{22}/g_{11}}$ is the interaction imbalance and $n_+ > 0$, $n_L < n_- < n_R$ with $n_L = -n_+\alpha$ and $n_R = n_+/\alpha$. After rotating $E_{\text{gc},0}$ into the new coordinate system, and including the Bogoliubov vacuum energy, $E_{\text{gc},0}$ reads [101]

$$E_{\text{gc},0} = \frac{\alpha + \alpha^{-1}}{2} g n_+^2 - \mu_+ n_+ + \frac{\delta g [n_+^2 - (\alpha - \alpha^{-1}) n_+ n_- - n_-^2]}{\alpha + \alpha^{-1}} - \mu_- n_- + E_B, \quad (3.96)$$

where $\delta g = g_{12} - g$ and¹¹ $g = \sqrt{g_{11}g_{22}}$. In the case for $g_{12} = g$ the negative branch c_- vanishes as before and c_+ becomes

$$c_+^2 = g \frac{(\alpha^3 + 1)n_+ + \alpha(\alpha - 1)n_-}{\alpha\sqrt{\alpha^2 + 1}}. \quad (3.97)$$

We now want to separately distinguish between the two cases of $g_{12} = \pm g$, starting with the negative case. While we restrict ourselves to the three-dimensional case, the following analysis is also valid in two- and one-dimensional systems [54]. On the mean-field level without the Bogoliubov vacuum energy density E_B , it is energetically favorable to minimize n_+^2 and maximize n_-^2 , i.e., having the ratio $n_1/n_2 = \alpha$ constant while increasing both densities. With a total increase of both densities, while including E_B , an intricate interplay of mean field interactions which scale with $\sim n^2$ and Bogoliubov vacuum energy $\sim n^{5/2}$ occurs. As $g_{12} - g$ is slightly smaller than g , the inter-component term effectively cancels the intra-component terms on the mean field level, and the system should collapse. It can, however, be stabilized by the Bogoliubov vacuum energy, leading to a zero-pressure environment in the bulk density [42]. We thus find a minimized energy for some finite densities n_1 and n_2 , allowing for the formation of a self-bound droplet state in the case of a finite particle number [42, 45, 46, 54].

Any self-bound system will have a zero-pressure environment in the bulk. In the grand canonical ensemble, one calculates the pressure as $P = -\partial E_{\text{gc},0}/\partial V$, where we have updated the chemical potentials as $\mu_i = \partial E_{\text{gc},0}/\partial N_i$. For the mass-balanced case, this gives the equilibrium density for zero pressure as

$$n_i^{(0)} = \frac{25\pi}{1024} \left(\frac{a + a_{12}}{\alpha^{1+i}} \right)^2 [a(\alpha^{-1} + 1)]^{-5}, \quad (3.98)$$

¹¹Note that dependent on whether the Bose gas is near collapse or separation δg is in the literature often defined as $g_{12} + g$ or $g_{12} - g$ respectively.

where $a = \sqrt{a_{11}a_{22}}$ is the average three-dimensional scattering length, which gives the interaction strength as $g = 4\pi\hbar^2 a / \sqrt{m_1 m_2}$. If we look at the energy terms contributing to the ground state for one-component dipolar systems, we see that they have a similar structure as in the two-component case with short-ranged interactions. While the contact term remains repulsive, the dipolar interaction may be attractive or repulsive, depending on the polarization angle due to its anisotropy. If it is attractive enough in the direction of head-to-tails, the Bose gas may collapse. Similar to the case in mixtures, the quantum fluctuations can now stabilize the system due to the $\sim n^{5/2}$ repulsive dependency [94–98, 114–116]. While we mentioned the existence of droplets in both, the two-component contact and one-component dipolar droplet, on a mean-field level, they also result from exact methods such as Monte-Carlo methods [117, 118] or exact diagonalization. We investigate droplet formation in mixtures using the Gross-Pitaevskii formalism in Papers I and II and using exact diagonalization in Paper V.

If we apply a compressional force to the droplet, it will deform to maintain its zero-pressure environment. Due to the anisotropy in the dipolar case, however, the energy cost for a widening of the droplet becomes too large, and it becomes energetically favorable to form multiple smaller droplets when compressed in the magnetic field direction [119]. Depending on the dimensionality of the trapping environment, the droplets then align themselves in an elongated one-dimensional array [119], or a hexagonal two-dimensional array [120]¹². We study such one-dimensional arrays in a toroidal trap in Papers IV and VI.

We can gain an intuitive understanding of the ground state behavior of two-component contact-based or one-component dipolar droplets by following a variational approach using a suitable trial-wavefunction [57, 59, 91]. By substituting the wave function with its variational parameters into an energy functional, we can minimize the energy functional with respect to the variational parameters. In this way one can understand the stability diagram, the formation of the droplets and their excitations [80, 94, 95, 122, 123] and the magnetostriction of dipolar systems [124, 125]. The variational approach is also applicable for mixtures [126] and arrays of droplets [119, 127, 128]. We use the variational ansatz for a symmetric two-dimensional droplet in Paper II.

Let us now consider the regime where $g_{12} \sim g$, following Ref. [101]. Then, the rotated density n_+ is independent of the system's phase in the mean-field approximation. We can see this if we minimize the mean field part of $E_{\text{gc},0}$ with respect to n_+ , such that

¹²See Ref. [121] for an extensive review on theoretical and experimental works on the self-bound systems discussed here.

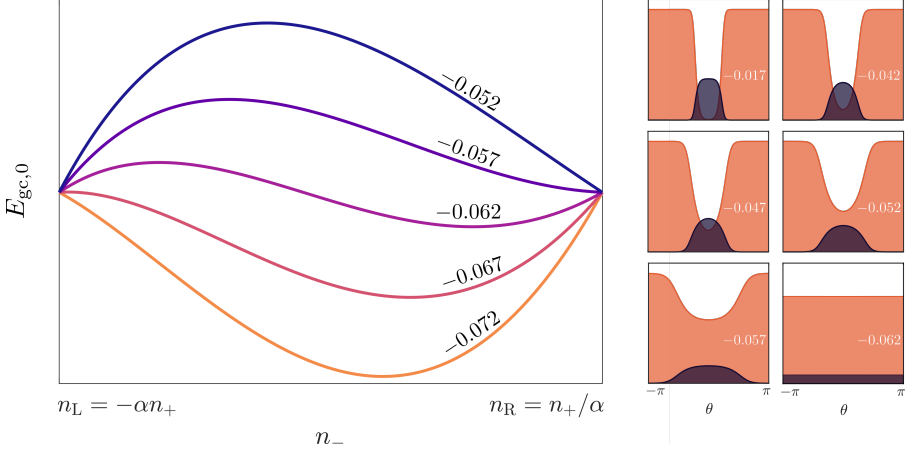


Figure 3.1: Bubble formation in a contact interacting Bose-Bose mixture: (left) Grand-canonical potential in arbitrary units as a function of n_- according to Eq. (3.96) for a one-dimensional system with $\alpha = 2.7$ and $g = 5.0$. Note that Eq. (3.96) is independent of total particle number and particle number imbalance. We chose μ_- and added an offset such that all lines have the same value at both endpoints without changing the underlying physics. (right) Density distributions for a mixed-bubble forming one-dimensional system on a ring. Note how the limits for the phase transitions of mixed-bubble formation change due to finite-size effects and $\nu = N_1/N_2 = 10 \neq \infty$ as discussed in the main text. All data were obtained by propagating Eq. (3.93) in imaginary time $\alpha = 2.7$, $g = 5.0$, $N_{\text{tot}} = N_1 + N_2 = 10^4$, $\nu = N_1/N_2 = 10$ and $\hbar = m_i = R = 1$. The parameter $\delta g \sqrt{n_+/g^3}$ is given in the respective figures.

$$n_+ = \frac{\mu_+}{g(\alpha + \alpha^{-1})} \quad (3.99)$$

and $E_{\text{gc},0}$ is then only dependent on n_- . Eq. (3.99) is the $g_{12} > 0$ analog of $n_1/n_2 = \alpha$ for the droplet formation.

The additional mean field terms with δg produce a correction of order $gn^2\eta$ where $\eta = \langle \hat{\vartheta}^\dagger \hat{\vartheta} \rangle / \langle \hat{\Psi}^\dagger \hat{\Psi} \rangle \ll 1$ is the total quantum depletion in Eq. (3.21). In the pure mean-field case, the transition is determined solely by $\delta g = g_{12} - g$. If $\delta g > 0$, the system separates, and $E_{\text{gc},0}(n_-)$ will minimize at the endpoints n_L and n_R , corresponding to fully separated components 2 and 1 respectively (see -0.052 line in Fig. 3.1). μ_- is then defined by $E_{\text{gc},0}(n_L) = E_{\text{gc},0}(n_R)$. For $\delta g < 0$ (but $g_{12} > 0$), $E_{\text{gc},0}(n_-)$ is convex and has only one minimum, resulting in a fully mixed phase, where both components share the same space (see -0.072 line in Fig. 3.1). The transition between miscibility and separation is behind two second-order phase transitions at $E'_{\text{gc},0}(n_R) = 0$ and $E'_{\text{gc},0}(n_L) = 0$. These two cases are exhaustive if we neglect the effects of quantum fluctuations.

Including E_B , however, $E_{\text{gc},0}(n_-)$ may be partially concave and convex [101] (see the three middle lines in Fig. 3.1), with the transition point in the interval $\delta g_{\text{min}} < \delta g < \delta g_{\text{max}}$. As $E''_{\text{gc},0}(n_-)$ is a monotonically increasing function, if $\alpha > 0$, the

concave region starts at n_L and ends at some n_- , which allows us to determine δg_{\min} by the emergence of the tangent point on n_L as $E''_{\text{gc},0}(n_L) \stackrel{!}{=} 0$. The upper end of the interval is then determined by whether the function is concave during the full interval as¹³ $E'_{\text{gc},0}(n_R) = (E_{\text{gc},0}(n_R) - E_{\text{gc},0}(n_L))/(n_R - n_L)$. Mixing several component-2 atoms into a large bath of component-1 atoms will lead to a uniform spread over the full system size for $\delta g < \delta g_{\min}$ (see -0.062 density plot in Fig. 3.1). Otherwise, it will either localize into a pure bubble for $\delta g > \delta g_{\max}$ (see -0.017 density plot in Fig. 3.1) or swim in a background of component 1 in between those two values. The transition from mixed to pure bubble occurs continuously, while from mixed phase to mixed bubble, it remains of first order. The boundaries of the mixed bubble phase in three dimensions are then

$$\begin{aligned} \frac{\delta g_{\min}}{\delta g} &= \frac{1}{\pi^2} \frac{(\alpha - 1)(\alpha^2 + 1)^{1/4}}{\alpha^{3/2}} \sqrt{\frac{m^3 g^3 n_+}{\hbar^3}}, \\ \frac{\delta g_{\max}}{\delta g} &= \frac{4}{15} \frac{3\alpha^{3/2} + 6\alpha + 4\alpha^{1/2} + 2}{(\sqrt{\alpha} + 1)^2} \delta g_{\min}. \end{aligned} \quad (3.100)$$

The mixed bubble phase occurs in $E_{\text{gc}}(n_-)$ and requires the fluctuation energy E_B , which depends on $(\alpha - 1)n_-$ in the rotated n_- - n_+ plane. The n_- term, however, vanishes at $\alpha = 1$, such that the n_- term vanishes together with the mixed bubble phase [101].

The above derivation for the mixed bubble is valid in the thermodynamic limit when $N_i \rightarrow \infty$, $V \rightarrow \infty$, $n_i = N_i/V = \text{const.}$ and $N_1/N_2 \rightarrow \infty$ for $\alpha > 1$. However, using the Bogoliubov-de Gennes equations for a one-dimensional system with periodic boundary conditions, we can calculate $\delta g_{\min}/\delta g$ by calculating the point of dynamic instability. Here, the lowest excitation branch acquires an imaginary part when crossing the phase transition via a critical parameter. The transition point then becomes

$$\lim_{N \rightarrow \infty} \sqrt{\frac{\hbar^2 n_+}{m}} \frac{\delta g}{g^{3/2}} = -\frac{1}{4\pi} \frac{(\alpha - 1)^2}{\sqrt{\alpha} \sqrt{\alpha^2 + 1}} \sqrt{\frac{\alpha + \nu}{\alpha^2 + \nu}}, \quad (3.101)$$

where $\nu = N_1/N_2$. Expanding this expression at $\nu \rightarrow \infty$ then recovers the original result for component 2 in a large bath of component 1 in the one-dimensional case and is a result of Paper III. One can see the difference between Eq. (3.101) and the $\nu \rightarrow \infty$ prediction in Fig. (3.1) when comparing the left panel with the right panels.

¹³This is just a Taylor expansion around n_R up to the first order. A function $f(x)$ is bounded from above by its first-order Taylor expansion if it is concave and differentiable.

Furthermore, one may modify the global mixing behavior of the system by introducing component-dependent local perturbations such as an optical lattice. Then, mixed bubbles with a size much larger than the periodicity of the lattice may form even without the inclusion of the Bogoliubov vacuum energy [129].

Chapter 4

Superfluidity

'by analogy with superconductors, [...] the helium below the λ -point enters a special state that might be called a 'superfluid''

- Kapitza, 1938 [16]

'any known formula cannot, from our data, give a value of viscosity which would have any meaning'

- Allen & Misener, 1938 [17]

Both superfluidity and superconductivity imply frictionless transport. In the case of superconductivity, this refers to the actual electrical charge, and in the case of superfluidity, to the mass of the moving particles.

In this chapter, we want to work out the phenomena associated with this frictionless flow in the context of a weakly interacting Bose gas. We start in Sec. 4.1 by reproducing Landau's criterion of superfluidity [24, 25] and specifying the two-fluid model's implications in Sec. 4.2. From here, we continue in Sec. 4.3 by extending the definition of a Bose-Einstein condensate to a macroscopic wavefunction with spontaneously broken $U(1)$ symmetry [130, 131] and global phase coherence. This immediately recovers Landau's criterion, specifically derived for a weakly interacting Bose gas. From here, we investigate in Sec. 4.4 the implications of phase coherence in the form of persistent currents and quantized vortices. Lastly, we extend this treatment in Sec. 4.5 to two components and discuss the so-called Andreev-Bashkin effect [132, 133], describing drag between superfluids.

4.1 Landau's Criterion for Superfluidity

At the beginning of the 1940s, two prevailing theoretical ideas tried to explain superfluidity. London and Tisza described it as an ideal Bose gas with the emergence of a two-fluid model for the condensed and non-condensed part [21–23]. The two-fluid model allowed each component to have its own velocity field, explaining the non-classical results in prior experiments [16–18, 134]. Landau, however, rejected the idea of relating an ideal Bose gas to superfluidity [24, 25] and pointed out that an ideal gas can not approximate the strongly interacting Helium molecules¹. To understand why interactions are necessary for superfluidity, let us follow Landau's approach and consider liquid Helium moving as an ideal Bose gas through a capillary with velocity \mathbf{v} , just like in Kapitza's experiment [16]. Additionally, we may have a frame of reference that moves with the Bose gas. In this frame of reference, the ideal gas has an energy E' , constituted by the internal energy E_0 and the kinetic energy $Mv^2/2$, where $M = Nm$ is the total mass of all particles:

$$E' = E_0 + Mv^2/2. \quad (4.1)$$

If the fluid is viscous, dissipation can occur by transferring kinetic energy into heating. Landau considered only dissipation via elementary excitations of two types of quasi-particles: phonons and rotons. It is important to understand that he postulated the existence of rotons as atomic-sized vortices based on the commutation relations of his newly quantized hydrodynamic equations [24]. For now, we ignore any specific form of quasi-particles and assume a generic excitation spectrum $E_{\mathbf{k}}$, which equals zero at all \mathbf{k} in the case of an ideal Bose gas. A single excitation in the gas will then add this energy $E_{\mathbf{k}}$ to E' . Through a Galilean transformation, the energy in the tube frame will then be

$$E'' = E_0 + Mv^2/2 + E_{\mathbf{k}} - \hbar\mathbf{k}\mathbf{v}. \quad (4.2)$$

Dissipation via elementary excitations is then favorable if $E'' < E'$, i.e., when $E_{\mathbf{k}} - \hbar\mathbf{k}\mathbf{v} < 0$. This always holds for an ideal Bose gas where $E_{\mathbf{k}} = 0$, such that it cannot support superfluidity. E'' minimizes if \mathbf{k} and \mathbf{v} are parallel, leading to the Landau critical velocity [24, 57, 59]

$$|\mathbf{v}_c| = \min_{|\mathbf{k}|} \frac{E_{\mathbf{k}}}{\hbar|\mathbf{k}|}. \quad (4.3)$$

¹London pointed this out himself in Ref. [21].

As already pointed out, an ideal gas whose particles are point-like and have no interactions, such as the ideal Bose gas as proposed by London and Tisza [21–23], will then have $E_{\mathbf{k}} = 0$ and, as such, will not be superfluid. Landau then postulated an excitation spectrum of weakly interacting quasi-particles consisting of phonons and rotons with $E_{\mathbf{k}} = c\hbar\mathbf{k}$ and $E_{\mathbf{k}} = \Delta + \hbar^2 k^2 / 2\mu$, where c is the sound velocity, μ an effective mass and Δ the minimum energy of rotons. He later modified the roton spectrum to be included in the phonon spectrum to $E_{\mathbf{k}} = \Delta + (\hbar\mathbf{k} - \hbar\mathbf{k}_0)^2 / 2\mu$ [135] to better represent the experimental data [15].

4.2 Two-Fluid Model & Second Sound

Let us now briefly return to the aforementioned two-fluid model, where each component can have its own velocity field according to

$$\mathbf{j} = \rho_s \mathbf{v}_s + \rho_n \mathbf{v}_n, \quad (4.4)$$

where \mathbf{j} is the momentum density and ρ_s and \mathbf{v}_s the superfluid density and velocity. The last term describes the normal component, which entails the system's viscosity, while the superfluid term carries zero viscosity. In Tisza's model [23], the superfluid and normal components were the Bose condensed and non-condensed parts, while in Landau's model [24, 25] they were parts without and with quasi-particles according to the description above.

A direct consequence of these separate velocity fields is their decoupling and moving in-phase and out-of-phase. When both superfluid and normal components move in-phase, this leads to the usual understanding of phononic sound waves, and we call this first sound. In the latter case, when both fields move out-of-phase, we refer to it as second sound, which can be understood as entropy or temperature waves, while the system remains undisturbed. The effect of second sound then explains the high thermal conductivity of superfluid Helium as the boiling process stops at the phase transition. Instead of diffusion, heat then moves via second sound in the system. Second sound was first measured by Peshkov in 1946 [136], while the sloshing of temperature waves has been recently visualized [137].

In this thesis, we only consider $T = 0$ K for a weakly interacting Bose gas where the normal component vanishes. Moreover, as such, one would expect no second sound in our systems. This changes, however, if the Bose gas experiences a density modulation. Here the system splits into a superfluid background, while the remaining particles can

move like a rigid body in the density modulation. We can then find an analogy of these two components with Eq. (4.4), where Ref. [138] describes the hydrodynamics in such a system. We will discuss a type of these density modulations further in Ch. 5, while we treat the resulting second sound in Paper VI.

4.3 Quasi-Averages, U(1) Symmetry Breaking & Phase Coherence

Due to the direct confirmation of the combined phonon-roton spectrum in Helium II via inelastic neutron scattering [139, 140], Landau's description quickly became the prevailing theory of superfluidity. London's and Tisza's idea still lacked a formal theoretical description [26, 55], which would eventually rely on the macroscopic order parameter we introduced in Ch. 1 and spontaneous breaking of U(1) symmetry. Both these concepts were only developed in the late 1950s [141]. Despite Bogoliubov introducing the bosonic macroscopic order parameter in Ref. [26], it took until the introduction of U(1) symmetry breaking [142–145] that both concepts together kick-started the study of weakly interacting Bose gases in connection with superfluidity². The goal of this section is now to combine Bogoliubov's work [26] with the symmetry-breaking macroscopic wavefunction in the form of Bogoliubov quasi-averages [63, 64, 146] to show that superfluidity in weakly interacting Bose gases emerges as a direct result of symmetry breaking and recovers Landau's criterion in Eq. (4.3).

In deriving the ground state properties of the weakly interacting Bose gas in Ch. 3, we used the Bogoliubov approximation and separated the system into a condensed and fluctuating part. There is a subtle detail when we assume a_0 and a_0^* to be complex numbers with an amplitude $\sqrt{N_0}$ and phase factor $\exp(\pm i\phi)$. We will now investigate how this phase factor emerges when explicitly deriving superfluidity in weakly interacting Bose gases.

Let us start with a one-component system where our general (grand canonical) Hamiltonian $\hat{H}_{gc} = \hat{H} - \mu\hat{N}$ conserves particle numbers $[\hat{H}_{gc}, \hat{N}] = 0$, and \hat{H} is the stationary one-component Hamiltonian as before. The Hamiltonian is then U(1) symmetric, which implies a degeneracy in \hat{H}_{gc} . In the Bogoliubov approximation, we can write the ground state operators $\hat{a}_0^{(\dagger)}/\sqrt{V} \sim \sqrt{n_0} \exp(\pm i\alpha)$, where α is a new arbitrary angle³, different from ϕ . Thus, in the Bogoliubov approximation, one has already assumed a ground state that spontaneously breaks U(1) symmetry.

²In fact, Bogoliubov's work mainly went under the radar [3], which lead to Lee, Huang and Yang coming to a similar result ten years later without citing Bogoliubov's work [141]. This is why the beyond mean-field energy correction is today known as the Lee-Huang-Yang correction [72].

³We now write α as we essentially want to derive the phase factor ϕ rigorously.

Let us now continue by taking the average⁴ of the operators $\langle \hat{a}_0^{(\dagger)} / \sqrt{V} \rangle$, which becomes exactly 0 due to selection rules in the occupation number basis $|n_0, \dots, n_{\mathbf{k}}, \dots\rangle$. If we treat $\hat{a}_0^{(\dagger)} / \sqrt{V}$ as a complex number and take the statistical average, this implies that we average over all α as well. Bogoliubov recognized this problem and remedied it by introducing what he called quasi-averages [63, 64, 146] $\prec \dots \succ$, such that

$$\prec \frac{\hat{a}_0^{(\dagger)}}{\sqrt{V}} \succ = \sqrt{n_0} \exp(\pm i\phi). \quad (4.5)$$

In the following, we want to introduce the concept of quasi-averages, starting from a non-interacting Hamiltonian, following Refs. [63, 64, 146]. Here, we will see that we can define quasi-averages as

$$\prec \dots \succ = \lim_{\nu \rightarrow 0} \langle \dots \rangle_{\nu, \phi}, \quad (4.6)$$

where $\langle \dots \rangle_{\nu, \phi}$ is the common average with respect to a new Hamiltonian $\hat{H}_{\nu, \phi}$ in Eq. (4.7), $\nu > 0$ some real parameter and ϕ the fixed angle of the phase factor above. As we will see later, we defined this conveniently with foresight. In general, ϕ could be some arbitrary symmetry-breaking quantity of the system under investigation and also occurs in other systems like superconductors and magnetism [63, 64].

To break U(1) symmetry, we introduce an additional term to our Hamiltonian that acts as source and drain terms and destroys the degeneracy⁵[63, 64, 146]

$$\hat{H}_{\nu, \phi} = \hat{H}_{\text{gc}} - \nu \left(\hat{a}_0^\dagger \exp(i\phi) + \hat{a}_0 \exp(-i\phi) \right) \sqrt{V}. \quad (4.7)$$

We can restore the quadratic properties of the Hamiltonian by introducing new operators \hat{a}'_0

$$\begin{aligned} \hat{a}_0 &= \hat{a}'_0 - \frac{\nu}{\mu} \exp(i\phi) \sqrt{V}, \\ \hat{a}_0^\dagger &= \hat{a}'_0{}^\dagger - \frac{\nu}{\mu} \exp(-i\phi) \sqrt{V}, \end{aligned} \quad (4.8)$$

⁴We can compute the expectation value of an operator as $\langle \hat{O} \rangle = \text{Tr}(\hat{O} \exp(-\hat{H}_{\text{gc}}/\theta)) / \text{Tr}(\exp(-\hat{H}_{\text{gc}}/\theta))$ while choosing the occupation number basis $|n_0, \dots, n_{\mathbf{k}}, \dots\rangle$ to sum over in the trace.

⁵Note that $\hat{a}_0^{(\dagger)}$ are operators again, as we now want to introduce the approximation as complex numbers formally.

while leaving the remaining $\hat{a}_{\mathbf{k}}^{(\dagger)}$ unchanged. After insertion, $\hat{H}_{\nu,\phi}$ then becomes

$$\hat{H}_{\nu,\phi} = -\mu \hat{a}_0'^{\dagger} \hat{a}_0' + \sum_{\mathbf{k} \neq 0} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \frac{\nu^2}{\mu} V. \quad (4.9)$$

Let us now calculate the average occupation number and determine the condition for a condensate:

$$\begin{aligned} \langle \hat{a}_0'^{\dagger} \rangle_{\nu,\phi} &= 0, \\ \langle \hat{a}_0'^{\dagger} \hat{a}_0' \rangle_{\nu,\phi} &= (\exp(-\beta\mu) - 1)^{-1}, \\ \langle \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} \rangle_{\nu,\phi} &= N_{\mathbf{k}} = \left(\exp \left(\beta \left(\frac{\hbar^2 k^2}{2m} - \mu \right) \right) - 1 \right)^{-1}, \end{aligned} \quad (4.10)$$

resulting in

$$N_0 = n_0 V + \langle \hat{a}_0'^{\dagger} \hat{a}_0' \rangle_{\nu,\phi}, \quad (4.11)$$

$$\frac{N}{V} = \frac{N_0}{V} + \frac{1}{V} \sum_{\mathbf{k} \neq 0} \langle \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} \rangle_{\nu,\phi}. \quad (4.12)$$

In the thermodynamic limit, $V \rightarrow \infty$ and $\nu \rightarrow 0$, this needs to recover the usual description of condensation of free bosons. At the same time, ν/μ needs to be of dimension $\sqrt{n_0}$. Thus we can write $\mu = -\nu/\sqrt{n_0}$. Taking the average $\langle \hat{a}_0'^{\dagger} \hat{a}_0'/V \rangle_{\nu,\phi}$ in the thermodynamic limit then becomes

$$\begin{aligned} \left\langle \frac{\hat{a}_0'^{\dagger} \hat{a}_0'}{V} \right\rangle &= \left\langle \left(\frac{\hat{a}_0^{\dagger}}{\sqrt{V}} - \sqrt{n_0} \exp(-i\phi) \right) \left(\frac{\hat{a}_0}{\sqrt{V}} - \sqrt{n_0} \exp(i\phi) \right) \right\rangle_{\nu,\phi} \\ &= \lim_{V \rightarrow \infty} \frac{1}{V} (\exp(\beta\nu/\sqrt{n_0}) - 1)^{-1} = 0, \end{aligned} \quad (4.13)$$

such that we have in the asymptotic limit $\hat{a}_0^{(\dagger)}/\sqrt{V} \sim \sqrt{n_0} \exp(\pm i\phi)$. It is this limit that defines the quasi-average as in Eq. (4.6), such that

$$\prec \hat{a}_0^{(\dagger)} \succ = \lim_{\nu \rightarrow 0} \langle \hat{a}_0^{(\dagger)} \rangle_{\nu,\phi}, \quad (4.14)$$

and thereby justifies writing $\hat{a}_0^{(\dagger)} \rightarrow a_0^{(*)}$. This way, for a Hamiltonian $\hat{H}_{\nu,\phi}$, the ground state amplitudes are fixed complex numbers in the limit $\nu \rightarrow 0$. Thus, the ground state spontaneously breaks the $U(1)$ symmetry in the Bogoliubov approximation by introducing the ν -term [63, 64, 146]. Let us take the limit $\nu \rightarrow 0$ after⁶ $V \rightarrow \infty$. We arrive at the usual description of condensation where, in the interacting case, the quasi-averages will also extend to the other amplitudes $\hat{a}_{\mathbf{k}}^{(\dagger)}$ besides $\hat{a}_0^{(\dagger)}$. This symmetry breaking of the ground state is called global phase coherence or global phase memory. We now want to investigate the consequences of this global phase ϕ by extending it to the local density approximation in a weakly interacting system.

In line with our local density approximation, let us assume that we still have a uniform Bose gas, but our newly acquired phase factor is position dependent $\phi \rightarrow \phi(\mathbf{r})$. Then, by using the system's translational invariance, we get

$$\hat{\Psi}(\mathbf{r}) = \frac{\exp(i\phi(\mathbf{r}))}{\sqrt{V}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} \exp\left(i \frac{\mathbf{k}\mathbf{r}}{\hbar}\right) \quad (4.15)$$

and the kinetic term in the thermodynamic and $\nu \rightarrow 0$ limit becomes

$$\sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \left(\frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 k}{2m} \nabla \phi(\mathbf{r}) + \frac{\hbar^2}{2m} (\nabla \phi(\mathbf{r}))^2 - \mu \right), \quad (4.16)$$

while the interaction term remains unchanged. If we use the current density operator⁷

$$\begin{aligned} \hat{\mathbf{j}}(\mathbf{r}) &= \frac{i\hbar}{2m} \left(\hat{\Psi}^\dagger(\mathbf{r}) \nabla \hat{\Psi}(\mathbf{r}) - \hat{\Psi}(\mathbf{r}) \nabla \hat{\Psi}^\dagger(\mathbf{r}) \right) \\ &= \frac{\hbar}{mV} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} (\mathbf{k} + \nabla \phi(\mathbf{r})), \end{aligned} \quad (4.17)$$

we can identify the velocity $\mathbf{v}(\mathbf{r}) = \langle \hat{\mathbf{j}}(\mathbf{r}) \rangle / n(\mathbf{r})$ via the current density operator expectation value $\langle \hat{\mathbf{j}}(\mathbf{r}) \rangle$ as

$$\mathbf{v}(\mathbf{r}) = \frac{\hbar}{m} \nabla \phi(\mathbf{r}), \quad (4.18)$$

⁶The non-commutativity between these two limits is sometimes seen as the defining property of spontaneous symmetry breaking [147].

⁷One can obtain the current density operator $\hat{\mathbf{j}}$ by calculating the equation of motion of the reduced one-particle density matrix.

where $\mathbf{v}(\mathbf{r})$ is the newly defined velocity of the Bose gas. The kinetic term then becomes

$$\sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \left(\frac{\hbar^2 k^2}{2m} + \hbar \mathbf{k} \mathbf{v} + \frac{1}{2} m v^2 - \mu \right). \quad (4.19)$$

After separating the system into its $\mathbf{k} = 0$ ground state and $\mathbf{k} \neq 0$ fluctuating terms, we get the ground state equation of state as $\mu = m v^2 / 2 + n_0 \Phi(0)$. While diagonalizing the fluctuating terms with the Bogoliubov transformations, we need to accurately discern between $T_{\pm \mathbf{k}} = T_{\mathbf{k}} \pm \hbar \mathbf{k} \mathbf{v}$, such that the system of equations to solve becomes

$$\begin{bmatrix} T_{\mathbf{k}} + \hbar \mathbf{k} \mathbf{v} & -U_{\mathbf{k}}^* \\ U_{\mathbf{k}}^* & -T_{\mathbf{k}} + \hbar \mathbf{k} \mathbf{v} \end{bmatrix} \begin{bmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{bmatrix} = E_{+\mathbf{k}} \begin{bmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{bmatrix} \quad (4.20)$$

and thus, the Bogoliubov excitation spectrum in Eq. (3.15) acquires an additional $\hbar \mathbf{k} \mathbf{v}$ term to become

$$E_{+\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}} + 2\Phi(\mathbf{k})n_0)} + \hbar \mathbf{k} \mathbf{v}. \quad (4.21)$$

While the depletion of the condensate (i.e., $\langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle = \lim_{T \rightarrow 0} |v_{\mathbf{k}}|^2$) remains unchanged by the additional velocity, the quasi-particles are still required to fulfill Bose-Einstein statistics, such that their average occupation number is

$$\langle \hat{N}_{\mathbf{k}} \rangle = (\exp(\beta(E_{\mathbf{k}} + \hbar \mathbf{k} \mathbf{v})) - 1)^{-1}. \quad (4.22)$$

Here $\langle \hat{N}_{\mathbf{k}} \rangle > 0$ and as such

$$E_{\mathbf{k}} + \hbar \mathbf{k} \mathbf{v} > 0, \quad (4.23)$$

which minimizes if \mathbf{k} and \mathbf{v} are antiparallel. We then replace the vectors with absolute values using the antiparallel property and get

$$|\mathbf{v}_c| = \min_{|\mathbf{k}|} \frac{E_{\mathbf{k}}}{\hbar |\mathbf{k}|}, \quad (4.24)$$

which is exactly Landau's criterion for superfluidity in Eq. (4.3), but derived specifically for a weakly interacting Bose gas that spontaneously breaks U(1) symmetry.

We now want to investigate the excitation spectrum more, starting with a purely contact-interacting Bose gas and later including dipolar interactions. For large momenta, $E_{\mathbf{k}}$ approaches the behavior of a free particle for both cases, while at low momenta, the excitation spectrum assumes the phononic form

$$E_{\mathbf{k}} = \hbar \mathbf{k} c (1 + \dots), \quad (4.25)$$

where c is the sound velocity

$$c = \sqrt{\frac{n_0 \Phi(\mathbf{k})}{m}}. \quad (4.26)$$

The phonon mode represents a gapped excitation, where the gap equals c and is the energy of a massless Goldstone-Nambu particle associated with the spontaneous breaking of U(1) symmetry [142–145]. For a contact interacting system the sound velocity also represents the upper bound for the superfluid critical velocity. The regime in which both the free-particle spectrum and the phonon mode become equally strong defines a characteristic momentum scale $1/\xi$, where

$$\xi = \hbar / \sqrt{4mg n_0} \quad (4.27)$$

is the healing length in a one-component contact-interacting Bose gas with interaction strength g and describes the length in which it recovers from 0 to its bulk density.

In the dipolar case, while for $\mathbf{k} \rightarrow 0$ and $\mathbf{k} \rightarrow \infty$ one observes the same behavior, there can be an additional minimum, depending on ϵ_{dd} . This minimum has the same shape as the roton spectrum proposed by Landau and was consequently dubbed the roton minimum. The excitation spectrum is then not monotonically increasing anymore and provides another option for dissipation. We focus on the roton minimum specifically in Sec. 5.2.

4.4 Persistent Currents & Vortex Lines

While quantizing the hydrodynamics equations to derive a microscopic description of superfluid Helium, Landau found that the system has irrotational states separated by

some discrete energy from the ground state [24, 25]. These irrotational states are the rotons we already mentioned, and Landau described them as atomic-size vortices. We here now want to introduce irrotational flow and vorticity in a superfluid based on the velocity in Eq. (4.18) and the work on vortices by Onsager [148] and Feynman [149].

The form of the velocity in Eq. (4.18) is a direct consequence of Bose-Einstein statistics and spontaneous U(1) symmetry breaking and is independent of temperature, interaction strength, or diluteness. We can readily see that the velocity is irrotational, meaning

$$\nabla \times \mathbf{v}(\mathbf{r}, t) = \frac{\hbar}{m} \nabla \times \nabla \phi(\mathbf{r}) = 0. \quad (4.28)$$

This irrotationality forces us to only consider distinct solutions for the order parameter that permit velocity and rotation, which we will explore next.

First, we look at a system that lives on a so-called simply connected region. This is a topology where one can reduce any closed line to a single point. Following the velocity and irrotationality, we can calculate the circulation $\kappa = \oint \mathrm{d}l' \mathbf{v}(\mathbf{r})$ along such a line and see that it naturally only permits one solution - $\kappa = 0$ [57, 148, 149]. The same is valid for multiply connected regions that consist of simply connected ones, but changes if we adapt our topology to the line integral using a toroidal geometry. Evaluating the same line integral then gives a quantized circulation κ around the loop:

$$\kappa = \oint \mathrm{d}l' \mathbf{v}(\mathbf{r}) = 2\pi \frac{\hbar}{m} s, \quad (4.29)$$

where s are non-negative integers, giving states of discrete angular momentum. Because of the quantization, at least in theory, these states are meta-stable against perturbations and thus allow for so-called persistent currents [29, 150–152]. We will now continue with two explanations for this meta-stability, one brought forth by Feynman [149] based on the irrotationality requirement itself and the other by Bloch [153, 154].

Because of irrotationality, the superfluid must rotate everywhere along the line at the same speed. So if it were to lose some velocity while maintaining irrotationality, it needs to lose the same amount of velocity δv everywhere, accompanied by a change in linear momentum δp of $M\delta v$ and energy $\delta E = v\delta p$. At $T = 0$ K, this energy can only dissipate as excitations with energy $\epsilon(p)$. Assume that there is an excitation

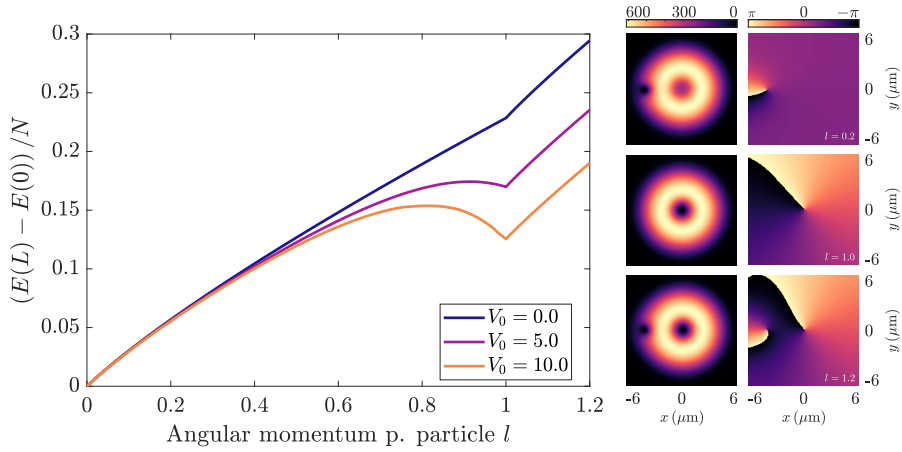


Figure 4.1: Superfluid dispersion relation for persistent current: (left) Ground state energy in units of $[\hbar^2/(39u(\mu\text{m})^2)]$ as a function of angular momentum in the laboratory frame for a contact-interacting one-component Bose gas in a harmonic trap permeated by a Gaussian as in Eq. (4.30). All data were obtained by propagating Eq. (3.25) in imaginary time for $\omega_r/(2\pi) = 178$ Hz, $\lambda = 248/178$, $N = 30 \times 10^3$, $a_s = 65a_0$ using ^{39}K atoms [155]. The Gaussian has V_0 as given in the legend and a width $w = 2.0 \mu\text{m}$. (right) Surface density plots for $V_0 = 10.0$ in the $z = 0$ -plane as $n(x, y) = \int dz n(x, y, z)$ for $l \in \{0.2, 1.0, 1.2\}$ (left column) and corresponding phase surfaces in the $z = 0$ plane (right column) for $V_0 = 10.0$. Colorbar either gives density in μm^{-3} or phase value.

Δ with momentum p_0 . Then the slowing down can only occur⁸ if $\delta E \geq \Delta \delta p/p_0$. At $T \neq 0$ K or in a non-isolated system, some excitations may be available that allow for dissipation at any velocity [149].

Let us now look at a one-dimensional torus and assume we are hypothetically allowed to violate irrotationality by giving a number N_l of particles angular momentum. Necessarily, this will not be a ground state of the system. Starting from a state where the angular momentum per particle $l = L/(N\hbar) = 0$, we give more and more particles one quantum of angular momentum until we reach some critical angular momentum l_c . Due to the associated local mass transport, the particle's movement comes at an energy cost. There will be a similar scenario if we start in the co-rotating frame of a state with $L/(N\hbar) = 1$ while finding some way to decrease the angular momentum to an angular momentum l'_c . With more particles coming to a standstill, they will lead to seemingly negative local mass transport, which comes at a similar energy cost. Naturally, the intersection point between the two scenarios is then $l_c = l'_c = 1/2$. In the co-rotating frame, the dispersion relation $E(l)$ is then a periodic function with minima at integer values of $L/(N\hbar)$, while in the lab frame the same function is engulfed by a $N\hbar^2 l^2/(2m\rho_0^2)$ function, where m is the mass of the particles and ρ_0 the radius of the torus. This argument was first brought forth rigorously in Ref. [154] and Fig. 4.1

⁸This is essentially yet another form of Landau's criterion, first formulated by Feynman and can be visualized by calculating the intersecting point between $\epsilon(p)$ and $\delta v p$ in an E-p plot.

shows the resulting dispersion relation $E(l)$. One refers to the states with the lowest energy for a given l as yrast states [156]. Note that for a two-component system, the periodicity depends on the mass imbalance between the two components [157, 158].

Fig. (4.1) shows how the persistent current develops as we move from a purely harmonic trap (simply connected region) to a toroidal geometry as we introduce a Gaussian bump with strength V_0 and width w into the harmonic trap's center:

$$V_{\text{trap}}(\rho, z) = \frac{1}{2}m\omega^2 \left((\rho^2 + \lambda^2 z^2) + V_0 \exp \left(-2\frac{\rho^2}{w} \right) \right). \quad (4.30)$$

We derived the quantization of circulation in Eq. (4.29) under the assumption that a geometry exists where the condensate density vanishes at the center, allowing the phase to wind around it. However, what if the system would create such a phase singularity itself? This scenario describes the case of vortex lines, first considered by Onsager [148] and Feynman [149]. Let us assume that we manage to rotate liquid Helium in a cylindrical container with frequency Ω . The most naive assumption would be that the angular velocity ω remains constant everywhere, such that $\mathbf{v}_{\text{rb}} = \boldsymbol{\Omega} \times \mathbf{r}$ - it rotates like a rigid body. It is immediately apparent that $\nabla \times \mathbf{v}_{\text{rb}} \neq 0$, and that a superfluid thus can not rotate like a rigid body in a continuous container.

However, because the particles are bosonic and angular momentum is a good quantum number as long as the Hamiltonian remains rotational symmetric, every particle needs to carry the same angular momentum $l = \langle \hat{L}_z \rangle / (N\hbar)$. This immediately rules out rigid body rotation but allows us to continue. In a classical system, $\mathbf{L} = m\mathbf{r} \times \mathbf{v}$, such that if we set $v_\phi \propto 1/r$, angular momentum remains constant for all distances around the rotational axis. This also emerges naturally from our irrotationality argument in cylindrical coordinates. Incidentally, a velocity of this shape diverges close to $\mathbf{r} = 0$, such that any particle near the rotation axis is pushed out by centrifugal forces - leaving a hole in the center, similar to the toroidal geometry before. The distance at which the vortex core recovers the non-rotating equilibrium density is the healing length ξ in Eq. (4.27) [57, 59].

We now want to calculate the energy of such a vortex line in the lab and rotating frame and see when it becomes energetically favorable to form a vortex state. In the laboratory frame, the vortex line energy of a weakly interacting Bose gas is then given by $E_v = E_{\text{gc}}(s \neq 0) - E_{\text{gc}}(s = 0)$ where E_{gc} is $\langle \hat{H}_{\text{gc},0} \rangle$ in Eq. (3.24a) [159]

$$E_v = \frac{nm}{2} \int_0^{2\pi} \int_0^R v^2 r dr d\theta = \frac{\pi N}{m} s^2 \hbar^2 \int_0^R \frac{dr}{r} = L\pi n \frac{\hbar^2 s^2}{m} \ln \frac{R}{r_c}, \quad (4.31)$$

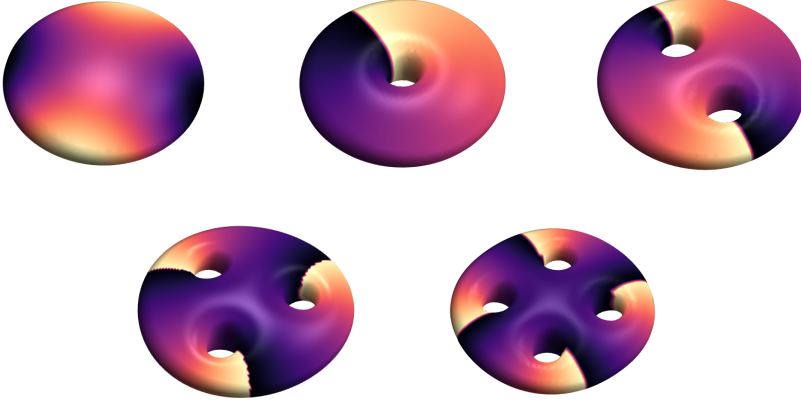


Figure 4.2: Ground state density isosurfaces for quantized vortex states: Isosurfaces with vorticity have the respective phase $\phi(\mathbf{r})$ overlaid. All data were obtained by propagating Eq. (3.25) with contact interactions including the rotation term $-\Omega\hat{L}_z$ in imaginary time for $\omega_r/(2\pi) = 178$ Hz, $\lambda = 248/178$, $N = 30 \times 10^3$, $a_s = 65a_0$ using ^{39}K atoms [155]. Isosurfaces taken at $n = 85 \times 10^{14} \text{ cm}^{-3}$.

where r_c is the vortex core size, which we introduce as a cut-off for the diverging integral.

The system can only reach equilibrium in a co-rotating frame, and as such, we need to evaluate whether a vortex state is preferable in this co-rotating frame. Following Eq. (3.22), the energy then becomes

$$E_{\text{gc}}(s \neq 0) - \Omega N \langle \hat{L}_z \rangle < E_{\text{gc}}(s = 0), \quad (4.32)$$

in other words, the energy cost E_v by introducing the vortex state needs to be smaller than the energy correction $\Omega N \langle \hat{L}_z \rangle$ in the co-rotating frame. Thus, the critical rotational frequency for a vortex state to be energetically favorable becomes

$$\Omega_{\text{cr}} = \frac{\hbar s}{mR^2} \ln \frac{R}{r_c}. \quad (4.33)$$

Due to the irrotationality condition in Eq. (4.28), the system's wavefunction is an eigenstate of the angular momentum operator, with $\langle \hat{L}_z \rangle = Ns\hbar$. This means that the system's angular momentum increases in steps of s , while E_v increases in steps of s^2 . By introducing a second vortex next to the first one, we can continue increasing the angular momentum when Ω increases, but at a lower energy cost, such that single vortices with $s > 1$ become energetically unfavorable, where in the simplest case

$E(s_1) + E(s_2) < E(s_1 + s_2)$, where we have ignored any interaction between the vortices themselves [59]. Due to the interaction, however, the vortices will align in a hexagonal pattern, commonly referred to as an Abrikosov lattice [59, 160–164]. Note that multiple singly quantized vortices will occur in harmonically trapped [165, 166], or uniform systems [159], while in anharmonic systems there may be multiply quantized vortices [167–169]. Fig. (4.2) shows an example system with up to four singly quantized vortices in a harmonic trap with their respective phase $\phi(\mathbf{r})$ overlaid if they carry angular momentum.

Furthermore, the number of vortices increases with Ω until some critical Ω' where the lattice breaks apart and enters a turbulent state [160, 170] or eventually the trap can not confine the rotating system any longer. For a weakly interacting system, this approximately mimics the scenario of a rotating spring with spring-constant k and a mass m . If the centrifugal force overcomes the spring's restoring force, the spring enters the regime of inelastic deformation, which is the case if $\Omega > \omega_c$, where ω_c is the spring's characteristic frequency. In other words, the condensate will break apart if we rotate faster than the harmonic oscillator frequency.

4.5 Three-Fluid Hydrodynamics

A big contention point in Landau's theory was that he made no statement on the type of particles required for superfluidity [24], while London and Tisza [21–23] assumed, and later Bogoliubov [26] showed that Bose statistics are crucial. A possible way to solve the scientific conflict between Landau and Tisza was to cool down fermionic ^3He . If it condenses and shows the same properties as ^4He , superfluidity would be independent of particle statistics.

Eventually, Bardeen, Baym, and Pines found [171] that at sufficiently low temperatures (in the order of mK), ^3He atoms may undergo a phase transition and start forming Cooper pairs, leading to the discovery of pure ^3He transitioning to a superfluid state [172–174] which then may be described as a weakly interacting Bose gas. So, while Fermions may form a superfluid, this only happens because they form bosonic Cooper-pairs, which form the superfluid [175]. This insight, in conjunction with the experimental discovery of ^3He being soluble in ^4He [171, 176], posed the question of how those two different superfluids would interact.

In analogy to Tisza's and Landau's two-fluid hydrodynamics of ^4He , one would expect some form of three-fluid hydrodynamics, describing the normal component, which, due to friction, can be described as one component for both constituents plus one superfluid component each. These types of systems, as shown by Khalatnikov [177],

Galasiewicz [178], and Mineev [179], experience a third sound similar to the first and second sounds in one-component superfluids. While first sound describes compression modes (i.e. sound waves) and second sound entropy waves, third sound describes a change in concentration between the two components.

Andreev and Bashkin [132] noted an oddity in the above paper by Khalatnikov [177]. According to Khalatnikov, the equations of motion for both superfluids remain independent. However, due to the strong interaction between ^3He and ^4He , a ^3He atom renormalizes to a quasi-particle with an effective mass 2.3 times greater than the ^3He mass itself. The renormalization only works if the motion of the quasi-particle not only moves ^3He but also co-transport ^4He . Additionally, this mass transport does not perturb the onset of superfluidity in ^3He due to the formation of Cooper Pairs [171, 176].

Earlier, we defined the expectation value of the probability density current of a component i as $\mathbf{j}_i(\mathbf{r}) = \mathbf{v}_i(\mathbf{r})/n_i(\mathbf{r})$. By definition, this immediately excludes the above effect of mass renormalization. Andreev and Bashkin [132] found a way around this when considering exactly this problem by introducing 'superfluid densities' $\rho_{ij}^{(s)}$, where densities of equal index describe the respective component and the unequal index introduces a coupling between the two components. In a frame where the normal component is at rest, the relative momenta \mathbf{p}_i can then be written using this symmetric superfluid density matrix as

$$\begin{aligned}\mathbf{p}_1 &= \rho_{11}^{(s)}(\mathbf{v}_1 - \mathbf{v}_n) + \rho_{12}^{(s)}(\mathbf{v}_2 - \mathbf{v}_n), \\ \mathbf{p}_2 &= \rho_{22}^{(s)}(\mathbf{v}_2 - \mathbf{v}_n) + \rho_{21}^{(s)}(\mathbf{v}_1 - \mathbf{v}_n).\end{aligned}\tag{4.34}$$

Using this in the equations derived by Khalatnikov [177] gives the mass-current \mathbf{j}_i of a component i as

$$\mathbf{j}_i = \left(\rho_i - \rho_{ii}^{(s)} - \rho_{ij}^{(s)}\right) \mathbf{v}_n + \rho_{ii}^{(s)} \mathbf{v}_i + \rho_{ij}^{(s)} \mathbf{v}_j.\tag{4.35}$$

One refers to this coupling of velocities via a drag coefficient as the Andreev-Bashkin effect [132]. For the ^3He - ^4He mixture, the symmetric matrix coefficients $\rho_{ij}^{(s)}$ emerge using BCS-theory [132]; the low miscibility of both isotopes, however, makes it challenging to achieve experimentally [176].

Let us now try to model the superfluid drag effect in a two-component bosonic mixture [133]. As before, we will use the Bogoliubov approximation and a spontaneously broken $U(1)$ symmetry in both components. In the local density approximation for

an infinite uniform system in the laboratory reference frame, the field operators then become

$$\hat{\Psi}_i(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k},i} \exp\left(i\frac{\mathbf{k}\mathbf{r}}{\hbar}\right) \exp(i\phi(\mathbf{r})). \quad (4.36)$$

As with the single-component system, the interaction term remains unchanged by the inclusion of the phase factor, while the kinetic term turns into

$$\sum_{\mathbf{k}} \hat{a}_{\mathbf{k},i}^\dagger \hat{a}_{\mathbf{k},i} \left(\frac{\hbar^2 k^2}{2m_i} + \hbar \mathbf{k} \mathbf{v}_i + \frac{1}{2} m_i \mathbf{v}_i \right). \quad (4.37)$$

Following the two-component diagonalization procedure in Sec. 3.4, while paying special attention to the specific $\pm \mathbf{k}$ terms, we end up with a similar set of equations to Eq. (3.59)

$$\begin{bmatrix} T_{+\mathbf{k},1} & U_{\mathbf{k},1} & C_{\mathbf{k}} & C_{\mathbf{k}} \\ -U_{\mathbf{k},1} & -T_{-\mathbf{k},1} & -C_{\mathbf{k}} & -C_{\mathbf{k}} \\ C_{\mathbf{k}} & C_{\mathbf{k}} & T_{+\mathbf{k},2} & T_{\mathbf{k},2} \\ -C_{\mathbf{k}} & -C_{\mathbf{k}} & -U_{\mathbf{k},2} & -T_{-\mathbf{k},2} \end{bmatrix} \begin{bmatrix} u_{\mathbf{k},1} \\ v_{\mathbf{k},1} \\ u_{\mathbf{k},2} \\ v_{\mathbf{k},2} \end{bmatrix} = E_{+\mathbf{k},\alpha} \begin{bmatrix} u_{\mathbf{k},1} \\ v_{\mathbf{k},1} \\ u_{\mathbf{k},2} \\ v_{\mathbf{k},2} \end{bmatrix}. \quad (4.38)$$

In the case of $\mathbf{v}_1 = \mathbf{v}_2 = \mathbf{v}$ the eigenvalues simply become $E_{\mathbf{k},\alpha} + \hbar \mathbf{k} \mathbf{v}$. If however, $\mathbf{v}_1 \neq \mathbf{v}_2$, the eigenvalues are determined by the characteristic polynomial

$$\begin{aligned} & \left[(T_{\mathbf{k},1}^2 - U_{\mathbf{k},1}^2) - (E_{\mathbf{k},\alpha} - \hbar \mathbf{k} \mathbf{v}_1)^2 \right] \left[(T_{\mathbf{k},2}^2 - U_{\mathbf{k},2}^2) - (E_{\mathbf{k},\alpha} - \hbar \mathbf{k} \mathbf{v}_2)^2 \right] \\ & - 4C_{\mathbf{k}}^2 (T_{\mathbf{k},1} - U_{\mathbf{k},1})(T_{\mathbf{k},2} - U_{\mathbf{k},2}) = 0. \end{aligned} \quad (4.39)$$

This is a true quartic polynomial: None of the a_i in $\sum_{i \leq 5} a_i x^i$ is zero. While quartic polynomials are the highest-order polynomials of which an exact solution exists, these solutions are too cumbersome for any practical purpose. As a remedy we expand $E_{\mathbf{k},\alpha(\beta)}$ around small velocities $\mathbf{v}_i(\mathbf{r}) = 0$ up to second order, which gives [133]

$$\begin{aligned}
E_{\mathbf{k},\alpha}^{(2)} &= E_{\mathbf{k},\alpha} \\
&+ \frac{1}{2} \hbar \mathbf{k} \mathbf{v}_1 \left(1 + \frac{E_{\mathbf{k},1}^2 - E_{\mathbf{k},2}^2}{E_{\mathbf{k},\alpha}^2 - E_{\mathbf{k},\beta}^2} \right) + \frac{1}{2} \hbar \mathbf{k} \mathbf{v}_2 \left(1 - \frac{E_{\mathbf{k},1}^2 - E_{\mathbf{k},2}^2}{E_{\mathbf{k},\alpha}^2 - E_{\mathbf{k},\beta}^2} \right) \\
&+ \frac{2C_{\mathbf{k}}^2(T_{\mathbf{k},1} - U_{\mathbf{k},1})(T_{\mathbf{k},2} - U_{\mathbf{k},2})(3E_{\mathbf{k},\alpha}^2 + E_{\mathbf{k},\beta}^2)}{E_{\mathbf{k},\alpha}(E_{\mathbf{k},\alpha}^2 - E_{\mathbf{k},\beta}^2)^3} \hbar^2 (\mathbf{k} \mathbf{v}_1 - \mathbf{k} \mathbf{v}_2)^2,
\end{aligned} \tag{4.40}$$

$$\begin{aligned}
E_{\mathbf{k},\beta}^{(2)} &= E_{\mathbf{k},\alpha} \\
&+ \frac{1}{2} \hbar \mathbf{k} \mathbf{v}_2 \left(1 + \frac{E_{\mathbf{k},1}^2 - E_{\mathbf{k},2}^2}{E_{\mathbf{k},\alpha}^2 - E_{\mathbf{k},\beta}^2} \right) + \frac{1}{2} \hbar \mathbf{k} \mathbf{v}_1 \left(1 - \frac{E_{\mathbf{k},1}^2 - E_{\mathbf{k},2}^2}{E_{\mathbf{k},\alpha}^2 - E_{\mathbf{k},\beta}^2} \right) \\
&+ \frac{2C_{\mathbf{k}}^2(T_{\mathbf{k},1} - U_{\mathbf{k},1})(T_{\mathbf{k},2} - U_{\mathbf{k},2})(E_{\mathbf{k},\alpha}^2 + 3E_{\mathbf{k},\beta}^2)}{E_{\mathbf{k},\beta}(E_{\mathbf{k},\alpha}^2 - E_{\mathbf{k},\beta}^2)^3} \hbar^2 (\mathbf{k} \mathbf{v}_1 - \mathbf{k} \mathbf{v}_2)^2.
\end{aligned}$$

The last term in both expressions includes a $\mathbf{v}_1 \mathbf{v}_2$ mixed-term, which couples the velocities. The second and third terms turn into $\hbar \mathbf{k} \mathbf{v}_i$ and cancel later with the same terms in $T_{+\mathbf{k},i}$ in Eq. (4.37).

Following a similar argument as in Sec. 4.3, where we obtained Landau's criterion for superfluidity in a single-component Bose gas by requiring that the quasi-particles also have to follow Bose-Einstein statistics, we can get a criterion for superfluidity for a two-component system using Eq. (4.39) [r80]. The resulting critical velocity $|\mathbf{v}_{c,i}|$ for component i then also includes the Andreev-Bashking effect [r80].

To determine the drag coefficient, we calculate the current \mathbf{j}_i via

$$\mathbf{j}_i = \frac{1}{V} \frac{\partial E_{\text{gc}}}{\partial \mathbf{v}_i} = (n_i - \rho_{\text{dr}}) \mathbf{v}_i + \rho_{\text{dr}} \mathbf{v}_j, \tag{4.41}$$

where the energy E_{gc} is

$$E_{\text{gc}} = E_{\text{gc},0} + \frac{V}{2} (n_1 \mathbf{v}_1^2 + n_2 \mathbf{v}_2^2 - \rho_{\text{dr}} (\mathbf{v}_1 - \mathbf{v}_2)^2). \tag{4.42}$$

Agnostic of the specific type of interaction, the drag coefficient then becomes for arbitrary masses

$$\rho_{\text{dr}} = \frac{1}{3V} \hbar^2 \sum_{\mathbf{k}} k^2 \frac{C_{\mathbf{k}}^2(T_{\mathbf{k},1} - U_{\mathbf{k},1})(T_{\mathbf{k},2} - U_{\mathbf{k},2})}{E_{\mathbf{k},\alpha} E_{\mathbf{k},\beta} (E_{\mathbf{k},\alpha} + E_{\mathbf{k},\beta})^3}. \tag{4.43}$$

For a purely contact-interacting mixture ρ_{dr} then has the following expression:

$$\rho_{\text{dr}} = \frac{4}{3V} \sqrt{m_1 m_2} \sum_{\mathbf{k}} \frac{g_{12}^2 n_1 n_2 (\epsilon_{\mathbf{k},1} \epsilon_{\mathbf{k},2})^{3/2}}{E_{\mathbf{k},\alpha} E_{\mathbf{k},\beta} (E_{\mathbf{k},\alpha} + E_{\mathbf{k},\beta})^3}. \quad (4.44)$$

After integration in the thermodynamic limit for equal masses, Eq. (4.44) becomes for $D = 3, 2, 1$

$$\rho_{\text{dr}} V = \begin{cases} \frac{2}{45\pi^2} \frac{m^2}{\hbar^2} g_{12}^2 n_1 n_2 \frac{c_-^2 + c_+^2 + 3c_- c_+}{(c_- + c_+)^3}, & \text{for } D = 3, \\ \frac{1}{48\pi} \frac{m}{\hbar^2} g_{12}^2 n_1 n_2 \frac{c_-^4 - c_+^4 + 4c_-^2 c_+^2 \ln\left(\frac{c_+}{c_-}\right)}{(c_-^2 - c_+^2)^3}, & \text{for } D = 2, \\ \frac{1}{18\pi} \frac{1}{\hbar} g_{12}^2 n_1 n_2 \frac{1}{(c_- + c_+)^3}, & \text{for } D = 1, \end{cases} \quad (4.45)$$

where c_{\pm} are the Bogoliubov sound modes in Eq. (3.77). Eq. (4.45) monotonically increases with g_{12}^2 such that close to the self-bound droplet and mixed bubble phase, where $g_{12}^2 = g_{11}g_{22}$ and thus $c_- = 0$ Eq. (4.45) becomes

$$\rho_{\text{dr}} V = \begin{cases} \frac{2}{45\pi^2} \frac{m^2}{\hbar^2} \frac{g_{12}^2 n_1 n_2}{(g_{11}n_1 + g_{22}n_2)^{1/2}}, & \text{for } D = 3, \\ \frac{1}{48\pi} \frac{m}{\hbar^2} \frac{g_{12}^2 n_1 n_2}{g_{11}n_1 + g_{22}n_2}, & \text{for } D = 2, \\ \frac{1}{18\pi} \frac{1}{\hbar} \frac{g_{12}^2 n_1 n_2}{(g_{11}n_1 + g_{22}n_2)^{3/2}}, & \text{for } D = 1. \end{cases} \quad (4.46)$$

Similarly to the Bogoliubov vacuum energy E_{B} before, we may include one of the two Eqs. (4.45) and (4.46) to determine the equation of state and ultimately include it in the Gross-Pitaevskii equation.

Due to its relatively small size, there is no direct observation of the Andreev-Bashkin effect in a two-component weakly interacting Bose-Bose mixture. Similarly to the inclusion of the Bogoliubov vacuum energy E_{B} that leads to the discovery of self-bound droplets and dipolar supersolids if the interactions are tuned suitably, one would also expect the Andreev-Bashkin effect to be most prevalent close to those systems due to the quadratic dependence on g_{12} [133, 181]. Possible options for detection are then the

measurement of the sound velocity c [182, 183], which experiences a shift in a moving system. Alternatively, a detection via the Josephson effect in a toroidal system with two weak links [133] or measuring the current-current response function via the system's susceptibility [182] seems likely. Outside of the mean-field framework presented here, the Andreev-Bashkin occurs in exact methods such as quantum Monte Carlo [184], or matrix product states [185], which show good agreement with the Bogoliubov approximation. Lastly, while no paper in this thesis covers the Andreev-Bashkin effect, it is subject to current work by the author.

Chapter 5

Supersolidity

'In view of the small value [...] it seems highly unlikely that these effects would have been discovered by accident even if 'superfluid solids' do exist at attained temperatures.'

- Legget, 1970 [48]

The previous chapter summarizes superfluidity as frictionless flow due to bosonic particles gaining phase coherence by forming a macroscopic wavefunction where they become indistinguishable. The term supersolidity then suggests combining this global phase coherence with the rigidity of a crystalline solid. In the latter, the rigidity occurs because, in a crystal, each particle sits in localized positions in space that are distinguishable.

One of the earliest ideas to detect supersolidity was to study quantum crystals, which may have vacancies at low temperatures [47, 186, 187]. These vacancies could then behave like particles and tunnel from site to site. If the atoms are bosons, the vacancies should obey bosonic statistics and turn superfluid for low enough temperatures. It took until 2004 [188, 189] until the first potential observation in solid ^4He , which subsequently was highly controversial [190], sparking a flurry of experimental and theoretical works¹.

In keeping with the rest of this thesis, we will focus on supersolidity in ultra-cold atomic systems², particularly the dipolar kind. In the following pages, we will develop what constitutes a solid in Sec. 5.1, the origin of supersolidity in dipolar Bose gases in Sec. 5.2 and how to measure supersolidity in Sec. 5.3. Lastly, in Sec. 5.4, we

¹see Ref. [49, 191] for comprehensive and detailed reviews on the history and physics involved.

²Experimentally first achieved in 2019 in three different groups at around the same period [50–52].

investigate how much of a superfluid is in a ring supersolid, building the foundations for Papers IV and VI.

5.1 What Makes a Solid?

If we want to know how to combine the notion of a superfluid with a crystalline solid, we first need to understand what makes a solid. Here we restrict ourselves to a three-dimensional system. In the common understanding of a macroscopic crystalline solid, we will encounter some periodic density modulation $\delta n(\mathbf{r}) = \bar{n} - n(\mathbf{r})$ across a set of lattice vectors $\{\mathbf{T}_i\}$, where \bar{n} is the system's average density,

$$\bar{n} = \frac{1}{V} \int d\mathbf{r} n(\mathbf{r}). \quad (5.1)$$

Naturally, an unperturbed fluid or gas will have $\delta n(\mathbf{r}) = 0$. The periodicity in the modulation $\delta n(\mathbf{r})$ with lattice vectors $\{\mathbf{T}_i\}$ can then be written as

$$\delta n(\mathbf{r}) = \delta n(\mathbf{r} + \mathbf{T}_i). \quad (5.2)$$

Moreover, in a macroscopic sample, we call this property diagonal long-range order [49], which shows in the reduced one-particle density matrix $n_1(\mathbf{r}, \mathbf{r}')$ as periodicity occurring along its diagonal. A supersolid then needs to fulfill diagonal long-range and off-diagonal long-range orders simultaneously and spontaneously for the same set of particles.

Additionally, it is essential to stress the periodicity argument, as there are also solids with disordered structure, referred to as glasses, which in the following would then lead to superglasses [192, 193] if combined with superfluidity³. The mentioned periodicity is further required to emerge via spontaneous breaking of translational symmetry. One could imagine a setting by which $V_{\text{ext}}(\mathbf{r})$ is shaped to induce the desired lattice vectors via an optical lattice. A weakly interacting Bose gas would represent the periodic solid structure we explicitly enforce while maintaining its superfluid characteristics. This, however, does not make a supersolid.

³In fact, the early experiments had a sizeable amount of disorder in the crystal. After decreasing the disorder via annealing, the difference to a regular crystal was below the measurement error [191].

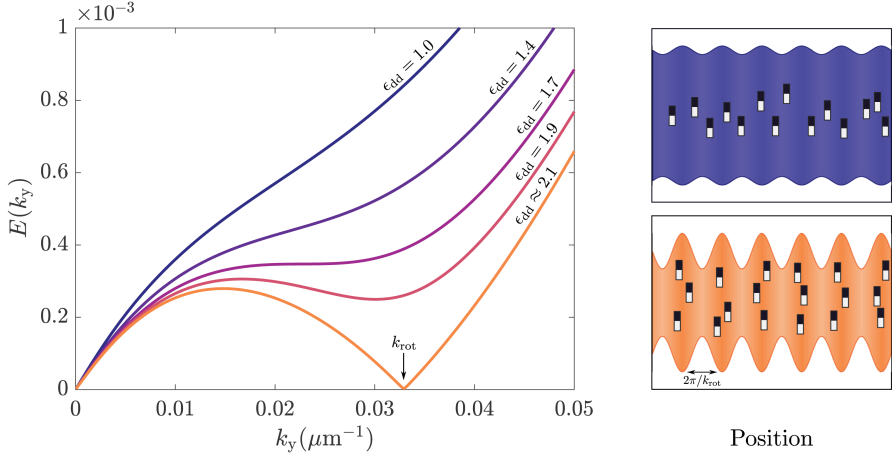


Figure 5.1: Dipolar excitation spectrum (left) and schematic density modulation (right): (left) Roton spectrum in units of $[\hbar^2/(162u(\mu\text{m})^2)]$ of a one-component dipolar Bose gas of ^{162}Dy atoms in a tube for different values of ϵ_{dd} . All data were obtained via $E_{\text{Q1D}}(k_y) = \sqrt{\epsilon(k_y)\Delta(k_y)}$, with $\Delta(k_y)$ as in Eq. (5.3), for $n = 733.0625 \mu\text{m}^{-1}$ from numerical simulations, $a_{\text{dd}} = 130a_0$, $\epsilon_{\text{dd}} = a_{\text{dd}}/a_s$, $\rho_0 = 1 \mu\text{m}$, $\omega/(2\pi) = 1 \text{ kHz}$ and $\lambda = 1.7$. (right) Schematic illustration of side-by-side alignment of dipoles (small boxes within the density) for low ϵ_{dd} (top) and head-to-tail alignment for large ϵ_{dd} (bottom), leading to a density modulation of $\lambda_{\text{rot}} = 2\pi/k_{\text{rot}}$. Figure inspired by Ref. [44].

5.2 Roton Instability & Dipolar Supersolids

We are now looking for a mechanism that spontaneously breaks translational symmetry and induces diagonal long-range order while maintaining global phase coherence. In ultra-cold gases, this has been achieved by using spin-orbit coupling [194] or by coupling to the modes of an optical cavity [195]. Here, we focus on the modern variant in dipolar gases [50–52], following the surprising observation of dipolar self-bound droplets [43, 114–116]. The culprit here is the roton-like excitation spectrum (see Fig. 5.1), where the roton is generally considered a precursor to crystallization [4, 196–198].

Eq. (3.41) gives the Bogoliubov excitation spectrum in a uniform Bose gas. This excitation spectrum changes drastically in a trapped geometry [199–203]. To illustrate the changes, let us consider a quasi-one-dimensional geometry, where we can integrate out the x - and z -direction by assuming harmonic confinement in these directions [202, 203] while leaving the gas unconfined in the y -direction with $n(\mathbf{r}) = \exp(-(\eta x^2 + z^2/\eta)/(2l^2))/(\sqrt{\pi}l)n(y)$, where $l^2 = \sqrt{\omega_x\omega_z}$ and $\eta = \sqrt{\omega_x/\omega_z}$ [202, 203]⁴. We can then write the excitation spectrum as $E_{\text{Q1D}}(k_y) = \sqrt{\epsilon(k_y)\Delta(k_y)}$,

⁴Note that this ignores the effective change of l and η by the anisotropic dipolar attractive interaction. The neglect of this change makes it a quasi-one-dimensional approximation, and one should consider l and η as variational parameters [202, 203]. The results in Fig. 5.1 without the full variational calculation are then only schematically correct, where it underestimates k_{rot} significantly.

where $\epsilon(k_y) = \hbar^2 k_y^2 / (2m)$ and

$$\Delta(k_y) = \epsilon(k_y) + 2n\tilde{U}(k_y) + 3g_{\text{QF}}n^{3/2}. \quad (5.3)$$

Here $g_{\text{QF}} = 256\hbar^2 / (15ml^3) \sqrt{a_s^5} (1 + 3/2\epsilon_{\text{dd}}^2)$ is the quantum fluctuation coefficient and

$$\tilde{U}(k_y) = \frac{2a_s\hbar^2}{ml^2} + \frac{2a_{\text{dd}}\hbar^2}{ml^2} \left(\frac{3Qe^Q \text{Ei}(-Q) + 3}{1 + \eta} - 1 \right) \quad (5.4)$$

is the two-body interaction for the field in k_y -space, where Ei is the exponential integral and $Q = \sqrt{\eta}k_y^2 l^2 / 2$ [202, 203].

At low momenta, the excitation spectrum in Eq. (5.3) increases stronger than the contact-based spectrum due to the side-by-side repulsion of the dipoles. At the same time, it approaches the free-particle limit for large momenta. The spectrum can develop a separate local maximum and minimum at intermediate values of k_y , depending on the exact values of ϵ_{dd} and n_0 . The maximum is known as the maxon, and the minimum is known as the roton in analogy to the roton spectrum of Helium II proposed by Landau [24]. In contrast to Helium, however, one can change the position k_{rot} and gap Δ of the roton minimum by modifying a_s via Feshbach resonances in an experiment with ultra-cold gases [57, 59, 204–206].

Let us now consider the case where we have a system with constant density and relatively low ϵ_{dd} such that there is no roton minimum (see $\epsilon_{\text{dd}} = 1.0$ line in Fig. 5.1). Here, the density is uniform, and excitations with finite momentum are too costly for dispersion. With increasing ϵ_{dd} , the roton minimum occurs (see $\epsilon_{\text{dd}} = 1.9$ line in Fig. 5.1) and eventually reaches $\Delta = 0$ as it deepens (see $\epsilon_{\text{dd}} \approx 2.1$ line in Fig. 5.1). The excitation modulates the ground state at zero energy cost with wavelength $\lambda_{\text{rot}} = 2\pi/k_{\text{rot}}$. This starts a feedback process where, due to the modulation, n_0 increases, pushing the spectrum into the imaginary, leading to a roton instability caused collapse⁵. Experimentally, however, the collapsing gas splits up into multiple self-bound droplets [43, 115, 116] where the quantum fluctuations in Eq. (3.41) stop the runaway process that would lead to collapse, as the repulsive term scales stronger with density than the dipole head-to-tail attraction (see Eq. (3.41)).

With $\Delta = 0$ and inclusion of the quantum fluctuation term, we have spontaneously broken translational symmetry with a wavelength of $\lambda_{\text{rot}} = 2\pi/k_{\text{rot}}$, and depending

⁵This feedback process is similar to other self-organizational processes [207–209] and fulfills all mathematical properties to be categorized as such [210, 211]. In molecular systems where a_{dd} itself is also tunable, this leads to a variety of different supersolid phases [212, 213].

on the system parameters, we either get self-bound isolated droplets [43, 114–116] or droplets that coherently couple via a background superfluid [50–52, 214].

We calculate the excitation spectrum in momentum space via the dynamic structure factor and the associated collective modes with symmetry arguments for a dipolar supersolid system on a ring in Paper VI.

5.3 Quantifying a Supersolid

One of the more startling consequences of a supersolid is the combination of the superfluid’s and solid’s response to small external rotations. Due to the superfluid’s zero viscosity, it will not respond to a small external rotation around its symmetry axis, meaning that its moment of inertia is zero. On the other hand, if set to rotate around its symmetry axis, a solid will pick up angular momentum according to its specific classical moment of inertia I_{cl} . Based on this, we can motivate the definition of a parameter describing non-classical rotational inertia (NCRI) f for a supersolid as [215]

$$f = 1 - \lim_{\Omega \rightarrow 0} \frac{I}{I_{\text{cl}}}, \quad (5.5)$$

where I is the total moment of inertia of the system. If we consider a system on a torus, $I = \lim_{\Omega \rightarrow 0} \langle \hat{L}_z \rangle / \Omega$, where Ω is the rotation frequency around its z-axis and $\langle \hat{L}_z \rangle$ the angular momentum expectation value in z . I_{cl} is the standard definition of classical moment of inertia $I_{\text{cl}} = \int d\mathbf{r} n(\mathbf{r}) r^2$. Then, for a superfluid, $f = 1$, and for a rigid body, $f = 0$. Assuming that f is neither of these values, and the system establishes diagonal long-range and off-diagonal long-range orders simultaneously and spontaneously, the system may be considered a supersolid.

In his seminal paper, Leggett [48] used the NCRI to suggest an experiment to indirectly measure supersolidity in a torsional oscillator [191]. Suppose we have a container with a supersolid above its transition temperature to a superfluid, meaning only the classical part exists. Further, suppose we set this container to small harmonic oscillations around its axis. In that case, the measurable resonant period of oscillations is then proportional to the square root of the system’s moment of inertia (vessel and substance therein). If we lower the temperature and observe the resonant period decreasing monotonously and continuously, this could be due to superfluidity emerging and the superfluid velocity field decoupling. While the vessel and solid part oscillate, the increasing superfluid part stays still. However, this may not immediately indicate a supersolid emerging, as the NCRI may lower due to any non-superfluid component,

such as a thermal one. The point that Leggett was making [48], however, is that at $T = 0$ K the NCRI can only be non-trivial if a broken translational symmetry exists, for which he derived an upper bound for f ,

$$f^u = \left(\frac{1}{C} \int_0^C \frac{dx}{n(x)/\bar{n}} \right)^{-1} \leq 1, \quad (5.6)$$

in the case of a one-dimensional ring, where we have ignored the curvature of the ring. Here $\bar{n} = 1/C \int_0^C dx n(x)$ is the average density and C the circumference of the ring. Note that one could alternatively also integrate only over a single supersolid cell. If $n(x)$ then has a density modulation, the NCRI in Eq. (5.6) subsequently lowers below 1. If there are regions where $n(x)$ almost vanishes, $f^u \rightarrow 0$, relating the separated parts to rigid motion.

The problem with measuring the NCRI is that it is a relatively ambiguous method of detecting supersolidity due to its indirectness, and several proposed mechanisms could have explained a non-trivial NCRI value in experiments with solid Helium [49]. However, in the case of a weakly interacting Bose gas, this method of detecting NCRI has been successfully combined with the scissors mode in a dipolar supersolid [216, 217].

In the previous section we have established that a supersolid features diagonal long-range order and off-diagonal long-range order simultaneously in its density matrix. While the off-diagonal long-range order will asymptotically approach n_0 for large $|\mathbf{r} - \mathbf{r}'|$, diagonal long-range order will lead to oscillatory behavior corresponding to the lattice periodicity. As such, the Fourier transform $n_1(\mathbf{k})$ shows peaks at the position of reciprocal lattice vectors. Measuring the momentum distribution, in principle, offers a way to assess whether a system is a supersolid. However, in Ch. 2, we also established that off-diagonal long-range order is a weak way of defining a Bose gas in experimentally feasible systems due to its finite size. An alternative way would be to demonstrate phase-coherence between the solid parts of the supersolid due to the underlying superfluid. Establishing phase coherence with the corresponding phase factor $\phi(\mathbf{r})$ is then equivalent to the spontaneous U(1) symmetry breaking discussed in Sec. 4.3.

For this purpose, we will choose a system in a ring geometry as in Paper IV and VI (and Ref. [214]). This geometry (or periodic boundary conditions for a 1D system) brings two main advantages. Firstly, due to its periodic nature, it is the closest experimentally feasible geometry to the infinite system we have been discussing in Ch. 3.3. In particular, this leads to a clear splitting of the collective modes in the form of an additional Goldstone mode, a Higgs mode, and a distinction between the first and

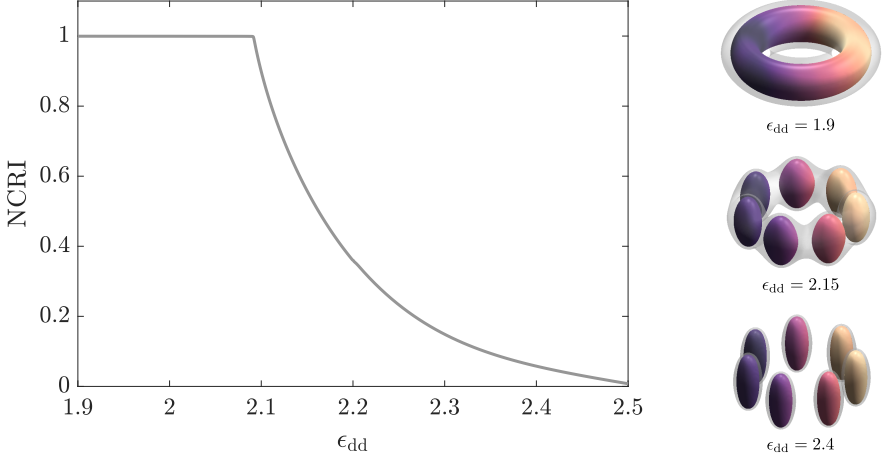


Figure 5.2: Fractional NCRI across superfluid-droplet transition: (left) Fractional NCRI as a function of ϵ_{dd} of a one-component dipolar Bose gas in a ring trap. (right) Ground state density isosurfaces for $\epsilon_{dd} \in [2.0, 2.15, 2.4]$. All data were obtained numerically by propagating Eq. (3.43) with quantum fluctuations in imaginary time for $N = 5 \times 10^3$ ^{162}Dy atoms, $a_{dd} = 130a_0$, $\epsilon_{dd} = a_{dd}/a_s$, $\rho_0 = 1 \mu\text{m}$, $\omega/(2\pi) = 1 \text{ kHz}$ and $\lambda = 1.7$. The solid and transparent isosurfaces are taken at $n = 6.5 \times 10^{14} \text{ cm}^{-3}$ and $n = 1.75 \times 10^{14} \text{ cm}^{-3}$. Figure inspired by Ref. [214].

second sound in a ring supersolid. Secondly, it offers an accessible platform to study the hallmarks of superfluidity, namely persistent currents, quantized vortex generation, and second sound. In the following subsection, we will discuss the first two hallmarks.

We start by calculating the ground state in imaginary time for $N = 5 \times 10^3$ ^{162}Dy atoms inside a ring trap $V_{\text{ring}}(\mathbf{r}) = m\omega^2[(\rho - \rho_0)^2 + \lambda^2 z^2]/2$, where ρ_0 is the radius of the ring, $\omega = 1 \text{ kHz}$ the trapping frequency and $\lambda = 1.7$ the trap-asymmetry in the azimuthal direction. The ^{162}Dy atoms have a dipolar scattering length $a_{dd} = 130a_0$, where a_0 is the Bohr radius. Experimentally we can tune the contact scattering length a_s and thereby ϵ_{dd} via Feshbach resonances [204, 206]. The system experiences two limiting cases, where for $\epsilon_{dd} \lesssim 2.09$ the system is a regular uniform Bose gas, and for large $\epsilon_{dd} \gtrsim 2.3$ ($f \lesssim 0.1$, see Fig. 5.2) the system separates into isolated droplets as explained in Sec. 3.5. The more interesting case lies between these two limits, where a Bose gas background immerses the isolated droplets, which may establish phase coherence between the droplets.

However, we first want to classify the density modulation occurring between the uniform Bose gas and isolated droplet phases. For this purpose, we use the NCRI in Eq. (5.5) adapted to the three-dimensional torus as $f = 1 - \lim_{\Omega \rightarrow 0} \langle \hat{L}_z \rangle / (NM \langle \rho^2 \rangle \Omega)$, by applying a small external rotation (numerically, $\Omega = 10^{-7} \omega$) and evaluate $\langle \hat{L}_z \rangle$ and $\langle \rho^2 \rangle$ numerically from the obtained ground state. Fig. 5.2 shows the result-

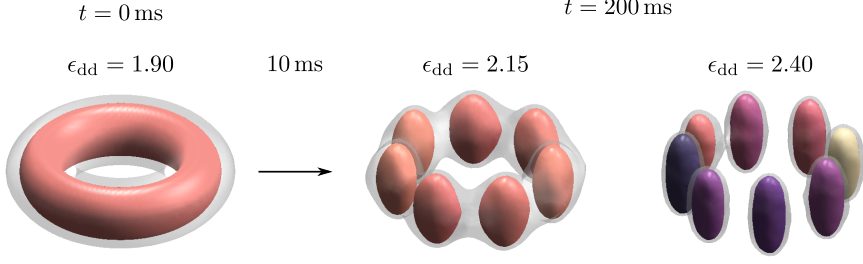


Figure 5.3: Phase coherence across superfluid-supersolid/droplet transition Isosurfaces of densities at given ϵ_{dd} and given t with phase $\phi(\mathbf{r})$ overlaid on inner isosurface. Starting from a phase-coherent superfluid ground state (left), we ramp a_s linearly within 10 ms to the target value corresponding to the respective ϵ_{dd} value. While the supersolid maintains phase coherence after 200 ms (middle), the droplets lose phase coherence (right). All data were obtained numerically by propagating Eq. (3.43) in imaginary and real time for $N = 5 \times 10^3$ ^{162}Dy atoms, $a_{dd} = 130a_0$, $\epsilon_{dd} = a_{dd}/a_s$, $\rho_0 = 1 \mu\text{m}$, $\omega/(2\pi) = 1 \text{ kHz}$ and $\lambda = 1.7$. The solid and transparent isosurfaces are taken at $n = 6.5 \times 10^{14} \text{ cm}^{-3}$ and $n = 1.75 \times 10^{14} \text{ cm}^{-3}$.

ing NCRI with density-isosurfaces. For values $\epsilon_{dd} \lesssim 2.09$ in the uniform regime, the NCRI is, as expected, equal to unity. With increasing ϵ_{dd} , a sudden jump occurs followed by a monotonous and continuous decrease in NCRI until we reach the droplet regime for $\epsilon_{dd} \gtrsim 2.3$ with $f \rightarrow 0$. Thus, we have a system with supersolid NCRI for intermediate values of ϵ_{dd} .

We now examine the phase coherence between the droplets. Interestingly, even for the isolated droplet case, all droplets are phase coherent in the ground state solution. This artifact of the time-independent Gross-Pitaevskii equation and the underlying macroscopic wavefunction ansatz changes if we dynamically induce the phase transition from the uniform ground state via an interaction quench into the desired regime. Starting from the uniform ground state at $\epsilon_{dd} = 1.9$, obtained via imaginary time propagation, we follow the protocol outlined in Ref [50–52] and ramp linearly to the target ϵ_{dd} within 10 ms. Then the picture changes and the isolated droplets have different phases, while the supersolid phase remains phase coherent as seen in Fig. 5.3.

5.4 Hallmarks of Superfluidity in a Supersolid

As we established in Sec. 4.4, the hallmarks of superfluidity are zero viscosity, leading to meta-stable persistent currents in toroidal geometries, irrotational flow, leading to quantized vortices, and a decoupling of the classic and superfluid velocity field, leading to the emergence of second sound. Here, we want to investigate the first two hallmarks, meta-stable persistent currents, and quantized vortices, building the bridge for Paper IV. In a supersolid, we may regard the solid component as the classical one in analogy with Tisza’s and Landau’s two-fluid model (see Sec. (4.2)). The second sound

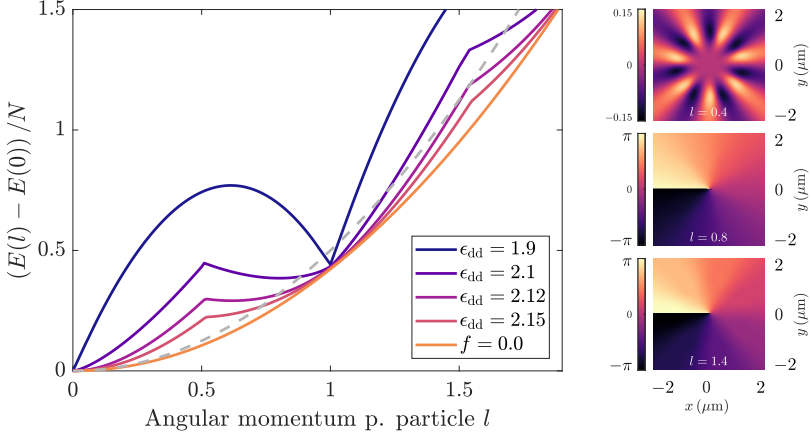


Figure 5.4: Dispersion relation comparing supersolid and superfluid: (left) Ground state energy difference per particle in units of $[\hbar^2/(162u(\mu\text{m})^2)]$ as a function of angular momentum per particle in the laboratory frame for a dipolar one-component Bose gas in a ring trap at different values of ϵ_{dd} . The dashed grey line shows Eq. (5.8) for $f = 0$ using the trap radius $\rho = 1 \mu\text{m}$. In contrast, the orange line uses the effective radius due to the long-range dipolar interaction $\sqrt{\langle r^2 \rangle} = \bar{\rho}_0 = 1.088 \mu\text{m}$. (right) Phase $\phi(x, y)$ at $z = 0$ for $l \in [0.4, 0.8, 1.4]$ and $\epsilon_{\text{dd}} = 2.12$. The color bar gives the phase value $\phi(x, y)$. All data were obtained numerically by propagating Eq. (3.43) in imaginary time for $N = 5 \times 10^3$ ^{162}Dy atoms, $a_{\text{dd}} = 130a_0$, $\epsilon_{\text{dd}} = a_{\text{dd}}/a_s$, $\rho_0 = 1 \mu\text{m}$, $\omega/(2\pi) = 1 \text{ kHz}$ and $\lambda = 1.7$.

then shows in the collective excitations of the system by an out-of-phase oscillation between the crystals and the superfluid background. This is one of the subjects of Paper VI.

We address the hallmark of meta-stable persistent currents by investigating the dispersion relation $E(l)$ in the laboratory frame, see Fig 5.4 [218], where $l = \langle \hat{L}_z \rangle / (N\hbar)$ is the angular momentum per particle as before. In the superfluid regime, the dispersion relation follows the same pattern as discussed in Sec. 4.4, namely that of a periodic function with local minima at integer values of l on top of a parabolic function representing the kinetic energy of the rotating system in the laboratory frame. The initial increase and later decrease of $E(l)$ is associated with a vortex entry into the ring.

The isolated droplet phase for $\epsilon_{\text{dd}} \gtrsim 2.3$ and $f \rightarrow 0$ then only acquires the parabolic branch $\sim l^2$ as it lacks any superfluid background. Necessarily, the supersolid phase has two options to pick up angular momentum: via rigid body rotation of the droplets and vortex entry of the superfluid. The resulting energy in the rotating frame is then [214, 218]

$$E = \frac{\hbar^2 N_s s^2}{2m\rho_0^2} + \frac{\hbar^2 N_c l_c^2}{2m\rho_0^2} + E_0, \quad (5.7)$$

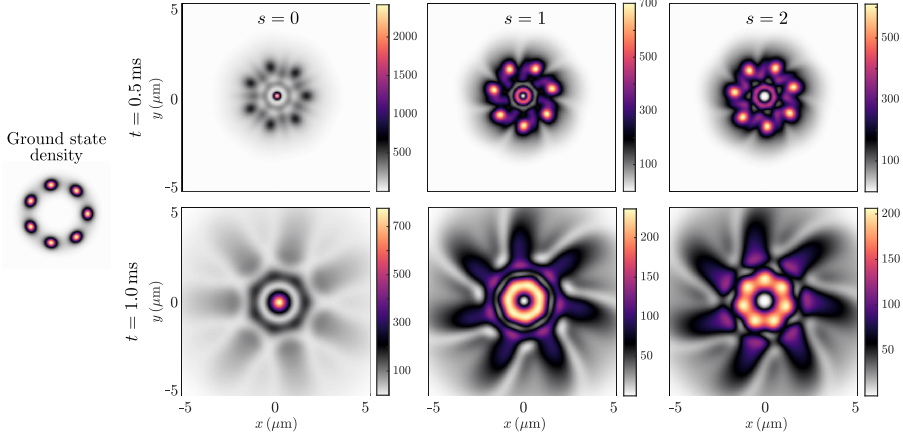


Figure 5.5: Time-of-flight expansion of supersolid with vorticity: Integrated density distributions $n(x, y) = \int dz n(x, y, z)$ for different vorticity s and times t . Systems with higher vorticity maintain a larger vortex core in the center. The color bar gives density in μm^{-3} . All data were obtained numerically by propagating Eq. (3.43) in imaginary and real time for $N = 5 \times 10^3$ ^{162}Dy atoms, $a_{\text{dd}} = 130a_0$, $\epsilon_{\text{dd}} = a_{\text{dd}}/a_s = 2.15$, $\rho_0 = 1 \mu\text{m}$, $\omega/(2\pi) = 1 \text{ kHz}$ and $\lambda = 1.7$.

where the first term describes the superfluid part with $N_s = fN$ the number of particles connected with vortex generation, s the circulation number originating from an order parameter $\sim e^{is\phi}$ and ρ_0 the system's radius. The second term describes the energy associated with rigid body rotation with $N_c = (1 - f)N$ and the classical angular momentum per particle l_c . The third term is the interaction energy, which we assume to be independent of l . We can then determine the angular momentum per particle associated with rigid body rotation l_c via $Nl = N_c l_c + N_s s$, such that

$$\frac{E(l)}{N} = \frac{\hbar^2}{m} \left[\frac{1}{2\rho_0^2} \left(fs + \frac{(l - fs)^2}{1 - f} \right) \right]. \quad (5.8)$$

The dispersion relation consists of intersecting parabolas, with intersection points at $l = s + 1/2$. Note that the intersecting branches are a general feature of the dispersion relation of a superfluid on a ring with an impurity [219]. In our case, the impurities are the self-forming droplets that interact attractively with their surrounding superfluid. The impurities may also be attractively acting particles or external potentials. Suppose we have a repulsive impurity, such as a repulsive particle, external potential [220–222], or even the localizing component in the mixed-bubble phase. In that case, the intersecting parabolas show an avoided level-crossing between the branches [220], resembling a qubit in an atomic superconducting quantum interference device (AQUID) [223–225]. As is visible in Fig 5.4, persistent currents may not appear at integer values of l in the supersolid phase compared to the superfluid phase. The local minima are then given in the interval $s - 1/2 < l < s + 1/2$ by $l = fs$, such that $f > (s - 1/2)/s$ is a requirement for the minimum to exist [218].

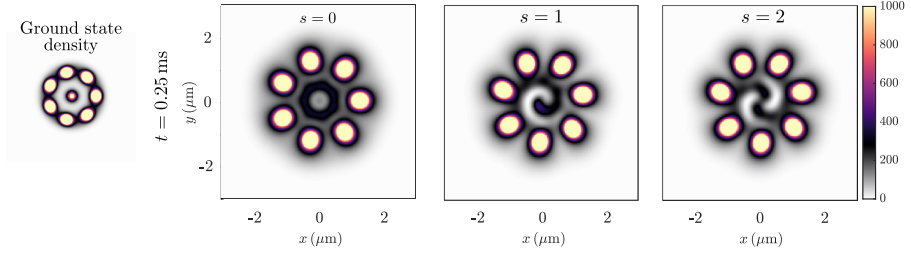


Figure 5.6: Interference pattern of supersolid with vorticity and a reference condensate: Integrated density distributions $n(x, y) = \int dz n(x, y, z)$ for different vorticity s at $t = 0.25$ s. Systems with higher vorticity maintain a larger vortex core in the center. The color bar gives density in μm^{-3} . All data were obtained numerically by propagating Eq. (3.43) in imaginary and real time for $N = 6 \times 10^3$ ^{162}Dy atoms, $a_{\text{dd}} = 130a_0$, $\epsilon_{\text{dd}} = a_{\text{dd}}/a_s = 2.15$, $\rho_0 = 1 \mu\text{m}$, $\omega/(2\pi) = 1 \text{ kHz}$ and $\lambda = 1.7$, with $V_{\text{ext}}(\mathbf{r}) = \min(V_{\text{ring}}(\mathbf{r}), V_{\text{harm}}(\mathbf{r}))$.

If we take ρ_0 in Eq. (5.8) to be the ring radius, the analytical model deviates from the numerical results. This deviation becomes evident if we compare the case $f = 0$ to the numerical results, where the parabola generated by $f = 0$ in Eq. (5.8) should form the support for the superfluid and supersolid periodic functions on top of it (see the grey-dashed line in Fig. 5.4). We can, however, remedy this deviation by noticing that for a dipolar system, the ring radius is not the system's actual radius due to the long-range interaction. The repulsive long-range interaction forces the Bose gas to assume an effective radius $\tilde{\rho}_0 > \rho_0$. For our system with $\rho_0 = 1 \mu\text{m}$ and $a_{\text{dd}} = 130a_0$, this effective radius becomes $\tilde{\rho}_0 \approx 1.088 \mu\text{m}$, which we evaluate numerically by calculating $\sqrt{\langle \rho^2 \rangle}$. When we insert $\tilde{\rho}_0$ into Eq. (5.8), we find that the expression agrees well with the numerical results.

In an experimental setup, one generally lacks direct access to the dispersion relation and needs to visualize the flow differently. If a vortex exists in the ring center, there will be a phase singularity with zero density due to irrotationality. Then, releasing the system radially from the trap and observing it in a time-of-flight expansion may reveal the vortex core [226]. For a system without a vortex, a high-density region forms at the center due to interference of the expanding condensate (see Fig. 5.5). To measure the circulation s , we introduce a reference condensate in the ring center, which remains at rest. When one removes the trap in the radial direction, including the barrier separating reference from outer condensate, spiral arms form due to interference of the superfluid components [222, 227–229]. The spiral arms' number and direction (clockwise or counter-clockwise) then give the circulation [222, 227–229]. Fig. 5.6 shows this process of spiral formation in a time-of-flight measurement, where we have increased the number of ^{162}Dy atoms to $N = 6 \times 10^3$ to compensate for the reference Bose gas in the center. Further, we amend the trap to be $V_{\text{ext}}(\mathbf{r}) = \min(V_{\text{ring}}(\mathbf{r}), V_{\text{harm}}(\mathbf{r}))$, with $V_{\text{harm}}(\mathbf{r}) = m\omega_0^2(\rho^2 + \lambda^2 z^2)/2$.

While the ring geometry lends itself to the study of persistent currents, it only sup-

ports multiply quantized vortices in a region where the density is already zero in the absence of vorticity. We may also want to observe multiple singly quantized vortices as they occur in harmonic traps for a weakly interacting Bose gas. Here, one can use the dipolar polarization direction to induce vorticity via magneto-stirring [230], which was recently applied to a dipolar Bose gas outside the supersolid phase for vortex generation [230]. In this experiment, the vortices aligned in a stripe phase compared to the triangular alignment in a non-dipolar Bose gas. This alignment is due to the anisotropy of the dipolar interaction and may have startling consequences if the vortices' inclination to align in a triangular pattern competes with the droplets' tendency to do the same in the supersolid phase [231–234]. The vortices should, however, form in the low-density region of the superfluid background, as it is energetically favorable (see Eq. (4.31)) [232].

Chapter 6

Outlook

This thesis describes the theoretical framework involved in the modern landscape of self-bound droplets, mixed bubbles, and dipolar supersolids in ultra-cold bosonic gases, particularly concerning their superfluid properties. As all these systems rely on the effects of quantum fluctuations on the condensed ground state, we spent a significant portion of the thesis on deriving these effects in Ch. 3. In particular, to the best of my knowledge, Sec. 3.4 in the fully interaction-type agnostic and mass-imbalanced regime has not been written down before with this level of detail. We also connected the definitions of a Bose-Einstein condensate to the defining property of a superfluid - global phase coherence and spontaneous $U(1)$ symmetry breaking. Lastly, we investigated how all these properties and effects come together in a dipolar supersolid.

As mentioned in the introduction, the goal was to provide the most helpful document if I were back at the beginning of my PhD studies. As such, it feels prudent to point out possible future research avenues.

A significant problem for all systems discussed in this thesis is the relatively short lifetime in an experiment [45, 46, 50–52]. This makes it challenging to observe superfluid properties as the high depletion and three-body losses near the Feshbach resonances [35–41] effectively destroy these systems before vortices or a persistent current could occur. Heteronuclear systems such as in Refs. [102, 235] offer a way out where the lifetime can be up to several orders of magnitudes larger. Investigating vortex formation and persistent currents could then become a feasible option.

A dipolar supersolid's lifetime may be increased similarly by introducing a second component. Here, the quantum fluctuation term becomes irrelevant as the interaction with the second component (which may be contact or dipolar interacting in

itself) stabilizes against collapse [236–242]. In analogy with the rigid and superfluid components of a one-component dipolar supersolid, we could find two superfluid components and two rigid ones (which couple together). The formation of these components could form an ideal playground to investigate the Andreev-Bashkin effect and its resulting third sound (see Sec. 4.5).

The superfluid drag originated from the mass-renormalization of ^3He in ^4He and emerged using BCS theory [132]. Ref. [100] introduced a similar pairing effect to correct some of the Bogoliubov theory deviations from exact diffusion Monte Carlo calculations [100]. One could assume that including a pairing mechanism may also amend some deviations in the drag for an attractive interspecies interaction. Similarly, to my knowledge, such an effect has not been investigated in the formation of dipolar droplets and supersolids.

Landau’s criterion for superfluidity can be written as $E_{\mathbf{k}} - \hbar \mathbf{k} \mathbf{v} > 0$, which enforces that the quasi-particles themselves fulfill bosonic particle statistics. Following a proposal by Pitaevskii [243, 244], we could apply some rotation to a dipolar system that is still fully superfluid but close to the supersolid phase, such that it has a roton minimum (see $\epsilon_{\text{dd}} = 1.9$ line in Fig. 5.1). Due to the applied rotation, we could lower the roton gap until a density modulation occurs, essentially rotating the superfluid system into a supersolid. A potential precursor of this effect exists in a dipolar toroidal supersolid in Ref. [214], which would help formalize this effect.

Lastly, let us turn to the mixed bubble. So far, there have been only two articles besides the original proposal [101], Paper III, and Ref. [129]. An experimental observation so far is missing and could be challenging to achieve due to the necessity of a fully flat trap. Here, we may turn to a strongly interacting one-dimensional system and investigate bubble formation via exact diagonalization (similarly to Paper V), quantum Monte Carlo [118], or matrix product states [245, 246]. This strongly interacting bubble could also offer a pathway for the superfluid drag.

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