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DYNAMICS OF ULTRA-COLD GASES

A THESIS SUBMITTED
FOR THE DEGREE OF DOCTOR IN PHYSICAL SCIENCES

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Abstract

The first part of this thesis devoted to establish a system of nonlinear differential equations describing the dynamics of the order parameter (the condensate wave function), the thermal cloud and the anomalous density, these equations often known as TDHFB (Time-Dependent-Hatree-Fock-Bogoliubov). The TDHFB equations are time-dependent variational equations derived using the Balian and Vénéroni principle. They are valid for any Hamiltonian and in any dimensions. We present the numerical solution of such equations in the static case in the presence of a spherical confining potential beyond the Thomas-Fermi approximation (taking into account the kinetic energy). We then examine the profiles of the different densities as function of the temperature and the interactions and compare them with the theoretical results existing in the literature, especially with those obtained by the approximation of HFB-BdG.

In order to shed some light on the anomalous density, remind us that the presence of this quantity in a Bose system indicates that the atoms are correlated. We again use our theoretical approach and varying interactions and temperature. Our results are in good agreement with those of HFB-BdG in a system of large number of particles. For a gas of weak interactions, our results start to deviate from the HFB-BdG, where we observe the disappearance of the "dip".

The study of the anomalous correlation function in two dimensional Bose gas was also among of our subjects in this thesis. We found that this quantity has a finite value in the limit of weak interactions at zero temperature. The effects of the anomalous density on some thermodynamic quantities such as the chemical potential (equation of state), the depletion and the superfluid fraction have been also highlighted. Our results show good agreements with Monte Carlo simulations and perturbative analytical methods. On other hand, by using the density-phase fluctuation, we found that the anomalous density does not exist at finite temperature in analogous manner with the true condensate.

In the second part of this thesis we turn to discuss effects of the rotonization in two dimensional dilute dipolar Bose gas. We have calculated in particular the density-density correlation function, fluctuation corrections to the chemical potential, compressibility, and the normal (superfluid) fraction. We have shown that the presence of the roton strongly enhances fluctuations of the density, and we establish the validity criterion of the Bogoliubov approach. At zero temperature the condensate depletion becomes significant if the roton minimum is sufficiently close to zero. At finite temperatures in the dilute regime where $nr_*^2 \ll 1$, exceeding the roton energy and the interaction between particles, the effect of thermal fluctuations is stronger and it may lead to a large normal fraction of the gas which may significantly reduce the superfluid fraction even at temperatures well below the Kosterlitz-Thouless transition temperature.

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Chapter 0

History of Ultacold Atoms

0.1. Introduction

The idea that the world around us is composed of small and fundamental building blocks goes back more than 2500 years. Already in the sixth century BC, philosophers in ancient India developed theories that described how these building blocks of matter could combine into more complex objects with different physical properties [1]. About a century later, the Greek philosophers Leucippus and Democritus came up with the idea that all physical objects are made of indivisible discrete units located in the void. These smallest pieces of matter were called *atomos*, which means *uncuttable* or *indivisible*, from which the modern name *atoms* is inherited. In the following years, Plato connected the notion of atoms to the basic elements - *fire, air, water and earth* - and postulated a geometrical basis underlying the structure of the atoms. However, his student Aristotle regarded the basic elements to be continuous and rejected the idea that atoms are the basic building blocks of reality. His natural philosophy continued to dominate the Western view of the world throughout the Middle Ages. Only in the late sixteenth century AD, experimental evidence in contradiction with the Aristotelian physics led to renewed interest in the atomic view of the world. Well known philosophers and early scientists, such as Bacon, Galilee, Descartes and Newton, developed physical theories that were based on the atomic or corpuscular nature of matter. With the great success of the kinetic theory of gases, developed independently by Maxwell and Boltzmann in the late nineteenth century, a modern atomic theory was born [2].

In the late nineteenth century, the physical world was thought to consist of matter and radiation. All material objects were considered to be formed by indivisible atoms, which could in turn form molecules and larger bodies. The wave theory of radiation was firmly established by a whole range of experiments on electric and magnetic phenomena and the success of geometrical optics, followed by the discovery of the

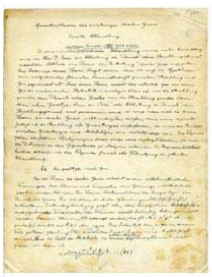
fundamental electromagnetic equations by Maxwell and the subsequent discovery of radio waves by Hertz. In 1859 Gustav Kirchhoff stated that there must be a black body radiation law that depends only on temperature and light frequency. However, there were insufficient experimental results to determine the formula for this law. Forty years later, experimental physicists finally probed the far infrared spectrum of black-body radiation.

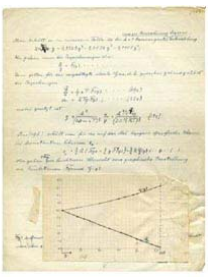
0.2. Development of the theory of weakly interacting bosons

In the following years, new experimental data was found to be in strong contradiction with the classical theories. In 1900, the measured spectrum of black body radiation could only be understood with the help of Planck's hypothesis that the interaction between matter and radiation is quantized. It became clear that the classical distinction between the corpuscular nature of matter on the one hand, and the wave character of radiation on the other, could not be maintained. Max Planck felt that this "quantization" of states was merely a "trick" to make the math work.

In 1905, Albert Einstein published a paper that showed that Plank's quantization could be used to explain the photoelectric effect, which is when electrons are emitted from metal after it absorbs electromagnetic radiation. Because he showed that Plank's quantization was not merely a "trick", but could be used to explain a new phenomenon, he received the Nobel Prize in 1921. Today we refer to these quantized electromagnetic states as photons.

Many experiments and a lot of new ideas eventually led to the development of the theory of quantum mechanics by Bohr, Heisenberg, Schrödinger, Dirac, Pauli and many others, ending the classical period and giving a completely new understanding, often mind-boggling, of the microscopic world. Within quantum mechanics particles have wave-like properties, while the quanta of radiation in many respects behave like particles. In 1911 (just three years after producing the world's first sample of liquefied helium), Kamerlingh Onnes discovered that the density of liquid helium, as a function of temperature, had a sharp maximum near 2.2 Kelvin [3].





In 1924, a young Indian physicist named Satyendra Nath Bose developed a new derivation of Planks law. His paper explaining this derivation was rejected for publication. Since this derivation used photons, he decided to send a copy of the paper to Einstein. This paper sparked Einstein's interest and he quickly

translated it into German. He submitted it for publication with the attached note, "In my opinion Bose's derivation of Planks formula constitutes an important advance [4]." In 1925, Einstein published three papers using the new statistical methods proposed by Bose. He made a few minor modifications so that he could apply the new statistics to matter as well as light. Using these statistics he showed that below a certain temperature there was a new phase of matter, in which a macroscopic number of particles are in the lowest quantum state. This phase of matter has become known as a Bose-Einstein condensate, and was the first purely quantum mechanical phase transition to be predicted [5].

In 1926 Onnes and Dana measured other strange maxima in the specific heat near the same above temperature i.e. T=2.2K [6] (this temperature later became known as the λ-point, due to the λ shaped specific heat curve of liquid helium). In 1928, Wolfke and Keesom expressed the opinion that these measurements were the result of a phase transition in liquid helium (the higher temperature phase being labeled He I, and the lower temperature phase He II) [7, 8]. In 1927, George Uhlenbeck [9,10] (a graduate student of Paul Ehrenfest) criticized Einstein's article explaining that mathematically the condensation could not occur in the fundamental mode because the process gas saturation was not valid; simply varying the temperature to change the particle density and vice versa. The Uhlenbeck's criticism was generally accepted.

It took until 1938 to update the idea of Einstein. Fritz London [11], noting the similarity of the λ-shaped heat capacity curve in liquid helium to the behavior of the heat capacity of an ideal gas near the BEC transition, proposed that superfluidity could be a manifestation of Bose-Einstein condensation. This proposal, and its later verification, constitutes a landmark in modern physics. For the very first time a system had been discovered which was described by a macroscopic wavefunction, and to this date the prediction of Einstein once called the "Bose-Einstein condensation" and superfluid helium continues to be the subject of a considerable amount of research.

In January, 1938, Kapitza [12] and, Allen and Misener [13,14], separately published their key experiments on superfluidity in Nature in which they showed that the viscosity of ^{4}He dropped to essentially immeasurable values when cooled below the λ-point. In the same period, Lazlo Tisza [15] developed a new idea "two-fluid hydrodynamics" based on the notion of a superfluid and normal fluid.

In the early of 1940's Landau's papers [16, 17] on superfluid ^{4}He changed how we think about all condensed matter systems. Landau introduced a "new" hydrodynamics to describe low frequency superfluid phenomena based on the motion of two fluids. He also introduced the phenomenological but powerful idea that the liquid could be described in terms of a "gas of weakly interacting quasiparticles", with a relatively simple energy spectrum for two kinds of quasiparticles: phonons and rotons.

Strange as it may seem, it took science more than 25 years from the discovery of the Bose-Einstein condensate to develop trustful predictions about interacting Bose gases and their condensation. This came true in 1947 when the first microscopic theory was published by Bogoliubov [18-20]. Bogoliubov's assumptions in this study based on the temperature was assumed to be zero, the "depletion" of the ground state was assumed to be small, and interactions were limited to mean-field interactions, binary collisions, or hard sphere interactions. Nevertheless, this work showed that (i) Bose condensation can occur in the presence of interactions, and (ii) the low-lying excitations of the ground state in this system are phonons.

Subsequently, by 1950, Landau and Lifschitz [21], Onsager and Penrose [22, 23], who proposed a physical theory explaining the weakly interacting gas case. However, it lacked a rigorous mathematical treatment.

In 1953, R. P. Feynman proposed a new concept to describe the Bose gas based on the formulation of quantum mechanics in path integral [24]. Under his assumption, he showed that for a gas interaction, as the ^{4}He, when one is at low temperature can form a Bose-Einstein condensate subject to certain sound approximations [24].

In parallel, the predictions of quantum vortices in superfluids by Onsager [25] and Feynman [26], for they appeared to be in perfect agreement with the experiments due to Hall and Vinen from 1956.

From 1957 to 1970 this period known as "the golden era" where during it the interacting Bose gas became a hot topic and attracted many theorists.

In 1957 a theory was presented in which pairs of fermionic electrons formed composite bosons in superconductors, linking superconductivity to phenomena very similar to Bose-Einstein condensation [27] which is often called BCS theory; proposed by John Bardeen, Leon Neil Cooper, and John Robert Schrieffer. An important work of Lee, Yang and Huang in period of 1957-59 on the low temperature properties of a dilute hard-sphere Bose gas [28]. However, their work involved very complex many-body calculations using exact wavefunctions.

Beliaev in 1958 [29,30] in his approach forms the basis of the systematic application of the quantum "field theory methods to boson systems with condensate, including anomalous propagators representing two particles going into or out of the condensate. Since the condensate is treated in the framework of Bogoliubov. In 1959, this approach was developed further by Hugenholtzand-Pines [31, 32], and was thoroughly reexamined in 1963 by Gavoret and Nozières [33, 34]. They showed that the singular character of interaction in the Bose systems with condensate remarked by Bogoliubov manifests itself in divergences of perturbation theory at small momenta (infrared divergences). Gavoret and Nozières scrutinized this question inspired by the higher-order calculations by Beliaev [35] and Hugenholtz-Pines [32,33]. They showed that infrared divergences cancel out in all physical quantities; the energy gap in elementary excitation spectrum vanishes to all order of perturbation theory; for further developments see [36, 37].

A key development relevant to trapped gases was due to Pitaevskii in the period 1959-61. Many of us now are very familiar with the famous Gross-Pitaevskii equation [38,39]. However, Pitaevskii's real contribution was not this particular equation rather it lies more in introducing the whole idea of a macroscopic wavefunction which could depend on both position and time. Pitaevskii's work, of course, was no doubt inspired by the use of a similar "wavefunction" by Ginzburg and Landau in their pioneering theory of spatially inhomogeneous superconductors [40]. In 1963, the Hugenholtz-Pines-Gavoret-Nozières theorem was discovered by Bogoliubov under the name $1/k^2$ theorem. Instead of perturbation theory Bogoliubov's proof of this theorem is based on local gauge transformations. He showed [41, 42] that the appearance of a gap in some models is a consequence of the lack of local gauge invariance of these models.

In 1965, Popov [43, 46] proposed a generalization of the Bogoliubov theory for $T \neq 0$ in which the density of thermal component can be taken into account this theory gives the elementary excitation spectrum similar to that for $T = 0$, but now with temperature-dependent condensate. This leads to the collapse of the low phonon-spectrum to free particles as $T \to T_c$. The Popov approximation leads to a jump of in the condensate at the transition point and thus predicts a first-order phase transition.

A craze for low dimensions started at this period by M. Girardeau in 1960 [47] in his study on the impenetrable one dimensional Bose gas. Furthermore, Lieb and Liniger

[48] solved exactly the zero-temperature interacting Bose gas with repulsive delta-function potential and showed that the derived ground state properties agree with Bogoliubov's perturbation theory only in the limit of very weak coupling constant. The time-dependent thermodynamic behavior for the Lieb-Liniger model was presented by Yang and Yang [49] through the use of the Bethe ansatz. Regarding the case of gas without interactions, all began with H. Casimir in 1968 [50] who studied the Bose-Einstein condensation of an ideal gas Bose in anisotropic boxes model.

0.1. Development of the experiment of weakly interacting bosons

The experimental studies on dilute Bose gases date to the 1970s when various laser techniques, such as magnetic and optical trapping, have been developed.

In 1976, Nosanow [51] used the quantum theory of corresponding states to conclude that spin-polarized hydrogen would remain gaseous down to zero temperature and should be a good candidate to realize Bose-Einstein condensation in a dilute atomic gas. These suggestions triggered several experimental efforts, most notably by Silvera and Walraven [52] in Amsterdam, by Greytak and Kleppner [53] at MIT, Hardy *et al.* [54]. By early 1980s with the development of modern methods of cryogenic refrigerators and very performance, it was hoped it would be possible to cool a gas of atoms or molecules at a temperature low enough to reach the threshold predicted by Einstein. But these methods, applied to an assembly of particles confined in an enclosure material, leading to a difficulty that seems insurmountable: at low temperatures, atoms stick on the walls of the container to form a liquid or a solid "ordinary" and the Bose-Einstein condensation cannot occur. To remedy this problem, the idea appeared to confine the atoms in immaterial boxes, made of magnetic fields or laser beams. In parallel, techniques for handling and cooling atoms by light beams have been developed.

The development of these methods has given rise to two Nobel Prize for physics in the two last decades. In 1997, S. Chu, C. Cohen-Tannoudji and WD Phillips were awarded for the development of cooling and trapping of atoms by light. In particular they invent the so-called optical molasses, where the atoms are cooled to very low temperatures by six perpendicular intersecting laser beams. The sub-Doppler temperatures of molasses found by Chu [55] Cohen-Tannoudji [56] and Phillips [57] were shown to be due to a combination of light-shifts and optical pumping that became known as Sysiphus cooling (Dalibard and Cohen-Tannoudji, 1989 [58]).

Indeed, the MOT had the essential elements needed for a widely useful optical trap: it required relatively modest amounts of laser power.

The success of trapping techniques and magneto-optical evaporative cooling as the criterion for Bose-Einstein condensation was carried out for relatively low densities and low temperatures. 1995 is the year of triumph, these successes led to the first direct observation of BEC in dilute gases of ultracold bosonic alkali atoms confined by magneto-optical trap. The discovery of such a condensation was carried out almost simultaneously by two American groups: Group E. A. Cornell C. W. Wieman (JILA, Boulder) on a gas of atoms of ^{87}Rb [59] and the group of W. Ketterle (MIT, Boston) on a gas of atoms of ^{23}Na [60]. Since then, the BEC has been reproduced in hundreds of laboratories around the world. This was done first with the same atomic species and with atoms having very different properties, such as hydrogen, produced in 1998 (MIT, Boston) [61], and ^{4}He in the metastable state in 2001 (ENS-Paris and Charles-Fabry laboratory Orsay) [62].

Related experiments in cooling fermions rather than bosons to extremely low temperatures have created degenerate gases, where the atoms do not congregate in a single state due to the Pauli Exclusion Principle [63]. To exhibit Bose-Einstein condensation, the fermions must "pair up" to form compound particles (e.g. molecules or Cooper pairs) that are bosons. The first molecular Bose–Einstein condensates were created in November 2003 by the groups of Rudolf Grimm at the University of Innsbruck [64], Deborah S. Jin at the University of Colorado at Boulder [65] and Wolfgang Ketterle at MIT [66]. Jin quickly went on to create the first fermionic condensate composed of Cooper pairs [67].

As of 2010, using ultralow temperatures of 10^{-7} K or below, Bose-Einstein condensates had been obtained for a multitude of isotopes, mainly of alkaline and alkaline earth atoms (^{7}Li, ^{23}Na, ^{39}K, ^{41}K, ^{85}Rb, ^{87}Rb, ^{133}Cs, ^{52}Cr, ^{40}Ca, ^{84}Sr, ^{86}Sr, ^{88}Sr, and ^{174}Yb).

0.2. Why cold atoms?

The study of Bose-Einstein condensation in ultracold gases has become one of the most active research areas in physics. To give an idea of the level of this activity, we just note that it simply results in the release of about a thousand articles per year. The reasons for this interest in condensed Bose gases are simple to understand. First, they are well controlled quantum systems, where the confrontation theory - experiment can be conducted with very good accuracy. The environment of atoms, formed by the

magnetic trap or laser beams can be changed at will and a wide range of geometries can be considered: the potential confining the atoms can form a single bowl, double sinks, or present a modulation periodic or random. We can therefore use the cold atomic gases to model more complex systems such as electrons moving in a solid (the quantum Hall effect), other analogies are also the subject of intensive research, as the study of Mott-insulator transition for materials which can be achieved by varying the distance between the atoms or the strength of the interactions between these particles in the crystal. One can hope to achieve through these cold atom quantum simulator imagined in the 1980s by Richard Feynman: starting from a problem that quantum theory cannot solve (e.g. a complex condensed matter), we perform an experiment with cold atoms in seeking to put in a situation such that the quantum equations of motion are formally the same as the original problem (although the magnitudes are in turn very different). The experiment with the atoms could then provide the answer sought. The harvest of results obtained on the bosonic atomic gases has stimulated course similar studies on gas of ultracold fermionic atoms. Each quantum state cannot contain more than one fermion, the distribution of atoms on the energy levels of the trap is very different from the bosonic case. If the spins of the fermions are all oriented in the same direction, one can show that these fermions interact hardly, making them outstanding candidates for metrology and manufacturing of high-performance atomic clocks. Indeed, one can accumulate a large number of these particles without interactions from disturbing the signal we want to measure on each of them. However, if we put in the same trap of fermions with different orientations possible for their spins, these fermions interact and this gives rise to new effects of particular interest. In fact, when we reach a situation strongly reminiscent of that of superconductivity, which occurs when an electron gas is cooled below a certain temperature. A very active area of research is the comparison of experiments with these fermionic atomic gases with existing theories of superconductivity, as the BCS theory. These atomic systems can help to understand the mystery of high temperature superconductivity observed in 25 years on certain materials. These questions illustrate how this research proves fruitful for the development to which it gives birth, 88 years after the publication of articles of Bose and Einstein.

Two amazing discoveries guide the current research: (i) it is now known how to change the strength of the interactions between ultracold particles by simple

adjustment of a magnetic field (Feshbach resonances), (ii) we can confine cold atoms in periodic electromagnetic potential, also called optical lattices, created by pairs of laser beams propagating in opposite directions.

Research on optical lattices is currently a very active area: the movement of atoms in these lattices is formally identical to that of electrons in a crystal, with the advantage that the parameters of optical networks can be changed at will and that atoms are observed individually. The idea is to build a "quantum simulator" in which we use cold atoms to model complex problems in condensed matter. The stakes are high hopes for it to run a better understanding of the phenomena of quantum magnetism and spin electronics.

Furthermore, in recent years considerable interest has been devoted to another aspect of the internal structure of the particles forming an ultracold gas, namely their dipole moment. If such dipole moment (either electric or magnetic) is sufficiently large, the resulting dipole-dipole forces may influence, or even completely change the properties of BEC in bosonic gases. This raises the experimental possibility of studying systems of many particles with long-ranged dipolar. The dipolar interaction opens up a range of interesting possible phases of matter (e.g. supersolid state).

A second area of research concerns the gas atoms in strong interaction, which is formally identical to quark-gluon plasma or neutron stars. A third way for quantum gases in low dimensions, hoping to simulate phenomena analogous to the quantum Hall effect for a two-dimensional system of electrons in a magnetic field, where it remains to be simulated with the equivalent atoms in the magnetic field acting on the electrons by developing artificial gauge fields.

At the interface between cold atoms and nanosciences, we also note the appearance of new objects: the polariton gas; hybrid particles composed of photons and electrons in semiconductor nanostructures, which can form and become superfluid condensate. We should also mention the recent development of nano-cooling by cold atoms. Another interface is that of "cold chemistry", providing unprecedented control over the parameters of the samples.

The use of cold atoms for precision measurements is a promising research topic, both in terms of fundamental physics and practical with the production of devices and

sensors considerably more efficient. The accuracy of cold-atom clocks is undergoing a dramatic improvement with the emergence of optical clocks. Launching into space will test Einstein's general relativity with unprecedented accuracy. Other laws, such as the principle equivalence, or the law of gravitation, may also be tested through the matter wave interferometers. The detection of gravitational waves is another area of major interest for which new type of interferometers are planned, with sensors on replacing the light beams. Finally the stability of fundamental constants over time will be tested and measured value with greater precision. The latter is a crucial issue for the next redesign of the international system of units, with strong implications for global trade.

Note that the cold ions are also well suited for measurements such as precision tests of fundamental symmetries violation. In addition to the single ion optical clocks are among the most accurate in the world.

In summary, it is expected that dramatic progress to be made soon on sensors based on cold particles: clocks, gyroscopes, gravimeters and magnetometers soon open up new possibilities in the field of measurement. This part of the activity will be strongly pushed in conjunction with industry and the development of physics in space. Among the most important applications of ultra-cold atoms is the realization of atom lasers, that is to say instruments capable of delivering a beam of atoms all in the same state, like the photons of a laser beam. This would make a great service to optics and atom interferometry, chemistry (study of reactions between two atomic beams under very well defined and controlled condensate of molecules, etc.). On the industrial side, several applications are involved such as transport economy electricity and rail (Maglev electrodynamics) very high speed moving in levitation by repulsion between the magnetic field of superconducting coils in the car (whose electrical resistance is almost zero if kept at low temperatures) and a magnetic field created by electromagnets located on the rails. Another application might be in the creation of lasers to shorter wavelength (in the field of UV or X-rays). The application, proposed by researchers at Bonn University after obtaining a condensate of photons could be used to include the miniaturization of printed circuit boards.

Part I. Dynamics of Ultracold Gases at Finite Temperature

General introduction

1. Topic of this thesis and literature reference

Following the first observation of Bose-Einstein condensation of dilutes gases, experimental and the theoretical efforts were mainly focused on the fundamental properties of such degenerate quantum gases, including spatial and momentum distributions, and collective excitations. Mean field theory was initially found to be impressively successful in most cases. Indeed, at temperatures well below the phase transition, nearly all atoms occupy one wave function that satisfies a nonlinear Schrödinger equation, the celebrated Gross- Pitaevskii equation (GPE) [38, 39]. The nonlinear term describes the mean field potential experienced by the atoms due to two-body interactions. In the language of quantum field theory, the GPE yields a zeroth-order approximation to the full matter-wave field where both the noncondensed component of the gas and quantum fluctuations are neglected. For trapped gases at zero temperature, the GPE equation constitutes the best model for studying the properties of Bose-Einstein condensation and provides excellent predictions for relevant experimental observations.

Nevertheless, it is important to remember that experiments actually take place at finite temperatures. A thermal cloud is always present, and as one increases the temperature towards T_c the influence of this on the system behavior will become progressively more important. In some situations the thermal cloud is absolutely central, for instance in the problem of condensate growth, or the heating of the gas under strong external perturbations. The effects of finite temperature also become particularly important in low dimensional systems, where the condensate exhibits fluctuations in its phase, and the usual picture of Bose-Einstein condensation needs to be revisited. Theoretical models of BEC at finite temperature are therefore of tremendous value. In order to be useful, such models should ideally accurately represent the important physics in a problem, while remaining feasible to solve either analytically, or numerically, using current computing resources. The development of dynamical finite temperature models that satisfy these conditions has proven to be a great challenge. Despite significant progress, research remains active, and much work remains to be done. A major problem that confronts newcomers to the field of Bose-

Einstein condensation at finite temperatures is the large number of seemingly very different approaches which have been applied to the problem. This is exacerbated by the fact that the major researchers have arrived from different backgrounds, and therefore speak different languages.

At finite temperature, the mean-field approximation is intensively used to describe the static and dynamic equilibrium properties of Bose-Einstein condensates. Depending on the regime at hand, different variants and different models do exist. Among them, we can cite in particular the Hartree-Fock-Bogoliubov theory [68-70], this theory has been successfully confronted to experiments as they predict correctly, among other things, the collective and single-particle excitations, the condensate fraction and also the transition temperature.

The condensate and thermal cloud are often treated as two subsystems that are coupled to each other by scattering processes that exchange particles and energy. Approaches based on such a splitting between condensate and thermal dynamics lead to a generalized Gross-Pitaevskii equation for the condensate dynamics that differs from its $T = 0$ counterpart through the inclusion of the thermal cloud mean field (Hartree-Fock potential). On the other hand, the thermal cloud itself is described by a quantum Boltzmann equation self-consistently coupled to the condensate in the so-called Gross-Pitaevskii-Boltzmann approach, which is often referred to as the “ZNG” scheme [71,72]. This kind of approximation known in the literature as kinetic theories. Despite their elegant formulation, kinetic theories based on mean field potentials have the drawback in lower dimensions of not fully capturing the large phase fluctuations in the quasi-condensate. In addition, so called anomalous averages (or pair correlations) in the thermal cloud, typically omitted in such approaches, are expected to become particularly relevant at lower dimensions. A modified mean field theory for low-dimensional quasi-condensates was developed by Stoof’s group [73-75], building on previous path-integral approaches pioneered by Popov. In this “modified Popov theory”, the infrared divergences due to phase fluctuations are systematically removed, leading to a gapless, convergent and computationally convenient scheme that applies in all dimensions, for homogeneous and trapped systems.

The condensate dynamics at nonzero temperature is a challenging problem as the Bogoliubov approximation becomes invalid, at least at large times, and large thermal phase fluctuations have to be taken into account even at low temperatures

where density fluctuations are small. Classical field methods [76-82] have been developed to simulate numerically those modes of the system that feature a macroscopic occupation. These methods rely upon the observation that for highly occupied modes, the field operator can be replaced by a classical complex field which evolves in time according to the GPE. Within the class of classical field techniques, we mention the projected GPE [78], the stochastic Gross-Pitaevskii equation [81,82] when implemented in the classical limit, and closely related classical field method. The above theories, although being quite satisfactory, suffer from several drawbacks and inconsistencies which restrict their applicability to certain regimes and not to others.

In the first part of our thesis we would like to proceed differently by using the time-dependent variational principle proposed by Balian and Vénéroni (BV) [83,84] a long time ago. The point is that this principle uses the notion of least biased state, which is the best ansatz compatible with the constraints imposed on the system. For our purposes, we will use a Gaussian density operator. This ansatz is reminiscent of the independent particle approximation and belongs to the class of generalized coherent states. It allows us to perform explicitly all the calculations since there exists a generalization of Wick's theorem to statistical physics. It is important to note however that despite its simple form, it by no means endows any further simplification on the interaction between particles. Indeed, the BV-principle, together with the trial Gaussian ansatz, lead to a set of coupled time-dependent mean field equations for the condensate, the thermal cloud and the anomalous average. We have to mention at this point that the equations that we have derived in our thesis are quite general and fully consistent as they do not require any simplifying assumption on the noncondensed or the anomalous densities. They may provide in this sense a kind of generalization to the previously discussed approximations, valid however, in the collisionless regime.

2. Outline

In chapter 1, we present general notions about the utracold Bose gases, where we give a short history and background of the domain. This includes a discussion of the early experiments. We also discuss some of the more recent experimental advances in the field, including the basic physics behind the optical and magnetic

cooling and trapping methods that led to the first experimental realization of a BEC and the first, most fundamental results that laid the foundation for the modern study of the ultracold physics of bosons. To give the reader an idea of how the Bose-Einstein condensate phase emerges statistically as a function of temperature, we also discuss the phenomenon of BEC in a both uniform and trapped, non-interacting (ideal) gas of bosons in a general *d*- dimensional form.

In chapter 2, we start from a second-quantized description of a quantum many-body system of interacting bosons and systematically derive the set of mean-field equations that describe the condensate field and the quantum fluctuations of the dilute, interacting Bose gas at zero-temperature, being the Gross-Pitaevskii equation and the Bogoliubov de Gennes equations, respectively. Additionally, we motivate the use of the short-range two-body interactions in the ultracold gas. Some thermodynamics quantities and correlations functions are also revealed in the framework of Bogoluibov at zero temperature. In addition, we expose other important finite temperature approximations like the HFB, kinetic theories such as the ZNG, Classical field methods and the stochastic approaches.

Chapter 3 is devoted to review the main steps used to derive the TDHFB equations from the Balian-Véneroni variational principle. The TDHFB equations are applied to a system of self-interacting trapped bosons to derive a coupled dynamics of the condensate, the non condensate and the anomalous densities. We then restrict ourselves to the local densities and discuss the properties of the underlying equations, their relevance to the finite temperature case as well as their relations with other known approximations such as the Bogoliubov-De Gennes equations (BdG). We present the static equations and the physical boundary conditions relevant to the trapped Bose gas. We then solve numerically these equations for a harmonic trap. We analyze the various densities as functions of the radial distance and the temperature. We find an overall good qualitative agreement with recent experiments as well as with the theoretical HFB-BdG predictions. In addition to investigate more deeply our formalism, we study the behavior and the formation of vortices at finite temperature. Surprisingly we find that the thermal gas forms a local minimum in the center of trap and appears as a tornado surrounds the condensate which leads to a coreless vortex (empty core) which is in disagreement with that predicted in the literature.

The investigation of the three-dimensional behavior of the anomalous density in both homogeneous and trapped cases is addressed in Chapter 4. We show that the

temperature dependence of the anomalous density agrees with the Hartree-Fock-Bogoliubov (HFB) calculations. In homogeneous case, the comparison between the normal and the anomalous fractions at low, intermediate and high temperatures low temperature, show that the latter remains higher and consequently the neglect of the anomalous density at zero and low temperatures may destabilize the condensate. We analyze the profiles of the anomalous density for different temperatures both for large and small values of the interaction parameter. Our results are in accordance with recent theoretical investigations. Surprisingly, we found that the dip in the central anomalous density is destroyed for sufficiently weak interactions.

Chapter 5 developed to treat the behavior of the anomalous correlation function in two dimensional Bose gas. In the local case, we find that this quantity has a finite value in the limit of weak interactions at zero temperature. The effects of the anomalous density on some thermodynamic quantities are also considered. These effects can modify in particular the chemical potential, the ground sate energy and the depletion. Our predictions are in good agreement with recent analytical and numerical calculations. We show also that the anomalous density presents a significant importance compared to the non-condensed one at zero temperature. The single-particle anomalous correlation function is expressed in the finite temperature two dimensional homogenous Bose gases by using the density-phase fluctuation. We then confirm that the anomalous average accompanies in analogous manner the true condensate at zero temperature while it does not exist at finite temperature. We also apply our formalism to analyze the behavior of the superfluid fraction. We then emphasize the importance of the anomalous density for the occurrence of superfluid transition.

Chapter1

Background: Theory and Experiment

1.1.What is Bose-Einstein Condensation?

Named for the theorists Satyendra Nath Bose and Albert Einstein who predicted its existence, a Bose-Einstein condensate is a new state of matter that arises because of quantum mechanical effects on a collection of entities called bosons. Everything is either a boson or a fermion. The spin of an object determines whether it is a boson or a fermion. The reason why it is important to differentiate between bosons and fermions is that they have vastly different quantum mechanical behavior. Identical fermions cannot occupy the same place. This is called the Pauli Exclusion Principle [63]. For example, you cannot put two electrons spinning in the same direction on top of one other. It is forbidden and never happens in nature. Bosons behave in almost the opposite way. They like to overlap.

In quantum mechanics, the position of an object is uncertain. An object has a definite probability of being at any given point in space. This probability is encoded in what-is-called a wave function. It is like a "cloud" that tells you the probability that an object has a certain location. The object is more likely to be found in denser parts of the "cloud" and is less likely to be found in the less dense parts. If a region of space has no "cloud," then there is zero chance that the object is there. If one concentrates a large number of identical bosons in a small region, then it is possible for their wave functions to overlap so much that the bosons lose their identity. This exotic state of matter is only possible at low temperatures. At high temperatures, the individual bosons not only have small wave functions but they move rapidly and fly apart. In summary, in a Bose-Einstein condensate, the individual bosons become indistinguishable. Two examples of materials containing Bose-Einstein condensates are superconductors and superfluids. Superconductors conduct electricity with virtually zero electrical resistance: Once a current is started, it flows indefinitely. The

liquid in a superfluid also flows forever. In effect, there is no friction. The nucleons in a neutron star are believed to form a superfluid. Scientists have been able to make superfluids in the laboratory by cooling materials to very low temperatures. Helium-4 below a temperature of 2.17 Kelvins is an example.

1.2.The ideal Bose gas in *d*-dimensions

We will consider an equilibrium gas at temperature T in the grand canonical ensemble, where the chemical potential μ is fixed and the number of particles N is fluctuating. In the thermodynamic limit ($N \to \infty$) this is equivalent to the description in the canonical ensemble (fixed N and fluctuating μ).

In any dimension and confining potential the gas is characterized by a set of eigenenergies of an individual particle, E_υ, with the index υ labeling quantum numbers of the particle eigenstates. The (average) total number of particles N is then related to the temperature and chemical potential by the equation

$$N = \sum_{\upsilon} \frac{1}{e^{\beta(E_\upsilon - \mu)} - 1}, \tag{1.1}$$

where $\beta = 1/T$.

1.2.1. Uniform gas

In an infinitely large uniform gas the particle eigenstates are characterized by the momentum k and the eigenenergy $E_k = \hbar^2 k^2 / 2m$, where m is the mass of a particle. For a numerical evaluation, we take the k 's to be sufficiently dense so that we may regard them as quasi-continuous. This allows us to change the sum to an integral via the general formula: $\sum_k \to V \int \frac{d^d k}{(2\pi)^d}$, Then Eq.(1.1) takes the form

$$N = N_c + \Omega \int \frac{d^d k}{(2\pi\hbar)^d} \frac{1}{e^{\beta(E_k - \mu)} - 1}, \tag{1.2}$$

with d being the dimension of the system, Ω the d -dimensional volume and N_c is the condensed number of particles.

We consider the transformation from Cartesian to spherical coordinates

$$\int_{-\infty}^{+\infty} dx_1 ... dx_d = S_d \int_0^{\infty} dr\, r^{d-1}, \tag{1.3}$$

where $S_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the surface of the d -dimensional unit sphere.

We use (1.3) to write the non condensed number of particles

$$\tilde{N} = N - N_c = \frac{\Omega}{\Gamma(d/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{d/2}\int_0^\infty dE\,\frac{E^{\frac{d}{2}-1}}{e^{\beta(E_k-\mu)}-1}\ . \tag{1.4}$$

Comparing (1.4) with the well known expression

$$\tilde{N} = \int_0^\infty dE\,\frac{g_d(E)}{e^{\beta(E_k-\mu)}-1}, \tag{1.5}$$

we obtain for the density of state

$$g_d(E) = \frac{\Omega}{\Gamma(d/2)}\left(\frac{m}{2\pi\hbar^2}\right)^{d/2} E^{\frac{d}{2}-1}. \tag{1.6}$$

It is convenient to express the thermodynamic quantities in terms of the thermal De-Broglie wavelength $\lambda = \sqrt{2\pi\hbar^2\beta/m}$ and the generalized Riemann zeta-function

$$\zeta_\alpha = \frac{1}{\Gamma(\alpha)}\int_0^\infty dx\,\frac{x^{\alpha-1}}{z^{-1}e^x-1}, \tag{1.7}$$

where $z = e^{\mu/k_BT}$ is the fugacity.

Therefore, the total number of particles can be rewritten as

$$N = N_c + \frac{\Omega}{\lambda^d}\zeta_{d/2}(z). \tag{1.8}$$

Varying the temperature, the chemical potential must adapt so that the total number of particles is conserved. On the other hand, the chemical potential is bounded from above by zero. For this critical value of the chemical potential, the number of excited states in (1.8) reaches a maximum. If the total number of particles N exceeds the available excited energy levels, all excess particles must be accommodated in the ground state E_0.

To calculate the limit $z \to 1$, we use the series representation of the generalized ζ-function for small negative values of the chemical potential, (see Appendix A)

$$\zeta_\alpha\left(e^{\beta\mu}\right) = \Gamma(\alpha-1)(-\beta\mu)^{\alpha-1} + \sum_{j=0}^{\infty}\frac{(\beta\mu)^j}{j!}\zeta(\alpha-j)\ . \tag{1.9}$$

Thus, in the limit $z \to 1$, the generalized zeta function reduces to the Riemann zeta-function

$$\underset{z\to 1}{\zeta_{d/2}(z)} = \zeta(d/2). \tag{1.10}$$

For temperatures higher than the critical temperature, $\tilde{N} \le N$ and the chemical potential has a negative value. As the system approaches the critical temperature, the

chemical potential increases until it reaches the limit $\mu \to 0$ as $z \to 1$. For temperatures below T_c, μ remains zero so that N_c increases while $\widetilde{N}$ decreases.

We now turn to calculate the critical temperature at the onset of the phase transition, where the chemical potential vanishes. Then, using (1.8) and (1.10), the maximum number of particles in the excited states is given by

$$\widetilde{N} = N = \frac{\Omega}{\lambda^d}\zeta(d/2). \tag{1.11}$$

We thus arrive at the following expression for the critical temperature

$$k_B T_c = \frac{2\pi\hbar^2}{m}\left(\frac{N}{\Omega\zeta(d/2)}\right)^{2/d}. \tag{1.12}$$

The condensed fraction as a function of temperature now follows immediately from (1.8) and (1.12):

$$\frac{N_c}{N} = 1 - \left(\frac{T}{T_c}\right)^{d/2}. \tag{1.13}$$

1.2.2. Trapped gas

In the presence of an isotropic trap, the density of states is modified and the thermal behavior differs from that of the free gas. The density of states for the harmonic trapping potential is given by

$$g_d(E) = \frac{E^{d-1}}{\Gamma(d)(\hbar\omega)^d}. \tag{1.14}$$

Using the methods described above, we calculate the number of thermal atoms as

$$\widetilde{N} = \frac{1}{(\hbar\omega\beta)^d\,\Gamma(d)}\int_0^\infty dE\,\frac{E^{d-1}}{e^{\beta(E_k-\mu)}-1} = \frac{\zeta_d(z)}{(\hbar\omega\beta)^d}, \tag{1.15}$$

where we have used (1.7). In analogy with the free gas, the maximum number of particles in the excited levels can be obtained from the limit $z \to 1$, so that we now get

$$\widetilde{N} = N = \frac{\zeta(d)}{(\hbar\omega/k_B T_c)^d}. \tag{1.16}$$

Hence, the critical temperature is given by

$$k_B T_c = \hbar\omega\left(\frac{N}{\zeta(d)}\right)^{1/d}, \tag{1.17}$$

and the temperature dependence of the condensate fraction is, in contrast to (1.13), expressed by

$$\frac{N_c}{N} = 1 - \left(\frac{T}{T_c}\right)^d . \tag{1.18}$$

Let us now apply general results obtained in these two last subsections to review briefly the three dimensional Bose gas.

1.3. Bose gas in three dimensions

It is well-known that Bose-Einstein condensation occurs in the three-dimensional free Bose gas. The occurrence of this phase transition was first described by Einstein [5] after the work of Bose [4] regarding the light quanta hypothesis and Planck's law.

1.3.1. Free case

We have derived all important quantities in the previous section, so that the results for the three-dimensional case are now obtained by setting $d = 3$ dimensions. The total particle number can be calculated using (1.8)

$$N = N_c + \frac{V}{\lambda^3}\zeta_{3/2}(z). \tag{1.19}$$

We now look at the critical properties for $z \to 1$. The condition for BEC to occur is that the number of excited particles reaches its maximum value, i. e. from (1.11)

$$n\lambda^3 = \zeta(3/2), \tag{1.20}$$

where we have introduced the density $n = N/V$. This means that there exists a critical temperature at that the phase transition. It is obtained from (1.12)

$$T_c = \frac{2\pi\hbar^2}{mk_B}\left(\frac{n}{\zeta(3/2)}\right)^{2/3}, \tag{1.21}$$

so that we get for the condensate fraction

$$\frac{N_c}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2} . \tag{1.22}$$

1.3.2. Trapped case

For the trapped gas, we get from (1.21) and (1.22) for the critical temperature

$$T_c = \frac{\hbar\omega}{k_B}\sqrt{N/\zeta(3)} \approx 0.94\hbar\omega\sqrt{N} . \tag{1.23}$$

The condensate fraction decreases with the temperature as

$$\frac{N_c}{N} = 1 - \left(\frac{T}{T_c}\right)^3 . \tag{1.24}$$

1.4. Bose gas in two dimensions

Unlike the 3D case, the function $\mu(T)$ is analytical and shows a monotonic increase of the chemical potential with decreasing temperature up to $T \to 0$. In the thermodynamic limit the population of the ground state ($k = 0$) remains microscopic. One thus can say that there is no BEC in a finite-temperature ideal uniform 2D Bose gas.

1.4.1. Free gas in 2D

In analogy to the three-dimensional case, we evaluate the results from Sections 1.1. The density of states in two dimensions is independent of the energy and is simply given by

$$g_2 = \frac{mA}{2\pi\hbar^2}, \tag{1.25}$$

where A is the area.

For the number of excited particles, we get

$$\widetilde{N} = \frac{A}{\lambda^2}\zeta_1(z). \tag{1.26}$$

This expression contains a significant difference with the three-dimensional case, since this ζ-function diverges at the pole $z = 1$. To look into this more closely, we again use Robinson's formula. However, one has to consider the mathematical correct limit in (1.9) for $\alpha \to 1$ [85,86]

$$\lim_{\alpha\to 1}\zeta_\alpha\left(e^{\beta\mu}\right) = -\ln(-\beta\mu) + \sum_{j=0}^{\infty}\frac{(\beta\mu)^j}{j!}\zeta(1-j) \quad . \tag{1.27}$$

We now substitute this into (1.26) and consider the limit $z \to 1$, $\mu \to 0$

$$\begin{aligned}\widetilde{N} &= \frac{A}{\lambda^2}\lim_{\mu\to 0}\left[-\ln(-\beta\mu) + \sum_{j=0}^{\infty}\frac{(\beta\mu)^j}{j!}\zeta(1-j)\right]. \\ &= -\frac{A}{\lambda^2}\lim_{\mu\to 0}\ln(-\beta\mu)\end{aligned} \tag{1.28}$$

From this we see that the integral over the density of states diverges logarithmically in two dimensions. Hence, there is no Bose-Einstein condensation at finite temperatures. This is true even when interactions are included and has been proved in the Hohenberg theorem [87]. Strictly speaking, BEC is only possible in the theoretical limit, $T = 0$, since in this case $\widetilde{N} = 0$, as can be seen from (1.26).

1.4.2. Trapped gas in 2D

We now turn to the inhomogeneous case, where BEC may occur if the two dimensional gas is trapped in a parabolic potential. From (1.16) the number of thermal particles is determined by

$$\widetilde{N} = \frac{A}{(\hbar\omega\beta)^2}\zeta_2(z). \tag{1.29}$$

We calculate the critical temperature from (1.17)

$$\widetilde{N} = N = \frac{\zeta_2(1)}{(\hbar\omega\beta)^2}, \tag{1.30}$$

from which we get

$$k_B T_c = \frac{\hbar\omega}{\pi}\sqrt{6N}, \tag{1.31}$$

where we have used $\zeta_2(1) = \pi^2/6$.

The temperature dependence of the condensate fraction follows from (1.18)

$$\frac{N_c}{N} = 1 - \left(\frac{T}{T_c}\right)^2. \tag{1.32}$$

The result of Eq. (1.32) is similar to that in the 3D case and it was first obtained by Bagnato and Kleppner [88]. They showed also that BEC can occur in general in two dimensions for any power law trapping potential $V = r^\eta$. In the vicinity of $\eta = 2$ (parabolic trapping potential), the critical temperature has a broad maximum [88].

1.5. Bose gas in one dimension

In 1D the situation is also very interesting. In this case, Bose-Einstein condensation cannot occur even in the presence of harmonic confinement because of the logarithmic divergence in the integral (1.5). In fact, in the thermodynamic limit the population of the ground state remains microscopic for any T indicating the absence of BEC in this system. One can define a degeneracy temperature T_d for lower-dimensional systems that indicates the transition from the classical regime to the regime where a quantum treatment is needed because the thermal de Broglie wavelength starts to exceed the average interparticle separation. For a homogeneous Bose gas in 1D, Eq.(1.11) yields

$$N = \frac{L}{\lambda}g_{1/2}(z). \tag{1.33}$$

Note that $g_{1/2}(z)$ diverges as $z \to 1$, consistent with the absence of a macroscopically occupied ground state in 1D in the semiclassical approximation. Degeneracy for a one-dimensional homogeneous Bose gas is thus reached for

$$T_d = \frac{\hbar^2 n^2}{2mk_B}, \tag{1.34}$$

where n is the 1D density.

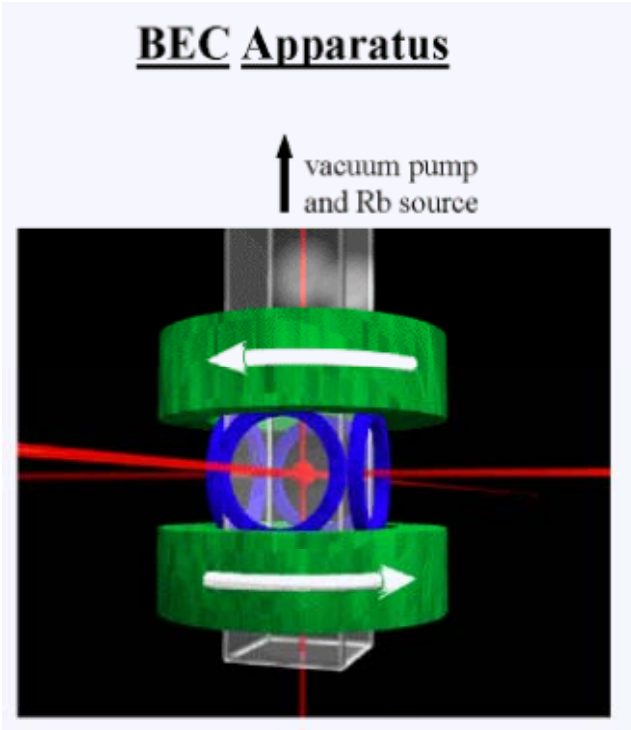
In a trapped 1D ideal Bose gas the critical temperature can be estimated to be [4]

$$k_B T_c = \frac{N}{\ln(2N)}\hbar\omega . \tag{1.35}$$

Despite the fact that one cannot have BEC in the thermodynamic limit, for finite values of N the system can nevertheless exhibit a large occupation of the lowest single-particle state in a useful interval of temperatures.

1.6.How to create BEC? Experimental realization

The general strategy to realize BEC in the 1995 experiment: first precool the gas by laser cooling techniques, then confine the gas in a magnetic trap, finally further cool the trapped gas by forced evaporative cooling to reach the critical temperature. The experimental apparatus is shown below:



In this experiment, six laser beams intersect in a glass cell, creating a magneto-optical trap (MOT). ^{87}Rb atomic gas is contained in the cell which is 2.5 cm square by 12 cm long, and the beams are 1.5 cm in diameter. The coils generating the fixed quadrupole magnetic field and rotating transverse components of the TOP trap magnetic fields are shown in green and blue, respectively.

After laser-cooling techniques achieved temperatures in the range of a few μK, evaporative cooling was carried out to further cool the atom gases. However, at that time there was a severe problem in the magnetic trap. The magnetic trap is shown in the figure below.

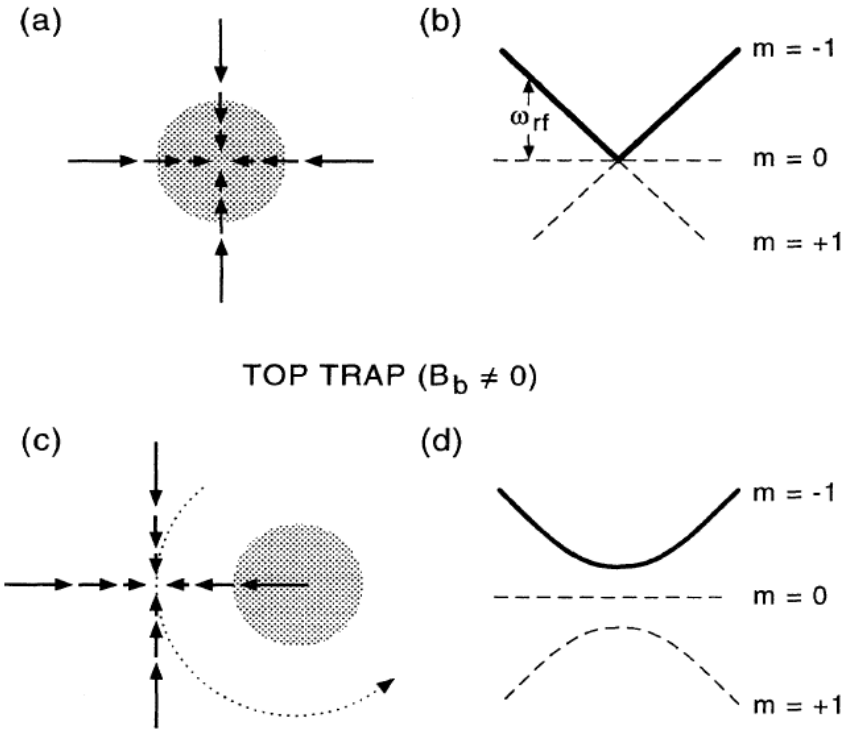


Figure 1.1. Magnetic trap, (a) is the magnetic configuration and (b) is the cylindrically symmetric potential of the quadrupole trap.

The magnetic trap has a zero field at the centre where atoms can undergo transitions and thus escape from the trap. As the cloud gets colder, atoms spent more time near the hole and are quickly lost from trap. Eric Cornell proposed a solution to the leaky trap problem: the time-orbiting potential (TOP) as shown in (c) and (d). The idea of TOP is like this: when you add a transverse magnetic field to the quadrupole trap, the hole will be moved away from the trap centre to a place in the direction of the transverse magnetic field. If you move the location of the hole faster than the average time taken for atoms to find it, the atoms will be constantly chasing the hole and will never find it. A smooth way to achieve this is to add a rotating field that moves the hole around in a circle. The time averaged pseudo-potential is then a smooth potential well with a non-zero minimum. To be concrete, the magnetic field in the quadrupole trap is

$$\begin{aligned} \vec{B} &= B'(x, y, -2z) \\ B &= B'\left(x^2 + y^2 + 4z^2\right). \end{aligned} \tag{1.36}$$

After adding a rotating, spatially-uniform magnetic field, the field becomes

$$\vec{B} = \left(B'x + B_0 \cos\omega t, B'y + B_0 \sin\omega t, -2B'z\right)$$

$$B(t) = \left[\left(B'x + B_0 \cos\omega t\right)^2 + \left(B'y + B_0 \sin\omega t\right)^2 + 4B'^2 z^2\right]^{1/2}$$

$$\approx \mathrm{B}_0 + B'\left(x\cos\omega t + y\sin\omega t\right) + \frac{B'^2}{B_0}\left[x^2 + y^2 + 4z^2 - \left(x\cos\omega t + y\sin\omega t\right)^2\right] . \quad (1.37)$$

$$\langle B \rangle = \mathrm{B}_0 + \frac{B'^2}{B_0}\left(x^2 + y^2 + 8z^2\right)$$

Plugging the leaky trap was the final hurdle in achieving BEC. In July 1995, Cornell and Wieman announced that they had observed BEC in a gas of ^{87}Rb atoms. The transition temperature was 170 nK. The researchers have imaged the cloud by first allowing it to expand and then illuminating with a pulse of resonant light. The light absorbed by the cloud cast a shadow on a CCD camera. The velocity distribution of the atom cloud is shown below.

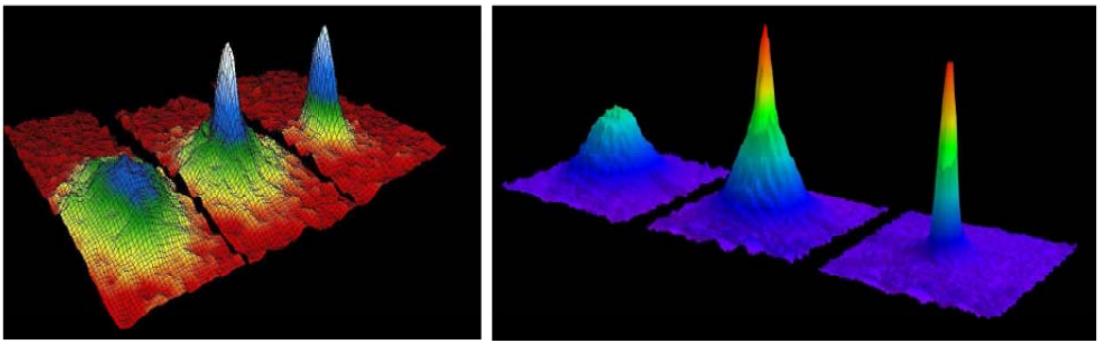


Figure 1.2. Images from the first BEC experiments of 87Rb at JILA (left) and 23Na at MIT (right). From left to right in each image, surface plots are shown of velocity distributions and real-space distrubutions, respectively, at temperatures just above, at, and below the critical temperature for BEC. The sharpening of the distribution below the critical temperature provides evidence BEC formation. Figures used with permission of E. A. Cornell from [67] (left) and W. Ketterle from [68] (right).

The striking feature of this experience was that there were three clear and distinct signature of BEC which made any skeptic immediately convinced:

(1) The appearance of the condensate was marked by a narrow, intense peak of atoms near the centre (zero-velocity region), corresponding to the ground state of the trap.

(2) As the temperature was lowered below the transition temperature, the density of atoms in the peak increased abruptly, indicating a phase transition.

(3) The atoms in the peak had a nonthermal velocity distribution as predicted by quantum mechanics for the ground state of the trap, thus indicating that all these atoms were in the same quantum state.

Chapter 2

Field Theory for Bose Gases

2.1. The Gross-Pitaevskii Equation

When describing a many-particle system, like the dilute Bose gas in a trap, it is impossible in practice to take the motion of every single particle into account. A characteristic of the phenomenon of Bose-Einstein condensation is the occurrence of a macroscopically occupied state that can be described by a classical wave function. At temperatures well below the critical temperature, where the phase transition to Bose- Einstein condensation occurs, this is an excellent description of the condensed state. Even at higher temperatures one can treat the thermal atoms as fluctuations of this classical field to a very good approximation. Important properties of the condensate, like its shape and its momentum distribution, can be described by a non-linear Schrödinger equation. The interactions between the atoms are accounted for by a term proportional to the condensate density $|\Phi(r)|^2$.

Let us consider a system of trapped bosons interacting via a two-body potential. The grand canonical Hamiltonian may be written in the form

$$H = \int d\vec{r}\hat{\Psi}^+(\vec{r},t)h^{sp}\hat{\Psi}(\vec{r},t) + \frac{1}{2}\int\int d\vec{r}d\vec{r}'\hat{\Psi}^+(\vec{r},t)\hat{\Psi}^+(\vec{r}',t)V(\vec{r},\vec{r}')\hat{\Psi}(\vec{r}',t)\hat{\Psi}(\vec{r},t)\,, \qquad (2.1)$$

where $h^{sp} = -\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(\vec{r})$ is the single particle Hamiltonian, $V(\vec{r},\vec{r}')$ is the two-body interaction potential, and $V_{\text{ext}}(\vec{r})$ the external confining field. $\hat{\Psi}^+(\vec{r})$ and $\hat{\Psi}(\vec{r})$ are the creation and annihilation operators satisfying to the usual commutation relations

$$\left[\hat{\Psi}(\vec{r}),\hat{\Psi}^+(\vec{r}')\right] = \delta(\vec{r},\vec{r}')\,, \qquad \left[\hat{\Psi}^+(\vec{r}),\hat{\Psi}^+(\vec{r}')\right] = \left[\hat{\Psi}(\vec{r}),\hat{\Psi}(\vec{r}')\right] = 0\,. \qquad (2.2)$$

This Hamiltonian is the starting point for all theoretical treatments of dilute Bose gases, and includes both thermal and quantum fluctuations. All theories appearing in the literature arise from distinct approximations for this Hamiltonian. For dilute gases at very low temperature, the usual procedure is to make a contact interaction approximation

$$V(\vec{r},\vec{r}') = g\delta(\vec{r}-\vec{r}') \ . \tag{2.3}$$

The potential (2.3) means that the two atoms undergo perfectly elastic local collisions, like two billiard balls. The strength of the interaction is given by $g = 4\pi\hbar^2 a/m$, where a is the s-wave scattering length for a particular atomic species, which can be determined from experiments. This is a somewhat idealized scenario, which can nonetheless be put on firm ground by a more careful treatment - the origin and validity of this approximation will be discussed later.

Substitution into the Hamiltonian (2.2) then gives:

$$H = \int d\vec{r}\hat{\Psi}^+(\vec{r},t)h^{sp}\hat{\Psi}(\vec{r},t) + \frac{g}{2}\int d\vec{r}\hat{\Psi}^+(\vec{r},t)\hat{\Psi}^+(\vec{r},t)\hat{\Psi}(\vec{r},t)\hat{\Psi}(\vec{r},t) \ . \tag{2.4}$$

The starting point for the dynamics of ultracold gases is to consider the equation governing the evolution of the bosonic field operator $\hat{\Psi}(\vec{r},t)$, i.e. the so-called equation of motion. The second-quantized form of the appropriate equation can be analyzed in one of three distinct pictures, known as the Schrödinger, and Heisenberg pictures, depending on whether the state-vectors, the operators corresponding to system observables, or both are time-dependent [89, 90]. In the Schrödinger picture, the state vectors are time-dependent and the operators are time-independent; in this picture, the solution of the Schrödinger equation at time t, given the initial solution at t_0, is given by the unitary transformation $|\Psi_S(t)\rangle = e^{-i\hat{H}(t-t_0)/\hbar}|\Psi(t_0)\rangle$ where $\hat{H}$ does not contain any explicit time-dependence, and the subscript `S' has been introduced to denote the Schrödinger picture. In the interaction picture, both operators and state vectors depend on time. Finally, in the Heisenberg picture the state vectors, which can be constructed from the corresponding Schrödinger picture state vectors via $|\Psi_H(t)\rangle = e^{i\hat{H}t/\hbar}|\Psi_S(t)\rangle$, are time-independent and all time dependence is contained in the operators.

While all three pictures can be used interchangeably, most subsequent discussion will be given in the Heisenberg picture in which the equation of motion of a general operator $\hat{O}_H$ obeys

$$i\hbar\frac{d\hat{O}_H}{dt} = \left[\hat{O}_H,\hat{H}\right]. \tag{2.5}$$

In studying the system dynamics, we will actually be concerned with the equations of motion of the Bose field operator $\hat{\Psi}$. For the Hamiltonian of Eq. (2.5), this evolves according to the Heisenberg equation of motion

$$i\hbar \frac{d\hat{\Psi}(\vec{r},t)}{dt} = \left[\hat{\Psi}(\vec{r},t), \hat{H}\right] = h^{sp}\hat{\Psi}(\vec{r},t) + g\hat{\Psi}^{+}(\vec{r},t)\hat{\Psi}(\vec{r},t)\hat{\Psi}(\vec{r},t). \tag{2.6}$$

In order to extract information from this equation, it is convenient to separate the condensate contribution, which corresponds to the macroscopic occupation of a single quantum state, from the remaining part of the Bose field operator. Hence the Bose-field operator is divided into two parts [18, 91]

$$\hat{\Psi}(\vec{r},t) = \Phi(\vec{r},t) + \hat{\tilde{\Psi}}(\vec{r},t), \tag{2.7}$$

corresponding respectively to a field operator for the condensate, $\hat{\Phi}$, and one for the non-condensed atoms, $\hat{\tilde{\Psi}}$. These could either correspond to thermally-excited atoms, quantum-mechanical fluctuations, or atoms promoted into higher energy states due to interactions. It is important to notice at this level that the condensate is described by a classical function and not by a field operator. This approximation is well justified since the ground state is macroscopically occupied [91].

Then we break down the full system Hamiltonian into various contributions based on the number of condensate and non-condensate factors contained in each of them. In particular, substitution of Eq. (2.7) into the system Hamiltonian (2.4) leads to

$$H = H_0 + H_1 + H_2 + H_3 + H_4, \tag{2.8}$$

where

$$\begin{aligned}
H_0 &= \int d\vec{r}\left[\Phi^{*}\hat{h}^{sp}\Phi + \frac{g}{2}|\Phi|^4\right] \\
H_1 &= \int d\vec{r}\left[\hat{\tilde{\Psi}}^{+}\left(\hat{h}^{sp}\Phi + g|\Phi|^2\right)\Phi + \Phi^{*}\left(\hat{h}^{sp}\Phi + g|\Phi|^2\right)\hat{\tilde{\Psi}}\right] \\
H_2 &= \int d\vec{r}\left[\hat{\tilde{\Psi}}^{+}\left(\hat{h}^{sp}\Phi + 2g|\Phi|^2\right)\hat{\tilde{\Psi}} + \frac{g}{2}\left(\Phi^{*2}\hat{\tilde{\Psi}}\,\hat{\tilde{\Psi}} + \hat{\tilde{\Psi}}^{+}\hat{\tilde{\Psi}}^{+}\Phi^{2}\right)\right] \\
H_3 &= g\int d\vec{r}\left[\Phi\hat{\tilde{\Psi}}^{+}\hat{\tilde{\Psi}}^{+}\hat{\tilde{\Psi}} + \Phi^{*}\hat{\tilde{\Psi}}^{+}\hat{\tilde{\Psi}}\,\hat{\tilde{\Psi}}\right] \\
H_4 &= \frac{g}{2}\int d\vec{r}\hat{\tilde{\Psi}}^{+}\hat{\tilde{\Psi}}^{+}\hat{\tilde{\Psi}}\,\hat{\tilde{\Psi}}
\end{aligned} \tag{2.9}$$

In the $T = 0$ limit, all of the particles are in the condensate, so that $N = N_0$ and the noncondensate operator can be neglected ($\hat{\tilde{\Psi}} = \hat{\tilde{\Psi}}^{+} = 0$); in other words, we set $\hat{\Psi}(\vec{r},t) \to \Phi(\vec{r},t)$. Hence, $\hat{\Psi}^{+}(\vec{r},t) \to \Phi^{*}(\vec{r},t)$, so in this case we consider only H_0.

The exact Heisenberg equation of motion (2.5) reduces then to the so-called Gross-Pitaevskii Equation (GPE) [38,39]

$$\begin{aligned} i\hbar\frac{d\Phi(\vec{r},t)}{dt} &= \left[\hat{h}^{sp}(\vec{r},t)+g\left|\Phi(\vec{r},t)\right|^2\right]\Phi(\vec{r},t) \\ &= \left[-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\vec{r},t)+g\left|\Phi(\vec{r},t)\right|^2\right]\Phi(\vec{r},t) \end{aligned} . \tag{2.10}$$

This equation is a nonlinear Schrödinger equation, corresponding to the zero temperature hydrodynamic description of Bose gases, first introduced to study vortex lines in an imperfect Bose gas. This equation is mathematically analogous to a Ginzburg-Landau-type approach [40], valid near the critical regime although the origin of the various contributions and the physical interpretation here is actually quite distinct. Remarkably, the GPE, which was first numerically implemented for dilute weakly-interacting trapped Bose gases was undertaken by Mark Edwards, Keith Burnett and collaborators [92-94], provides a good description of the dynamics of a Bose-Einstein condensate for a wide class of problems at temperatures as high as $T \approx T_c/2$. The GPE can be used, at low temperature, to explore the macroscopic behavior of the system, characterized by variations of the order parameter over distances larger than the mean distance between atoms.

One can find static solutions by eliminating the time-dependence via the transformation:

$$\Phi(\vec{r},t)=\Phi(\vec{r})e^{-i\mu t/\hbar}, \tag{2.11}$$

where μ is the chemical potential (which is equal to the energy per particle only for non-interacting particles). Substituting (2.11) into (2.10) yields the time-independent GPE:

$$\mu\Phi(\vec{r})=\left[-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\vec{r})+g\left|\Phi(\vec{r})\right|^2\right]\Phi(\vec{r}). \tag{2.12}$$

In the form given above, the wavefunction is normalized to the total number of particles, i.e. $\int\left|\Phi(\vec{r},t)\right|^2 d\vec{r}=N$.

Alternatively, the Gross-Pitaevskii equation (2.10) can also be obtained using a variational procedure:

$$i\hbar\frac{d\Phi}{dt}=\frac{\delta E}{\delta\Phi^*}, \tag{2.13}$$

where the energy functional E is given by

$$E[\Phi] = \int dr\left[-\frac{\hbar^2}{2m}|\nabla\Phi|^2 + V_{ext}(r)|\Phi|^2 + \frac{g}{2}|\Phi|^4\right]. \\ = E_{kin} + E_p + E_{int} \tag{2.14}$$

The first term in the integral (2.14) is the kinetic energy of the condensate E_{kin} , the second is the trapping energy E_p, while the last one is the mean field interaction energy E_{int}. In the case of nonnegative and finite-range interatomic potentials, rigorous bounds for this term have been obtained by Dyson [95], and Lieb and Yngvason [96].

2.1.1. Ground state Solution of GPE

Let us consider a system of interacting bosons confined in a spherical harmonic trapping potential given by $V_{ext} = \frac{1}{2}m\omega^2 r^2$. In order to find the ground state condensate wavefunction, one should solve Eq. (2.10) which now takes the form

$$-\frac{\hbar^2}{2m}\Delta_r\Phi(\vec{r}) + \frac{m\omega^2 r^2}{2}\Phi(\vec{r}) + g|\Phi(\vec{r})|^2\Phi(\vec{r}) - \mu\Phi(\vec{r}) = 0. \tag{2.15}$$

2.1.1.a. Ideal gas

For an ideal gas ($g = 0$) the ground state solution is simply the ground state wavefunction of the harmonic oscillator

$$\Phi(\vec{r}) = \frac{\sqrt{N}}{\pi^{3/4}a_{H0}^{3/2}}\exp\left(-\frac{r^2}{2a_{H0}^2}\right), \tag{2.16}$$

where $a_{H0} = \sqrt{\hbar/m\omega}$ is the oscillator length. The solution (2.16) has orbital angular momentum $l = 0$, and the chemical potential is $\mu = 3\hbar\omega/2$. The energy per particle in the first excited state is higher by $\hbar\omega$.

2.1.1.b. Thomas-Fermi limit

In the case of atoms with repulsive interaction ($a > 0$), the limit $Na/a_{H0} >> 1$ is particularly interesting, since this condition is well satisfied by the parameters N, a and a_{H0} used in most of current experiments. Moreover, in this limit the predictions of mean-field theory take a rather simple analytic form Edwards and Burnett [94]; Baym and Pethick [97]. As regards the ground state, the effect of increasing the parameter Na/a_{H0} is clearly seen in Figure1.1, the atoms are pushed outwards, the central density becomes rather flat, and the radius grows. As a consequence, the kinetic term in the Gross-Pitaevskii takes a significant contribution only near the

boundary and becomes less and less important with respect to the interaction energy. If one neglects completely the kinetic term in Eq. (2.15), one gets the density profile in the form

$$n(r) = [\mu - V_{ext}(r)]/\, g\,, \tag{2.17}$$

in the region where $\mu > V_{ext}(r)$, and $n = 0$ outside. This is often referred to as Thomas-Fermi (TF) approximation. The normalization condition on $n(\mathbf{r})$ provides the relation between chemical potential and number of particles:

$$\mu = \frac{\hbar\omega}{2}\left(\frac{15Na}{a_{H0}}\right)^{2/5}. \tag{2.18}$$

Note that the chemical potential $\mu = \partial E / \partial N$, the energy per particle turns out to be $E/N = (5/7)\mu$. This energy is the sum of the interaction and oscillator energies, since the kinetic energy gives a vanishing contribution for large *N*.

The density profile Eq.(2.17) has the form of an inverted parabola, which vanishes at the classical turning point R defined by the condition $\mu = V_{ext}(r)$. For a spherical trap, this implies $\mu = m\omega^2 R^2/2$ and, using the result (2.18) for μ, one finds the following expression for the radius of the condensate

$$R_{TF} = a_{H0}\left(\frac{15Na}{a_{H0}}\right)^{1/5}, \tag{2.19}$$

which grows with *N*.

It is interesting to note at this stage that the application of the TF approximation to the trapped Bose gases was pioneered by the earlier work of Goldman, Silvera and Legget [98], by Oliva [99] and by Chou, Yang, and Yu [100], by Timmermans, Tommasini and K. Huang [101] and P. Schuck *et al* [102].

It is worth mentioning at this stage that a finite temperature version of the Thomas-Fermi approximation was also investigated by using the Time dependent Hartree-Fock-Bogoliubov equations [103]. Where in particular extended analytic expressions for the condensate, the noncondensate and anomalous densities are derived. The exploration of these equations at finite temperature leads to the fact that all the thermodynamics quantities deviate from the standard values in the TF regime. The results are quite encouraging owing to the simplicity of the formalism [104].

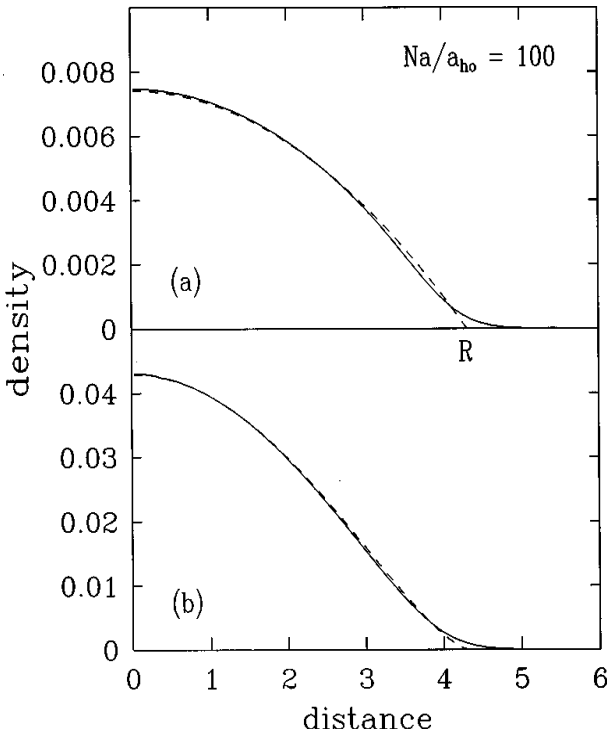


Figure 2.1. Density profile for atoms interacting with repulsive forces in a spherical trap, with $Na/a_{Ho}=100$. Solid line: solution of the stationary GPE. Dashed line: Thomas-Fermi approximation. In the upper part, the atom density is plotted in arbitrary units, while the distance from the center of the trap is in units of a_{Ho}.

For a system of noninteracting bosons in a harmonic trap, the condensate has the form of a Gaussian of average width a_{Ho} and the central density is proportional to *N*. If the atoms are interacting, the shape of the condensate can change significantly with respect to the Gaussian. The scattering length entering the Gross-Pitaevskii equation can be positive or negative, its sign and magnitude depending crucially on the details of the atom-atom potential. Positive and negative values of a correspond to an effective repulsion and attraction between the atoms, respectively. The numerical solution of the GP Eq. (2.12) shows that the change can be dramatic when the interaction energy is much greater than the kinetic energy, that is, when $Na/a_{Ho} >> 1$. The central density is lowered (raised) by a repulsive (attractive) interaction and the radius of the atomic cloud consequently increases (decreases). Note that the effect of the interaction has important consequences, not only for the structure of the ground state, but also for the dynamics and thermodynamics of the system, as we will see later on.

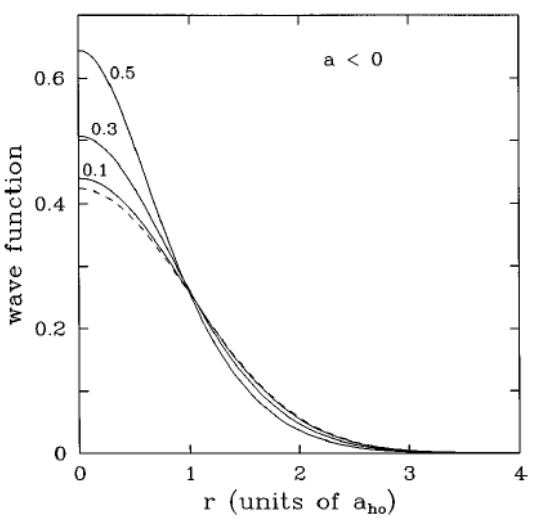


Figure 2.2. Condensate wave function, at *T*=0, obtained by solving numerically the stationary GP Eq. (39) in a spherical trap and with attractive interaction among the atoms ($a<0$). The three solid lines correspond to Na/a_{Ho} 0.1, 0.3, 0.5. The dashed line is the prediction for the ideal gas. Here the radius *r* is in units of the oscillator length a_{Ho} and we plot $\sqrt{a_{H0}^3/N}\Phi(r)$, so that the curves are normalized to 1.

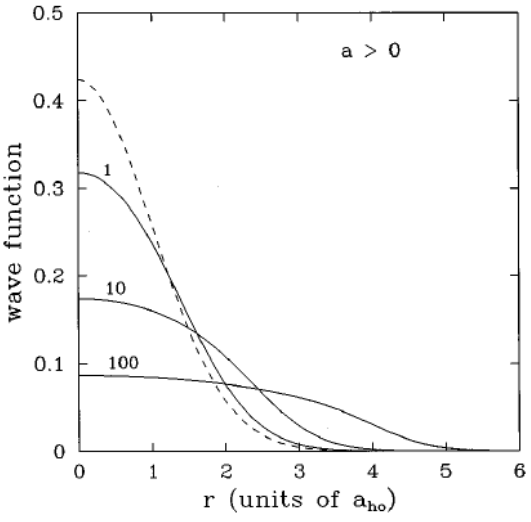


Figure 2.3. Same as in Fig. 2, but for repulsive interaction ($a>0$) and Na/a_{Ho} 1, 10, 100.

2.1.2. Hydrodynamic approach

Solving the time-dependent Gross-Pitaevskii Eq. (2.10) is not always the most adequate way to study the properties of Bose-Einstein condensates. When it comes to the low-lying excitations, for example, it is often useful to switch to an equivalent treatment which is provided by the hydrodynamic equations.

In a homogeneous system, the hydrodynamic excitations are sound waves, i.e. density fluctuations in the sample. For trapped gases the excitations are not plane waves anymore and have to be classified according to the symmetries present in the trap geometry. Besides the low-lying excitations, which are studied by shaking the gas out of the ground state into the lowest excited states, it is also important to consider time-of-flight experiments, in which the sample is released from the trap, and expands freely in space. Both types of phenomena can be investigated within the hydrodynamic formalism, which we derive now starting from the time-dependent Gross-Pitaevskii Eq. (2.10).

A useful reformulation of the Gross-Pitaevskii equation is obtained by factorizing the condensate wave function according to the Madelung transformation: $\Phi(\vec{r},t)=\sqrt{n(\vec{r},t)}e^{i\theta(\vec{r},t)}$, with n the atomic density and θ the phase of the order

parameter and it is a real quantity, related to the superfluid velocity field by $v = (\hbar / m)\nabla\theta$. Substituting this expression in Eq. (2.10) and separating real and imaginary parts, one gets the following set of hydrodynamic equations:

$$\frac{dn}{dt} + \nabla.(nv) = 0\,, \tag{2.21}$$

$$-\hbar\frac{d\theta}{dt} = \frac{\hbar^2}{2m}(\nabla\theta)^2 - \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{n}}{\sqrt{n}} + V_{ext}(r) + gn\,. \tag{2. 22}$$

If the repulsive interaction among atoms is strong enough, then the density profiles become smooth and one can safely neglect the kinetic-pressure term, proportional to $\hbar^2$, in the equation for the velocity field, which then takes the form

$$-\hbar\frac{d\theta}{dt} = \frac{\hbar^2}{2m}(\nabla\theta)^2 + V_{ext}(r) + gn\,. \tag{2. 23}$$

This result corresponds to the equation of potential flow for a fluid whose pressure and density are related by the equation of state $P = gn^2/2$. Equations (2.21) and (2.22) have the typical structure of the dynamic equations of superfluids at zero temperature (see, for example, Pines and Nozieres, 1966, Vol. II [105]) and can be viewed as a particular case of the more general Landau's theory of superfluidity.

2.1.3. Superfluidity

Superfluidity is closely related to Bose-Einstein condensation. In a phenomenological level, superfluid can flow through narrow capillaries or slits without dissipating energy. Superfluid does not possess the shear viscosity. The superfluid of liquid ^{4}He, below the so-called λ-point, was discovered by Kapitza [12] and independently by Allen and Misener [13]. Soon after Landau explained that if the excitation spectrum satisfies certain criteria, the motion of the fluid does not cause the energy dissipation [16, 17]. These Landau criteria are met by the Bogoliubov excitation spectrum associated with the Bose-Einstein condensate consisting of an interacting Bose gas and thus establish the first connection between superfluidity and BEC. The connection between the two phenomena is further established in a deeper level through the relationship between irrotationality of the superfluid and the global phase of the BEC order parameter.

2.1.3.a. The Landau's criteria

We consider a fluid at zero temperature, in which all particles are in the ground state and flowing along a capillary at constant velocity v. If the fluid is viscous, the motion will produce dissipation of energy via friction with the capillary wall and decrease of

the kinetic energy. We assume that such dissipative processes take place through the creation of elementary excitation, which is the Bogoliubov quasi-particle ε_k (see below) for the case of an interacting Bose gas. The Landau's criteria of superfluidity satisfy the following condition:

$$v_c = \min_k \frac{\varepsilon_k}{|k|} \ , \tag{2.24}$$

where the minimum is calculated over all the values of k. If instead the fluid velocity v is smaller than (2.24), then no elementary excitation will be spontaneously formed. Thus, the Landau's criterion of superfluidity is summarized as the relative velocity between the fluid and the capillary is smaller than the critical value $v \le v_c$.

2.1.3.b. Quantized vortices in superfluids

The story of quantized vortices provides an important insight into the problem of rotations in superfluids. Quantized vortices were first predicted by Onsager [23] and Feynman [24]. In fact, it is well known that a superfluid cannot rotate. In usual rigid systems, the tangential velocity corresponding to a rotation is given by $v = \Omega \times r$, where Ω is the angular velocity vector and r is the distance vector from the origin of rotation. The circulation of the tangential velocity over a closed contour around the *z*-axis is given by

$$\oint v_s d\ell = 2\pi \frac{\hbar}{m} \ell \ , \tag{2.25}$$

which is quantized in units of $\hbar / m$, independent of the radius of the contour. This is called "Onsager-Feynman quantization condition".

2.2. The Bogoliubov approximation

The Hamiltonian of Eq. (2.1) thus represents, in the occupation number representation of second quantization the basic system Hamiltonian corresponding to the original position representation. For a uniform gas occupying a volume V, the field operator $\hat{\Psi}(\vec{r})$ can be expanded by the plane waves:

$$\hat{\Psi}(\vec{r}) = \sum_{\vec{k}} \frac{1}{V} e^{i\vec{k}.\vec{r}} \hat{a}_{\vec{k}} \text{ and } \hat{\Psi}^+(\vec{r}) = \sum_{\vec{k}} \frac{1}{V} e^{-i\vec{k}.\vec{r}} \hat{a}^+_{\vec{k}} \ , \tag{2.26}$$

which are summed over the complete set of single-particle quantum numbers. Upon plugging (2.26) in (2.1), we get

$$\hat{H} = \sum_k \frac{\hbar^2 k^2}{2m} \hat{a}^+_{\vec{k}} \hat{a}_{\vec{k}} + \frac{1}{2V} \sum_{\vec{k},\vec{k}',\vec{q}} \tilde{V}(\vec{q}) \hat{a}^+_{\vec{k}+q} \hat{a}^+_{\vec{k}'-q} \hat{a}_{\vec{k}'} \hat{a}_{\vec{k}} \ . \tag{2.27}$$

Here $\tilde{V}(\vec{q}) = \int V(\vec{r}) e^{-i\vec{q}.\vec{r}} d\vec{r}$ is the Fourier transform of the two body scattering potential.

In real systems $V(\vec{r})$ always contains a short-range term, which makes it difficult to solve the Schrödinger equation at the microscopic level. However, by virtue of the above assumptions on dilute and cold gases, one can conclude that the actual form of $V(\vec{r})$ is not important for describing the macroscopic properties of the gas, as far as the assumed fictitious potential $V_{eff}(\vec{r})$ gives the correct value for the low momentum value of its Fourier transform . It is therefore convenient to replace the actual potential $V(\vec{r})$ with an effective, smooth potential. Since the macroscopic properties of the system depend on $V(q=0) = g$, this procedure will provide the correct answer to this complicated many-body problem as far as the system is dilute and cold.

Replacing $\tilde{V}(q=0) = g$ in (2.27), yields a new simpler Hamiltonian

$$\hat{H} = \sum_{k} \frac{\hbar^2 k^2}{2m} \hat{a}_{\vec{k}}^{+} \hat{a}_{\vec{k}} + \frac{g}{2V} \sum_{k} \hat{a}_{\vec{k}+q}^{+} \hat{a}_{\vec{k}'-q}^{+} \hat{a}_{\vec{k}'} \hat{a}_{\vec{k}} \ . \tag{2.28}$$

Since the lowest energy state is macroscopically occupied by number of particles in BEC, one can neglect the quantum fluctuation of this state and replace the operator a_0 by a *c*-number: $a_0 = a_0^{+} = \sqrt{N}$. The Hamiltonian (2.28) separates into eight distinct parts

$$\begin{aligned}
E_0 &= \frac{1}{2} V n^2 \tilde{V}(0) \\
V_1 &= \frac{1}{2} n \sum_{k} \tilde{V}(q) \hat{a}_{\vec{k}} \hat{a}_{-\vec{k}} \\
V_2 &= \frac{1}{2} n \sum_{k} \tilde{V}(q) \hat{a}_{\vec{k}}^{+} \hat{a}_{-\vec{k}} \\
V_3 &= \frac{1}{2} n \sum_{k} \tilde{V}(q) \hat{a}_{\vec{k}}^{+} \hat{a}_{\vec{k}} \\
V_4 &= \frac{1}{2} n \sum_{k} \tilde{V}(0) \hat{a}_{\vec{k}}^{+} \hat{a}_{\vec{k}} \\
V_5 &= \sqrt{\frac{n}{V}} \sum_{k} \tilde{V}(q) \hat{a}_{\vec{k}+\vec{q}}^{+} \hat{a}_{\vec{k}} \hat{a}_{\vec{q}} \\
V_6 &= \sqrt{\frac{n}{V}} \sum_{k,q} \tilde{V}(q) \hat{a}_{\vec{k}}^{+} \hat{a}_{\vec{q}}^{+} \hat{a}_{\vec{k}+\vec{q}} \\
V_7 &= \frac{1}{2V} \sum_{k,k',q} \tilde{V}(q) \hat{a}_{\vec{k}+\vec{q}}^{+} \hat{a}_{\vec{k}'-\vec{q}}^{+} \hat{a}_{\vec{k}'} \hat{a}_{\vec{k}} \ .
\end{aligned} \tag{2.29}$$

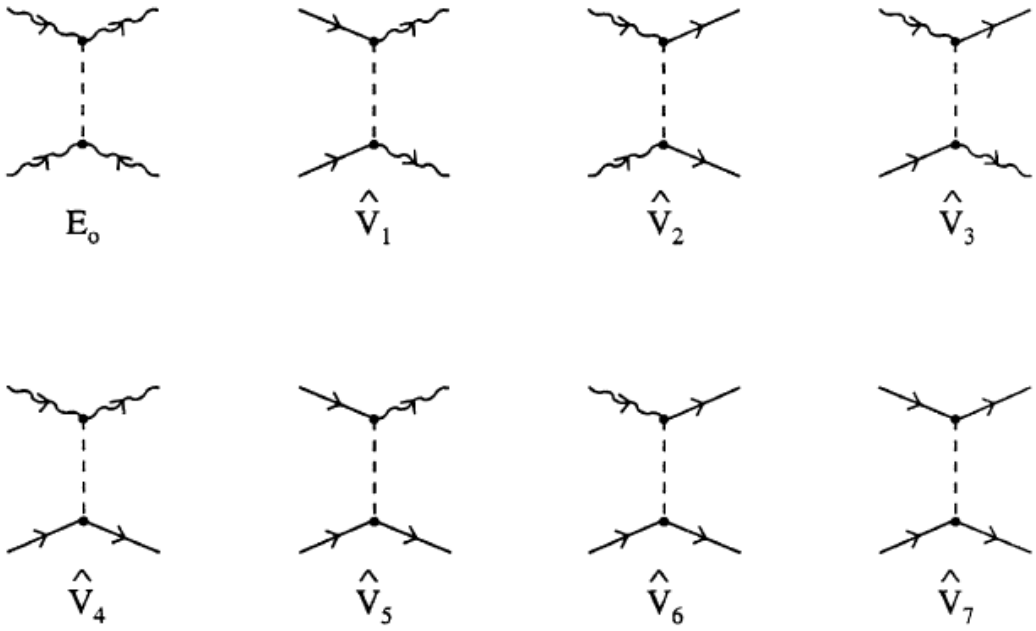


Figure 2.4. Eight distinct processes involved in the interaction *V*. A solid line denotes $\hat{a}$ or $\hat{a}^+$. A wavy line corresponds to a condensate atoms or factor $\sqrt{n}$ and dashed line denotes the interaction $\tilde{V}$.

These parts are represented by the vertex diagrams in figure 2.4. We note that $\hat{H}$ has no term containing a single $\hat{a}_{\vec{k}}$ or $\hat{a}^+_{\vec{k}}$ because these would violate momentum conservation.

By using the normalization relation,

$$\begin{aligned} a_0^+ a_0 &= \hat{N}_c = N - \sum_{k\neq 0} \hat{a}_k^+ \hat{a}_k \\ \left(a_0^+ a_0\right)^2 &= \left(N - \sum_{k\neq 0} \hat{a}_k^+ \hat{a}_k \right)^2 \approx N^2 - 2N \sum_{k\neq 0} \hat{a}_k^+ \hat{a}_k \end{aligned} . \tag{2.30}$$

Substitution of (2.29) and (2.30) into (2.28) yields the following expression for the Hamiltonian:

$$\hat{H} = \frac{1}{2} gnN + \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\vec{k}}^+ \hat{a}_{\vec{k}} + \frac{1}{2} gn \sum_{\vec{k}\neq\vec{0}} \left[2\hat{a}_{\vec{k}}^+ \hat{a}_{\vec{k}} + \hat{a}_{-\vec{k}}^+ \hat{a}_{\vec{k}}^+ + \hat{a}_{\vec{k}} \hat{a}_{-\vec{k}} \right]. \tag{2.31}$$

The third term of this Hamiltonian represents the self-energy of the excited states due to the interaction, simultaneous creation of the excited states at momenta k and $-k$, and simultaneous annihilation of the excited states, respectively (see chapter 4).

Equation (2.31) can be diagonalized by the following linear transformation

$$\begin{aligned} \hat{a}_{\vec{k}} &= u_k \hat{b}_{\vec{k}} - v_k \hat{b}^+_{-\vec{k}} \\ \hat{a}^+_{-\vec{k}} &= u_k \hat{b}^+_{-\vec{k}} - v_k \hat{b}_{\vec{k}} \end{aligned} , \tag{2.32}$$

which known as the Bogoliubov transformation. The two parameters, u_k and v_k, are determined uniquely by the following requirements. The quasiparticles, described by the new operators, $\hat{b}_{\vec{k}}$ and $\hat{b}^+_{\vec{k}}$ are sometimes called *bogolons*. They are assumed to obey the same bosonic commutation relation as the real particle operators, $\hat{a}_{\vec{k}}$ and $\hat{a}^+_{\vec{k}}$

$$\left[\hat{b}_{\vec{k}}, \hat{b}_{\vec{k}'}\right] = \delta_{\vec{k}\vec{k}'}. \tag{2.33}$$

This commutation relation imposes the constraint for the two parameters u_k and v_k:

$$u_k^2 - v_k^2 = 1, \tag{2.34}$$

or equivalently $u_k = \cosh\theta_k$ and $v_k = \sinh\theta_k$. Then the Hamiltonian (2.31) writes

$$\begin{aligned}\hat{H} = \frac{1}{2}gnN + \sum_{\vec{k}\neq 0}\left[\frac{\hbar^2 k^2}{2m}v_k^2 + gn\left(v_k^2 - u_k v_k\right)\right] \\ + \sum_{\vec{k}\neq\vec{0}}\left[\frac{\hbar^2 k^2}{2m}\left(v_k^2 + u_k^2\right) + gn\left(v_k^2 + u_k^2 - 2u_k v_k\right)\right]\hat{b}^+_{\vec{k}}\hat{b}_{\vec{k}} \\ + \sum_{\vec{k}\neq\vec{0}}\left[\frac{\hbar^2 k^2}{2m}u_k v_k + \frac{1}{2}gn\left(v_k^2 + u_k^2 - 2u_k v_k\right)\right]\left(\hat{b}^+_{-\vec{k}}\hat{b}^+_{\vec{k}} + \hat{b}_{\vec{k}}\hat{b}_{-\vec{k}}\right)\end{aligned} \tag{2.35}$$

The value of θ_k must be chosen in order to make the coefficients of the non-diagonal terms $\hat{b}_{\vec{k}}$ and $\hat{b}^+_{\vec{k}}$ in (2.35) vanish. This condition is rewritten as

$$u_k, v_k = \frac{1}{2}\left(\sqrt{\frac{E_k}{\varepsilon_k}} \pm \sqrt{\frac{\varepsilon_k}{E_k}}\right), \tag{2.36}$$

where the Bogoliuibov spectrum is

$$\varepsilon_k = \sqrt{E_k^2 + 2ngE_k}, \tag{2.37}$$

and $E_k = \hbar^2 k^2 / 2m$ is the free particle energy.

Eq.(2.37) is the famous Bogoliubov excitation spectrum. Substituting Eqs. (2.37) and (2.36) into (2.35). The resulting diagonal Hamiltonian is

$$H = E_0 + \sum_{\vec{k}\neq\vec{0}}\varepsilon_k \hat{b}^+_{\vec{k}}\hat{b}_{\vec{k}}, \tag{2.38}$$

where the ground state energy is

$$E_0 = \frac{1}{2}gnN + \sum_{\vec{k}\neq 0}\left(\varepsilon_k - gn + E_k\right). \tag{2.39}$$

Results (2.37)-(2.39) have a deep physical meaning. The original system of interacting particles can be described by the Hamiltonian for non-interacting quasi-particles (collective excitations) having a dispersion law ε_k.

2.2.1. Bogoliubov excitation spectrum, sound velocity and healing length

For small momenta $k << mc_s = \sqrt{mgn}$ the Bogoliubov dispersion law (2.37) is well approximated by the phonon-like linear dispersion form

$$\varepsilon_k = \hbar c_s k , \tag{2.40}$$

where $c_s = \sqrt{gn/m}$ is the sound velocity. According to the Bogoliubov theory, the long wavelength (low momentum) excitations of an interacting Bose gas are the sound waves.

In the opposite limit $k >> mc_s$, the Bogoliubov dispersion law (2.37) is reduced to the free-particle form:

$$\varepsilon_k \approx E_k . \tag{2.41}$$

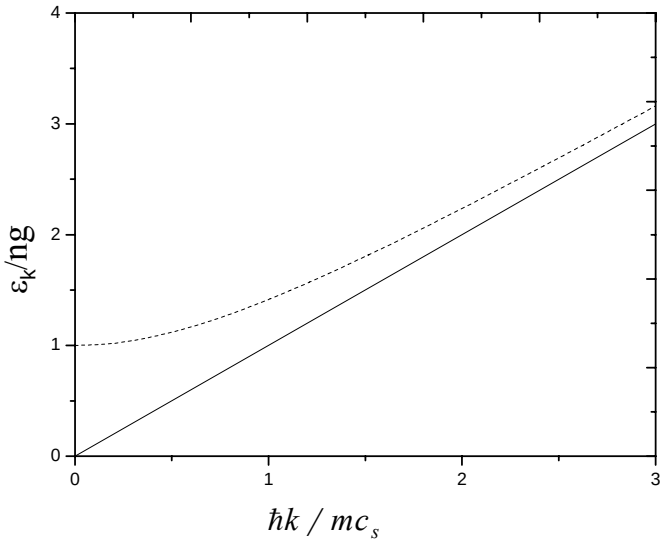


Figure 2.5. Excitation spectrum of homogeneous Bose gas (full line) plotted as a function of the wave number expressed as the dimensionless variable $\hbar k / mc_s$. The expansion (for high wave number is shown as dotted line).

The transition from the phonon regime to the free particle regime takes place near the point where $\hbar^2 k^2 / 2m = gn$ is satisfied. If we use $k = 1/\xi$ in this equation, the characteristic length can be written as

$$\xi = \hbar / \sqrt{2mgn} = \frac{1}{\sqrt{2}} \frac{\hbar}{mc_s} , \tag{2.42}$$

which is often referred to as "healing length". In such a length scale the density and phase fluctuations in the condensate are removed by the interaction between condensed particles. The healing length plays an important role in the superfluidity. The Bogoliubov dispersion law (2.37) is schematically shown in figure2.5.

The first observation of the Bogoliubov excitation spectrum was reported in 1998, using the two photon Bragg scattering spectroscopy technique in atomic BEC [106].

2.2.2. Depletion of the condensate

The particle number of the gas is given by Eq.(2.30) which rewritten in terms of $\hat{b}_k$ and $\hat{b}_k^+$, has the from

$$n = n_c + \sum_k v_k^2 + \sum_{k\neq 0}\left(v_k^2 + u_k^2\right)\left\langle \hat{b}_k^+ \hat{b}_k \right\rangle - \sum_{k\neq 0} u_k v_k \left(\left\langle \hat{b}_k^+ \hat{b}_{-k}^+ + \hat{b}_{-k}\hat{b}_k \right\rangle\right), \tag{2.43}$$

where

$$\begin{aligned} \left\langle \hat{b}_k^+ \hat{b}_k \right\rangle &= N_k = \frac{1}{\exp\left(\varepsilon_k / T\right) - 1} \\ \left\langle \hat{b}_k \hat{b}_k^+ \right\rangle &= 1 + N_k \\ \left\langle \hat{b}_k^+ \hat{b}_k^+ \right\rangle &= \left\langle \hat{b}_k \hat{b}_k \right\rangle = 0 \end{aligned} \quad . \tag{2.44}$$

The physical interpretation of the expression (2.43) is that the first term is the number of atoms in the condensate. The second term represents the depletion of the condensate by interactions when no real excitations are present. In the ground state of the interacting gas, not all particles are in the zero momentum state because the two-body interaction mixes into the ground state components with atoms in other state. Consequently, the probability of an atom being in the zero-momentum state is reduced. For states which contain a defined number of elementary excitations, the expectation value of $\hat{b}_k^+ \hat{b}_{-k}^+$ and its hermitian conjugate vanishes, and operator may equivalently be written as

$$n = n_c + \sum_k v_k^2 + \sum_{k\neq 0}\left(v_k^2 + u_k^2\right) N_k \ . \tag{2.45}$$

At zero temperature we have $N_k = 0$ since almost of the atoms are in the ground state and thus excitations are note present. Then we obtain for depletion

$$\frac{\tilde{n}}{n} = \frac{n - n_c}{n} = \sum_k v_k^2 \ . \tag{2.46}$$

Replacing the sum over k by an integral $\sum_k \Rightarrow \int \frac{d^3k}{(2\pi)^3}$.

Using Eq.(2.46) and then we substitute the relation (2.36) one obtains

$$\frac{n - n_c}{n} = \int_0^\infty \left(\frac{\varepsilon_k}{E_k} + \frac{E_k}{\varepsilon_k} - 2 \right) \frac{k^2 dk}{2\pi^2} \ . \tag{2.47}$$

Thus, the integration over the dimensionless variable $x = k\xi$, yields for the ground-state depletion

$$\frac{n - n_c}{n} = \frac{8}{3\sqrt{\pi}} \left(na^3\right)^{1/2}. \tag{2.48}$$

In deriving this result we have assumed that the depletion of the condensate is small. In most experiments that have been carried out, the ground-state depletion is of the order of one per cent. Recent experiment on ^{85}Rb near a Feshbach resonance achieved very large value of the scattering length corresponding to a depletion of 10% thus opening up the possibility of measuring effects beyond the validity of the mean field [107].

2.2.3. Ground state energy

The expression of the ground state energy E_0 is obtained from Eq.(2.39). Formally the sum is of order of g^2, as one can see by expanding the summand for large k: the leading term in the summand is of order $1/k^2$, and the sum over momentum space when converted to an integral gives a factor $k^2 dk$. This difficulty is due to the fact that we have used the effective interaction g, which is valid only for small momenta. To make a consistent calculation of the ground state energy one must use an effective interaction $g(k_c)$ in which all intermediate states with momenta in excess of sum cut-off value k_c are taken into account. The ground state is therefore

$$E_0 = \frac{1}{2} gnN + \sum_{\vec{k}(k<k_c)} \left(\varepsilon_k - gn + E_k\right). \tag{2.49}$$

The effective interaction is given

$$g(k_c) = g + \frac{g^2}{V} \sum_{\vec{k}(k<k_c)} \frac{1}{2E_k}, \tag{2.50}$$

with this expression one finds

$$E_0 = \frac{1}{2} gnN + \frac{1}{2} \sum_{\vec{k}(k<k_c)} \left(\varepsilon_k - gn + E_k - \frac{(ng)^2}{2E_k} \right) \quad . \tag{2.51}$$

After integration over the momentum, we obtain

$$E_0 = \frac{gn^2}{2} \left[1 + \frac{128}{15\pi^{1/2}} \left(na^3\right)^{1/2} \right] \quad . \tag{2.52}$$

The first form of the correction term indicates that the order of magnitude of the energy change is the number of states having wave numbers less than the inverse coherence length, times the typical energy of an excitation with this wave number, as one would expect from the form of the integral. This result was first obtained by Lee and Yang [28].

2.2.4. One body correlation function

The one body correlation function is defined as the probability of finding any particle in position $\vec{r}$. It can be rewritten as follows

$$\tilde{n}(\vec{r},\vec{r}';t,t') = g^{(1)}(\vec{r},\vec{r}';t,t') = \left\langle \hat{\Psi}^{+}(\vec{r},t)\hat{\Psi}(\vec{r}',t') \right\rangle . \tag{2.53}$$

At equal times, $t = t'$, so that $g^{(1)}$ is independent of t and we may put $t = t' = 0$. In the uniform case $g^{(1)}$ depends only on the difference $|\vec{r} - \vec{r}'|$ and we may set $\vec{r}' = 0$. Representing the field operator as a sum of condensate wavefunction and non-condensed part as given previously and taking into account that $|\Phi| = \sqrt{n_c}$ we thus have

$$g^{(1)}(\vec{r},\vec{r}') = n_c + \left\langle \hat{\tilde{\Psi}}^{+}(\vec{r},0)\hat{\tilde{\Psi}}(0,0) \right\rangle . \tag{2.54}$$

For the second term in the right hand side of this equation, using Eqs. (2.26) and (2.36), one finds

$$\left\langle \hat{\tilde{\Psi}}^{+}(\vec{r},0)\hat{\tilde{\Psi}}(0,0) \right\rangle = \int \frac{d^3k}{(2\pi)^3} v_k^2 \exp\left(i\vec{k}.\vec{r}\right). \tag{2.55}$$

Using Eq.(2.36) and turning to integration variable $x = k\xi$, we obtain

$$g^{(1)}(\vec{r},0) = n_c + \frac{1}{4\pi^2\xi^2 r}\int_0^{\infty} \sin x(r/\xi)\left\{\sqrt{x^2+4} - x - \frac{2}{\sqrt{x^2+4}}\right\}dx . \tag{2.56}$$

Integrating by parts we then get an expansion in powers of $1/r$. For $r \to \infty$, keeping only the leading terms of expansion, we obtain

$$g^{(1)}(r) = n_c + \frac{1}{4\pi^2\xi^3}\left(\frac{\xi}{r}\right)^2 . \tag{2.57}$$

It is important that $g^{(1)}$ tending to a constant value for $r \to \infty$. This type of behavior called (off diagonal) long-range order.

2.3. Finite temperature approximations

We now extend the formalism to finite temperatures, by explicitly retaining the noncondensate operator $\hat{\tilde{\Psi}}(\vec{r},t)$ in Eq. (2.41). We proceed via the technique of

Hamiltonian diagonalization already discussed in this section. In order to go beyond the zero temperature discussion, we must additionally include the remaining contributions

$(\hat{H}_3 + \hat{H}_4)$ of Eqs.(2.9) to the system Hamiltonian. This Section discusses their approximate mean field inclusion, which amounts to a static thermal cloud approximation.

In order to reduce the full Hamiltonian of Eq. (2.8) to a desired quadratic form, one may use Wick's theorem for the non-condensate operators in $\hat{H}_4$ [91, 109], which states that at equilibrium, an average over multiple operators can be approximated by sums of averages of pairwise contracted operators, i.e.

$$\left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} \hat{\tilde{\Psi}} \right\rangle = \left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}}^+ \right\rangle \left\langle \hat{\tilde{\Psi}} \hat{\tilde{\Psi}} \right\rangle + 2 \left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} \right\rangle \left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} \right\rangle . \tag{2.58}$$

The above approximation maintains correlations of non-condensate operators only to quadratic order. One may thus also wish to approximate products of three noncondensate operators appearing in $\hat{H}_3$ by their corresponding quadratic form,

$$\begin{aligned} \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} &= \left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}}^+ \right\rangle \hat{\tilde{\Psi}} + 2 \hat{\tilde{\Psi}}^+ \left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} \right\rangle \\ \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} \hat{\tilde{\Psi}} &= 2 \left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} \right\rangle \hat{\tilde{\Psi}} + \left\langle \hat{\tilde{\Psi}} \hat{\tilde{\Psi}} \right\rangle \hat{\tilde{\Psi}}^+ \end{aligned} . \tag{2.59}$$

Since by construction $< \hat{\tilde{\Psi}} > = < \hat{\tilde{\Psi}}^+ > = 0$, the approximation of Eq. (2.59) implies that $\left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} \right\rangle = 0$.

We have already seen that the system may be split into two sub-components, namely the condensate contribution, $n_c = |\Phi|^2$ and the thermal cloud $\tilde{n} = \left\langle \hat{\tilde{\Psi}}^+ \hat{\tilde{\Psi}} \right\rangle$ satisfying: $n = n_c + \tilde{n}$ Similarly, the approximations of Eqs. (2.58), (2.59) motivate the definition of an additional mean field contribution $\tilde{m} = \left\langle \hat{\tilde{\Psi}} \hat{\tilde{\Psi}} \right\rangle$. This is often referred to as the pair anomalous average. Such quantity will be studied in details both in 3D and 2D Bose gas in the chapters 4 and 5 respectively.

Popov approximation

One neglects the anomalous average $\tilde{m} = \left\langle \hat{\tilde{\Psi}} \hat{\tilde{\Psi}} \right\rangle$ [68,110]. This simplification often called Popov approximation in which the condensate wavefunction is coupled to the noncondensed density

$$\mu\Phi = \left[-\frac{\hbar^2}{2m}\Delta + V_{ext}(\vec{r}) + g\left(n_c + 2\tilde{n}\right) \right] \Phi . \tag{2.60}$$

The usual Bogoliubov transformation $\hat{\tilde{\psi}}(\vec{r}) = \sum_k \left[u_k(\vec{r})\hat{b}_k - v_k(\vec{r})\hat{b}_k^+ \right]$, leads to the coupled Bogoliubov-de Gennes equations

$$\begin{pmatrix} \hat{\mathrm{L}} & \hat{\mathrm{M}} \\ -\hat{\mathrm{M}}^* & -\hat{\mathrm{L}}^* \end{pmatrix} \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} = \varepsilon_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix}, \tag{2.61}$$

where $\hat{\mathcal{L}} = -\frac{\hbar^2}{2m}\Delta + V_{ext}(r) + 2gn - \mu$, $\hat{\mathrm{M}} = g\Phi^2$ and $n = n_c + \tilde{n}$ is the total density.

The equilibrium thermal cloud density is given by

$$\tilde{n} = \frac{1}{2}\sum_k \left[\frac{E_k + gn_c}{\varepsilon_k} \coth\left(\varepsilon_k / 2T\right) - 1 \right]. \tag{2.62}$$

The Popov approximation is a finite temperature approximation, since it endows condensate interactions with both condensate and thermal atoms. The set of equations (2.61) predicts excitations at finite temperatures with no gap in the energy spectrum for uniform gas and therefore that reason we term it gapless theory. They have advantage of being in agreement with Goldstone's theorem.

2.3.1. Hartree-Fock-Boboliubov approximation

To realize practical calculations, it is necessary to resort to some approximation. The Bogoliubov approximation [19, 20] is valid for low temperatures and asymptotically weak interactions. The more general approximation, that would be valid for all temperatures and any interaction strength, is the Hartree-Fock-Bogoliubov (HFB)[68-70] approximation. Early works employing this approximation, confronted the inconsistency problem, which will be discussed in next section, because of a gap in the particle spectrum.

In the frame of HFB formalism, the condensate wave function $\Phi(\vec{r})$ is defined within the generalized Gross-Pitaevskii equation.

$$\mu\Phi = \left[-\frac{\hbar^2}{2m}\Delta + V_{ext}(\vec{r}) + g\left(n_c + 2\tilde{n}\right) \right] \Phi + g\,\tilde{m}\,\Phi^* . \tag{2.63}$$

Using the above Bogoliubov transformation, we get the generalized coupled Bogoliubov-de Gennes equations

$$\begin{pmatrix} \hat{\mathcal{L}} & \hat{\mathcal{M}} \\ -\hat{\mathcal{M}}^* & -\hat{\mathcal{L}}^* \end{pmatrix} \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} = \varepsilon_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix}, \tag{2.64}$$

where $\hat{\mathcal{L}} = -\frac{\hbar^2}{2m}\Delta + V_{ext}(r) + 2gn - \mu$, $\hat{\mathcal{M}} = g\left(\Phi^2 + \tilde{m}\right)$ and $n = n_c + \tilde{n}$ is the total density.

These equations define the Bogoliubov energy spectrum ε_k and the quasiparticle amplitudes u_k and v_k. Once these quantities have been determined, the noncondensed and the anomalous densities for homogeneous Bose gas are obtained from the following expressions

$$\tilde{n} = \frac{1}{2}\sum_k \left[\frac{E_k + g\left(n_c + \tilde{m}\right)}{\varepsilon_k} \coth\left(\varepsilon_k / 2T\right) - 1 \right], \tag{2.65}$$

$$\tilde{m} = -\sum_k \left[\frac{g\left(n_c + \tilde{m}\right)}{\varepsilon_k} \coth\left(\varepsilon_k / 2T\right) \right], \tag{2.66}$$

where

$$\varepsilon_k = \left[\left(E_k + 2gn - \mu\right)^2 - g^2\left(n_c + \tilde{m}\right)^2 \right]^{1/2}, \tag{2.67}$$

Making use of the HFB chemical potential μ given by (2.63)

$$\mu = g\left(n + \tilde{n} + \tilde{m}\right), \tag{2.68}$$

one sees that there is a finite energy gap at $k = 0$

$$\varepsilon_k = 2g\sqrt{|\tilde{m}| n_c}\,. \tag{2.69}$$

Clearly the HFB does not satisfy the Hugenholtz-Pines theorem. The spectrum (2.67) should be gapless in the long wavelength limit. This is indeed provided an ad hoc procedure [68] for the chemical potential

$$\mu = g\left(n + \tilde{n} - \tilde{m}\right). \tag{2.70}$$

It is useful now to summarize how one would solve numerically the HFB equations given by (2.63) and (2.64), for a given anisotropic parabolic potential-well trap and temperature [68,69]:

a. First calculate $n_c(r) = |\Phi(r)|^2$ and $\tilde{n}(r)$ for a non-interacting gas ($g = 0$). In this case, the off-diagonal correlation functions $\tilde{m}(r) = 0$.
b. Use these non-interacting gas results in (2.64) to solve for u_k, v_k and ε_k. With these excited states, one can calculate $\tilde{n}(r)$ and $\tilde{m}(r)$ from (2.65, 2.66) and use these in (2.63) to find $\Phi(r)$.
c. Iterate the above procedure to self-consistency.

2.3.2. Problems of HFB

The difficulties of the generalized HFB theory are summarized in the following:

1. The anomalous pair average is ultraviolet divergent. Physically this comes from the approximate parameterization of collisions through a hard sphere interaction potential, which treats collisions of different momenta with the same probability. In reality, however, collisions with high energies are much more unlikely in the Bose condensed system and this unequal treatment leads to the divergence in the anomalous average.
2. The HFB theory is not gapless. The excitation spectrum contains a finite energy gap ($\varepsilon_k = 2g\sqrt{|\tilde{m}|n_c}$, see Eq.2.69) [68,69], which is a relic of divergences in the homogeneous case at low momenta. Genuine divergences, though, are only a feature of the homogeneous case, since the trap naturally introduces a low-energy cutoff. Goldstone's theorem [111], however, requires the theory to be gapless. It predicts a mode with energy vanishing linearly with the wave number for a system with a spontaneously broken symmetry, and, hence, in the long wavelength limit, a zero energy mode must exist. This mode corresponds to a rotation of the condensate phase. Technically, the reason for the occurrence of the energy gap can be found to be the approximate factorization of the operator averages and the resulting inconsistent treatment of interactions [111].

2.3.3. Other finite temperature approaches

In order to circumvent the well-kwon HFB problems, many approaches were proposed in these two last decades. Among them we can cite, the so-called self-consistent, coupled Gross-Pitaevskii-Boltzmann approach, which is often referred as the Zaremba-Nikoni and Griffin (ZNG) theory [71, 72]. In such approach, the thermal cloud itself is described by a quantum Boltzmann equation self-consistently coupled to the condensate [71]. This method reproduces the two-fluid hydrodynamics in the collisional and hydrodynamic regime [112, 113], and has been tested successfully against experiment for collective modes [113–116] and macroscopic excitations [117, 118]. Despite their elegant formulation, kinetic theories based on mean field potentials have the drawback in lower dimensions of not fully capturing the large phase fluctuations in the quasi-condensate. In addition, so called anomalous averages (or pair correlations) in the thermal cloud, typically omitted in such approaches, are

expected to become particularly relevant at lower dimensions. It is not entirely clear, however, how to obtain a gapless excitation spectrum for the system in the homogeneous limit, as required by the Hugenholtz-Pines theorem [31].

Classical field methods have been developed to simulate numerically those modes of the system that feature a macroscopic occupation. These methods rely upon the observation that for highly occupied modes, the field operator can be replaced by a classical complex field which evolves in time according to the GPE [119-120]. This description extends the $T = 0$ GPE, by adding stochastic elements that describe fluctuations of the condensate modes; these may be further coupled to the thermal cloud where the mean occupation numbers are small. (In fact, too small to be treated in the classical field approximation and more appropriately described by quantum Boltzmann equations [73].) Within the class of classical field techniques, we mention the projected GPE [76, 77], the truncated Wigner method [78,79] the stochastic Gross-Pitaevskii equation [81,82, 122-124], when implemented in the classical limit and closely related classical field methods. Hybrid simulation techniques were also recently developed that attempt to go beyond the classical limit.

In the stochastic approaches, the relation between them and other kinetic theories and their respective applications have been reviewed in Refs [122, 125, 126]. A key appeal is that they provide an approximation to the full distribution function of the ultracold gas and give access to physics beyond the mean field. They have been used, e.g., to probe the large critical fluctuations near the phase transition [127-128], to study dynamical effects of fluctuations on condensate growth [129] and macroscopic excitations [130-132]. Another quantity of interest is the counting statistics of the condensate mode [133-135], which is analogous to the photon number distribution in quantum laser theory [136-137].

Another kind of finite temperature approximation was proposed by Yukalov. Such approach based on the general notion of representative statistical ensembles [138] which is formulated for arbitrary statistical systems, equilibrium or not. The main idea of this notion is the necessity of taking into account all imposed conditions that uniquely define the given statistical system. Employing such a representative ensemble for Bose condensed systems removes all paradoxes, yielding both conserving and gapless in any approximation.

This theory has been used to study the static and the dynamics behavior of the normal and anomalous densities [138]. System of Bose-Einstein condensed gases in random

potentials is also investigated in the context of this theory [139]. In addition, this theory has been used to analyze the behavior of the Bose-Einstein condensates in optical lattices [139].

Alternatively, in the next chapter, we will explore the variational TDHFB formalism which does not require any simplifying assumption on the thermal cloud or the anomalous density and it is valid for any Hamiltonian and in any dimension. TDHFB equations allow us to obtain a coherent and consistent dynamics to treat the Bose-Einstein condensate at finite temperature.

Chapter 3

Time Dependent Hatree-Fock-Bogoliubov Theory

3.1.Introduction

Variational principles sometimes appear to be as old as the questions that they answer. In a mathematical language, variational principles were elaborated more than two thousand years ago (not without metaphysical connotations) for the propagation of light or for dynamics.For a historical introduction, see Lanczos, 1970 [140], Yourgrau and Mandelstam [141]. Often they have been introduced on metaphysical grounds, as eloquently expressed by Euler (we borrow the quotation from Ref. [142]): “the fabric of the universe is most perfect..., nothing at all takes place... in which some rule of maximum or minimum does not appear.” We recall that, beside perturbation theory, variational methods are among the most efficient approaches to study many-variable systems.

Furthermore, variational approaches are flexible; they allow expressing the principles in a concise and global way. There is no need to emphasize the central role played by the lagrangian formulation and the Hamilton principle of least action for the understanding of fundamental theories. We shall use a variational principle adapted to an optimal evaluation of a quantity of interest. This method, which is extremely general [143], has found applications in many domains of physics.

In static situations, the question may be to optimize the expectation value or the fluctuation (or both) for a given observable, through the determination of a “best” state chosen among some trial class. Out of equilibrium the question may be to predict this expectation value at time t, from the knowledge of some properties of the system at an earlier time to. (The calculation of transition probabilities belongs to this class [144].)

The essence of a variational procedure is to determine, within a trial subspace, a “best” estimate for a given quantity of particular interest. For instance, in the Hartree-Fock (HF) method, extensively used in atomic, molecular and nuclear physics, the HF state is determined by minimizing the free enegy (or, at zero temperature, the energy) within the trial class of independent-fermion states. The free energy thus obtained is the best approximation for this class of states. However, it is tempting to view the HF state as the “closest” independent-

particle state to the exact state and then to use it to compute different physical properties. This common practice escapes a genuine variational framework: nothing tells us that for quantities other than the free energy the smallest error is attained, within the independent-particle class. We are, for instance, particularly interested in correlation functions for which HF provides trivial answers. A natural question then arises: would it be possible, still using a trial state of the independent-particle type, to optimize the evaluation of correlation functions through a variational procedure? a positive answer is given to this question through the optimization of the characteristic functions.

At zero temperature the literature on the applications to many-body physics of the Dirac-Frenkel principle [145,146] is extensive. At non-zero temperature, to our knowledge, the variational approaches are sparser. A variational criterion to find approximate eigenfunctions and eigenvalues of the Liouville operator has been proposed by Zwanzig [147]. In the spirit of the Lippmann-Schwinger principle [148], Nakano [149] and collaborators in a series of papers have designed variational principles suited to the evaluation of response functions, with special emphasis on irreversible processes. A review of this approach, and of VPs in thermodynamics, is given by Ichiyanagi, 1994 [150] (see also Nakano and Hattori, 1990 [151]; Nakano, 1993 [152]). A noticeable difference with the approach which we shall use lies in the nature of the variational objects. While they will be for us respectively akin to a density operator and to an observable, they are two density matrices in Nakano's formulation. From our point of view this is not without questioning the meaning of the boundary conditions. In the realm of classical statistical mechanics, Gross (1973) [153], using the Laplace transform of the Liouville equation, has constructed a VP of the Lipmann-Schwinger type, the stationary value of which is the autocorrelation function. Sauermann and Turschner (1981) [154] have extended the Gross functional to quantum mechanics. By this means they have evaluated expectation values, derived TDHF and showed the connection with the projection method; Sauermann and Zhang (1982) [155] discussed the case of driven systems.

First-order variational functional have been used in the theory of the optimal control of quantum systems (see for example Tersigny *et al.*1990 [156]; Gaspard and van der Pals, 1994 [157]). Some works have been directly inspired by the present approach (Kim and Girardeau 1995 [158]; Schirmer *et al*., 2000 [159]).

3.2.The Balian-Véneroni variational principle

The Balian-Véneroni **(**BV) variational principle has several applications in different area of physics. First, it has been applied to various quantum problems including heavy ion reactions [160-164], quantum fields out of equilibrium [165] attempts to go beyond the Gaussian

approximation for fermion systems [166]. Therefore, the BV principle has been used to provide the best approximation to the generating functional for two and multi-time correlation functions of a set of bosonic and fermionic observables [167-170]. More recently, it was used to derive a set of equations governing the dynamics of trapped Bose gases [171, 173]. Moreover, the BV variational principle is used at the mean-field level to determine the particle number fluctuations in fragments of many-body systems of fermions [174].

The BV variational principle [83, 84,160-164] is based on the Liouville equation. It addresses the following question:

Given the state of system described by the density operator $\mathcal{D}_0$, at an initial time t_i what will be the expectation value of an observable $\mathcal{A}$ at a final time t_f ?

The answer can be stated as follows: take two variational spaces, one for observables denotes $\mathcal{A}$ and one for the density operator denotes $\mathcal{D}$, the optimal value of $Tr(\mathcal{A}\mathcal{D})_{t_f}$ is given by the stationary value of action-like functional [172],

$$I = Tr(\mathcal{A}\mathcal{D})_{t_f} - \int_{t_i}^{t_f} dt Tr\ \mathcal{A}\left(\frac{d\mathcal{D}}{dt} - i[H,\mathcal{D}]\right), \tag{3.1}$$

with the two mixed boundary conditions:

$$\mathcal{D}(t_i) = \mathcal{D}_0;\ \mathcal{A}(t_f) = \mathcal{A}\ , \tag{3.2}$$

The symbol Tr stands for a trace taken over a complete basis of the Fock space, and H is the Hamiltonian of the system assumed time independent.

The variation of I in (3.1) provides evolution equations for the operators $\mathcal{D}$ and $\mathcal{A}$, which are in general coupled. This forbids the interpretation of the solution $\mathcal{D}(t)$ as a density operator; this is not very strange since the variational principle aims at giving a number: an approximate value of $Tr(\mathcal{A}\mathcal{D})_{t_f}$. However, in order to have a better understanding of all these quantities, we shall choose the variational space for $\mathcal{A}$ to be linear in its parameters, thus the evolution of $\mathcal{D}$ will decouple, and we can interpret $\mathcal{D}(t)$ as an approximate solution for the exact density operator but only suited for predictions of expectation values of observables belong to the variaional space of $\mathcal{A}$. In almost all physical cases, $\mathcal{D}$ is parameterized nonlinearly, thus the evolution of $\mathcal{A}(t)$ is still dependent on $\mathcal{D}(t)$ and can explain, among other things, the energy conservation. In order to get a closed system of differential equations, the trial spaces must have the same dimensionality. The question whether these spaces are relevant or not

depends on the aspects of dynamics we want to preserve and on the tractability of the corresponding evolution equations.

When the allowed variation $\delta\mathcal{A}(t)$ and $\delta\mathcal{D}(t)$ are unrestricted, the stationary conditions of the BV functional (4.1) lead to the exact Liouville-von Neumann equation for $\mathcal{D}(t)$ and the (backward) Heisenberg equation for $\mathcal{A}(t)$.

3.3.Trial spaces and the TDHFB equations

Let us first introduce the trial class of operators which we shall use throughout this work for $\mathcal{D}(t)$ and $\mathcal{A}(t)$. To this end, we define the 2^n- component operator α

$$\alpha = \begin{pmatrix} \Psi \\ \Psi^+ \end{pmatrix}, \tag{3.3}$$

where Ψ and Ψ^+ denote boson field creation and annihilation operators in a given single-particle space of dimension n. The commutation relations can be expressed in the compact form $(i, j = 1 \ldots 2n)$

$$\left[\alpha_i, \alpha_j\right] = \tau_{ij} \text{ and } \tau = \sigma_2 = \begin{pmatrix} 0 & 1_n \\ -1_n & 0 \end{pmatrix}, \tag{3.4}$$

where 1_n is the $(n \times n)$ unit matrix and σ_2 is the $(2n \times 2n)$ second Pauli matrix.

With this notation, our trial class for the operator $\mathcal{D}(t)$, the exponentials of the linear plus quadratic forms in α, can be written in the factorized form [169-173]

$$D(t) = \exp(\upsilon)\exp\left(\tilde{\lambda}\tau\alpha\right)\exp\left(\frac{1}{2}\tilde{\alpha}\tau S\alpha\right), \tag{3.5}$$

with υ is a c-number, λ is a $2n$-component vector and S is a $(2n \times 2n)$ symplectic matrix (τS is symmetric). The tilde symbol denotes vector or matrix transposition. For any operator O, let us denote the average value $\langle O \rangle$ and the shifted operator O by $\langle O \rangle = Tr(O\mathcal{D})/z$ and $\overline{O} = O - \langle O \rangle$. Then, $\mathcal{D}$ is completely specified by the knowledge of "the partition function" $z = Tr\,\mathcal{D}$, the vector $\langle\alpha\rangle$ and contraction matrix ρ (which we shall also call the single-particle density matrix) defined as

$$\rho_{ij} \equiv \left\langle (\tau\overline{\alpha})_j \overline{\alpha}_i \right\rangle. \tag{3.6}$$

For our purpose, the parameterization of the operator $\mathcal{D}$ by z, $\langle\alpha\rangle$ and ρ is more convenient than that by υ, λ and S. In particular, we will see that the evolution equation for the former variables take a simple form.

With the same notation, we take as our variational choice [169-173] for the operator $\mathcal{A}(t)$ a linear plus quadratic form in the operator α;

$$\mathcal{A}(t) = \upsilon_a + \tilde{\lambda}_a(t)\tau\alpha + \frac{1}{2}\tilde{\alpha}\tau S_a(t)\alpha, \tag{3.7}$$

To which we shall loosely refer as a single-particle operator.

With the choices (3.5) and (3.7), it is possible to write explicitly the functional (3.1) in terms of the variational parameters z, $\langle\alpha\rangle$, ρ, υ_a, λ_a and S_a. Indeed, we find

$$I = Tr\,\mathcal{A}\mathcal{D}(t_f) - \int_{t_i}^{t_f} dt\left(Tr\,\mathcal{A}\mathcal{D}\frac{\dot{z}}{z} - iz\left\{\tilde{L}_a\tau\left(i\langle\dot{\alpha}\rangle - \tau\frac{\partial\mathcal{E}}{\partial\langle\alpha\rangle}\right) - \frac{1}{2}trS_a\left(i\dot{\rho} + 2\left[\rho, \frac{\partial\mathcal{E}}{\partial\rho}\right]\right)\right\}\right), \tag{3.8}$$

with $L_a = \lambda_a - S_a\langle\alpha\rangle$. The equation of motion for z, $\langle\alpha\rangle$ and ρ are now obtained by writing the stationary of the BV functional (3.8) with respect to υ_a, λ_a and S_a. These equations take the simple form

$$i\dot{z} = 0, \tag{3.9.a}$$

$$i\langle\dot{\alpha}\rangle = \tau\frac{\partial\mathcal{E}}{\partial\langle\alpha\rangle}, \tag{3.9.b}$$

$$i\dot{\rho} = -2\left[\rho, \frac{\partial\mathcal{E}}{\partial\rho}\right]. \tag{3.9.c}$$

In these equations, $\mathcal{E} = \langle H\rangle$ is the mean field energy and the dots denote d/dt. We have used the usual convention $\left(\frac{\partial}{\partial\rho}\right)_{ij} = \frac{\partial}{\partial\rho_{ji}}$.

We see from equation (3.9.a) that the partition function z is a constant of motion. One of the most noticeable properties is that the evolution of ρ preserves the trace of any function of the single particle matrix. A related property is the equation

$$i\frac{d}{dt}\rho(\rho+1) = \left[\rho(\rho+1), \frac{\partial\mathcal{E}}{\partial\rho}\right], \tag{3.10}$$

which implies in particular the conservation of the von-Neumann entropy $S = -\mathrm{Tr}\,\mathcal{D}\ln\mathcal{D}$ and the fact that an initially pure state, satisfying $\rho(\rho+1) = 0$, remains pure during the evolution. The two last equations (3.9.b) and (3.9.c) entail that the energy $\mathcal{E}$ is conserved when the Hamiltonian H does not depend explicitly on time. Within the BV formalism, this conservation law has a special status in the sense that it does not result from general properties of the variational spaces. We may notice at this point that the system (3.9) is closed and does not require any further ingredients. The truncation of the full hierarchy is no longer

brutally performed but rather obtained by softly restricting the full Hilbert space to the single particle one. Other properties of the TDHFB equations (3.9) is that they admit a Lie-Poisson structure [175, 176], and in the zero temperature limit, can be cast in an Hamiltonian form.

3.4.Application of the TDHFB formalism to trapped Bose gases

Let us first write the single-particle density matrix (3.6) in explicit form as

$$\rho(\vec{r},\vec{r}',t)=\begin{pmatrix} <\overline{\Psi}^{+}(\vec{r}')\overline{\Psi}(\vec{r})> & -<\overline{\Psi}(\vec{r}')\overline{\Psi}(\vec{r})> \\ <\overline{\Psi}^{+}(\vec{r}')\overline{\Psi}^{+}(\vec{r})> & -<\overline{\Psi}(\vec{r})\overline{\Psi}^{+}(\vec{r}')> \end{pmatrix}. \tag{3.11}$$

In the preceding definitions, $\Psi(\vec{r})$ and $\Psi^{+}(\vec{r})$ are the boson destruction and creation field operators (in the Schrödinger representation) satisfying the usual canonical commutation rules

$$\left[\overline{\Psi}(\vec{r}),\Psi^{+}(\vec{r}')\right]=\delta(\vec{r}-\vec{r}'), \tag{3.12}$$

and $\overline{\Psi}(\vec{r})=\Psi(\vec{r})-<\Psi(\vec{r})>$.

Upon introducing these variational parameters into the BV principle, one obtains dynamical equations for the expectation values of the one and two boson field operators [173]

$$i\frac{\partial<\Psi>}{\partial t}(\vec{r},t)=\frac{\partial\mathcal{E}}{\partial<\Psi^{+}>(\vec{r},t)}, \tag{3.13.a}$$

$$i\frac{\partial<\Psi^{+}>}{\partial t}(\vec{r},t)=-\frac{\partial\mathcal{E}}{\partial<\Psi>(\vec{r},t)}, \tag{3.13.b}$$

$$i\frac{\partial\rho}{\partial t}(\vec{r},\vec{r}',t)=-2\left[\rho,\frac{\partial\mathcal{E}}{\partial\rho}\right](\vec{r},\vec{r}',t). \tag{3.13.c}$$

Moreover, our formalism provides a direct link between different components of matrix density as

$$I(\vec{r},\vec{r}')=\int d\vec{r}''\left[\rho_{11}(\vec{r},\vec{r}'')\rho_{22}(\vec{r}'',\vec{r}')-\rho_{12}(\vec{r},\vec{r}'')\rho_{21}(\vec{r}'',\vec{r}')\right]. \tag{3.14}$$

Notice that Eq.(3.14) is often known as the Heisenberg invariant, it is a direct consequence of the conservation of the von-Neumann entropy. As it stands, *I* describes the degree of mixing of the system. For the pure state in *d*-dimension, Eq.(3.14) takes the form $I(\vec{r},\vec{r}')=\delta^{d}(\vec{r}-\vec{r}')$ [169,173,176].

Let us apply the previous equations (3.13) to a system of trapped bosons interacting via a two-body potential. The grand canonical Hamiltonian is given by

$$H = \int d\vec{r}\Psi^{+}(\vec{r})h^{sp}\Psi(\vec{r}) + \frac{1}{2}\int d\vec{r}d\vec{r}'\Psi^{+}(\vec{r})\Psi^{+}(\vec{r}')V(\vec{r},\vec{r}')\Psi(\vec{r}')\Psi(\vec{r}), \tag{3.15}$$

where $h^{sp} = \left(-\hbar^2/2m\right)\Delta + V_{\text{ext}}(\vec{r}) - \mu$ is the single-particle Hamiltonian, $V_{\text{ext}}(\vec{r})$ is the external trapping potential and μ is the chemical potential.

For the sake of clarity, we will omit writing explicitly the time dependence whenever evident. Next, we introduce the order parameter $\Phi(\vec{r}) = <\Psi(\vec{r})>$ and the non-local densities

$$\begin{aligned}\tilde{n}(\vec{r},\vec{r}') &\equiv \tilde{n}^{*}(\vec{r},\vec{r}') = <\Psi^{+}(\vec{r})\Psi(\vec{r}')> - \Phi^{*}(\vec{r})\Phi(\vec{r}') \\ \tilde{m}(\vec{r},\vec{r}') &\equiv \tilde{m}(\vec{r}',\vec{r}) = <\Psi(\vec{r})\Psi(\vec{r}')> - \Phi(\vec{r})\Phi(\vec{r}')\end{aligned}, \tag{3.16}$$

where we note that $\tilde{n}(\vec{r},\vec{r}) \equiv \tilde{n}(\vec{r})$ and $\tilde{m}(\vec{r},\vec{r}) \equiv \tilde{m}(\vec{r})$ are respectively the non condensate and the anomalous densities. The energy may be readily computed to yield

$$\begin{aligned}\mathcal{E} &= \int d\vec{r}h^{sp}(\vec{r})\left[\tilde{n}(\vec{r},\vec{r}) + \Phi(\vec{r})\Phi^{*}(\vec{r})\right] + \int d\vec{r}d\vec{r}'V(\vec{r},\vec{r}')\left|\Phi(\vec{r})\right|^2\left|\Phi(\vec{r}')\right|^2 \\ &+ \frac{1}{2}\int d\vec{r}d\vec{r}'V(\vec{r},\vec{r}')\left[\tilde{m}^{*}(\vec{r},\vec{r}')\tilde{m}(\vec{r},\vec{r}') + \tilde{n}(\vec{r},\vec{r}')\tilde{n}(\vec{r}',\vec{r}) + \tilde{n}(\vec{r},\vec{r})\tilde{n}(\vec{r}',\vec{r}')\right] \\ &+ \frac{1}{2}\int d\vec{r}d\vec{r}'V(\vec{r},\vec{r}')\left[\tilde{n}(\vec{r},\vec{r}')\Phi(\vec{r})\Phi^{*}(\vec{r}') + \tilde{n}(\vec{r}',\vec{r})\Phi^{*}(\vec{r})\Phi(\vec{r}') + \tilde{n}(\vec{r},\vec{r})\Phi(\vec{r}')\Phi(\vec{r}') + \tilde{n}(\vec{r}',\vec{r}')\Phi(\vec{r})\Phi(\vec{r})\right] \\ &+ \frac{1}{2}\int d\vec{r}d\vec{r}'V(\vec{r},\vec{r}')\left[\tilde{m}^{*}(\vec{r},\vec{r}')\Phi(\vec{r})\Phi(\vec{r}') + \tilde{m}(\vec{r},\vec{r}')\Phi^{*}(\vec{r})\Phi^{*}(\vec{r}')\right]\end{aligned} \tag{3.17}$$

Now, one inserts the expression (3.17) in the general equations of motion (3.13), we get the explicit form of the TDHFB equations for a trapped Bose gas [177,178]:

$$\begin{aligned}i\hbar\dot{\Phi}(\vec{r}) &= h^{sp}(\vec{r})\Phi(\vec{r}) \\ &+ \int d\vec{r}'V(\vec{r},\vec{r}')\left[\left|\Phi(\vec{r}')\right|^2\Phi(\vec{r}) + \Phi^{*}(\vec{r}')\tilde{m}(\vec{r},\vec{r}') + \Phi(\vec{r}')\tilde{n}(\vec{r},\vec{r}') + \Phi(\vec{r})\tilde{n}(\vec{r}',\vec{r}')\right],\end{aligned} \tag{3.18a}$$

$$\begin{aligned}i\hbar\dot{\tilde{n}}(\vec{r},\vec{r}') &= \left[h^{sp}(\vec{r}) - h^{sp}(\vec{r}')\right]\tilde{n}(\vec{r},\vec{r}') \\ &+ \int d\vec{r}''V(\vec{r}',\vec{r}'')\left[a(\vec{r}'',\vec{r}')\tilde{n}(\vec{r},\vec{r}'') + a(\vec{r}'',\vec{r}'')\tilde{n}(\vec{r},\vec{r}') + b(\vec{r}',\vec{r}'')\tilde{m}(\vec{r}'',\vec{r})\right] \\ &- \int d\vec{r}''V(\vec{r}',\vec{r}'')\left[a(\vec{r},\vec{r}'')\tilde{n}(\vec{r}'',\vec{r}') + a(\vec{r}'',\vec{r}'')\tilde{n}(\vec{r},\vec{r}') + b(\vec{r},\vec{r}'')\tilde{m}(\vec{r}'',\vec{r}')\right],\end{aligned} \tag{3.18b}$$

$$
\begin{aligned}
i\hbar\dot{\tilde{m}}(\vec{r},\vec{r}') &= \left[h^{sp}(\vec{r})+h^{sp}(\vec{r}')\right]\tilde{m}(\vec{r},\vec{r}') \\
&+\int d\vec{r}''V(\vec{r}',\vec{r}'')\left[a(\vec{r}'',\vec{r}')\tilde{m}(\vec{r},\vec{r}'')+a(\vec{r}'',\vec{r}'')\tilde{m}(\vec{r},\vec{r}')+b(\vec{r}',\vec{r}'')\left(\tilde{n}^{*}(\vec{r},\vec{r}'')+\delta(\vec{r}-\vec{r}'')\right)\right], \\
&+\int d\vec{r}''V(\vec{r}',\vec{r}'')\left[a(\vec{r}'',\vec{r})\tilde{m}(\vec{r}',\vec{r}'')+a(\vec{r}'',\vec{r}'')\tilde{m}(\vec{r},\vec{r}')+b(\vec{r},\vec{r}'')\tilde{n}(\vec{r}'',\vec{r}')\right].
\end{aligned}
\tag{3.18.c}
$$

$$
\begin{aligned}
a(\vec{r},\vec{r}') &= \tilde{n}(\vec{r},\vec{r}')+\Phi^{*}(\vec{r})\Phi(\vec{r}') \\
b(\vec{r},\vec{r}') &= \tilde{m}(\vec{r},\vec{r}')+\Phi(\vec{r})\Phi(\vec{r}')
\end{aligned}
\quad . \tag{3.19}
$$

It is worth noticing that similar equations have been derived elsewhere using quite different approaches. For instance, Stoof [179] used a variational plus perturbative effective action, Proukakis [180,181] a truncation of the Heisenberg equations and Chernyak *et al*. [182] the generalized coherent state representation. The latter approach yields equations very close to ours, but the authors did not pursue further their analysis.

For a short-range interaction potential and sufficiently dilute gas, the TDHFB equations can be written in *d*-dimensions as [183]

$$
i\hbar\dot{\Phi}(r)=\left[h^{sp}+gn_{c}(r)+2g_{d}\tilde{n}(r)\right]\Phi(r)+g_{d}\,\tilde{m}(r)\,\Phi^{*}(r), \tag{3.20.a}
$$

and consequently, the equations of motion for $\tilde{n}(\vec{r},\vec{r}')$ and $\tilde{m}(\vec{r},\vec{r}')$ may be written in compact form

$$
i\hbar\frac{d\rho}{dt}=\Im\rho-\rho\Im^{+}, \tag{3.20.b}
$$

where we have defined the 2×2 matrices

$$
\Im(r.r')=\begin{pmatrix} h(r,r') & \Delta(r',r') \\ -\Delta^{*}(r,r) & -h^{*}(r,r') \end{pmatrix}, \qquad \rho(r.r')=\begin{pmatrix} \tilde{n}(r,r') & \tilde{m}(r,r') \\ \tilde{m}^{*}(r,r') & \tilde{n}^{*}(r,r')+\delta(r,r') \end{pmatrix}
$$

and

$$
\begin{aligned}
h(r,r') &= h^{sp}(r)+2ga(r',r') \\
\Delta(r,r) &= gb(r,r)
\end{aligned}
\quad .
$$

Eqs. (3.20) constitute the TDHFB equations for the contact interaction potential approximation in real space in any dimensions.

Among the advantages of the TDHFB equations is that the three densities are coupled in a consistent and closed way. Second, they should in principle yield the general time, space and

temperature dependence of the various densities. Furthermore, they satisfy the energy and number conserving laws. In addition, the most important feature of the TDHFB equations is that they are valid for any Hamiltonian H and for any density matrix operator. Interestingly, our TDHFB equations can be extended to provide self-consistent equations of motion for the triplet correlation function by using the post Gaussian ansatz.

It is well known that in the HFB theory the issues of the ultraviolet divergence of the anomalous density arise from the zero-point occupation of quasiparticle modes [69,70]. In our case, the diverging term appears in the equation (13.8c) and becomes highly non trivial when considers the contact potential. This is precisely the term which leads to UV-divergences in the anomalous density in the HFB theory [69,70]. Having identified the origin of this divergence, we can habitually eliminate it from the problem, by regularizing the anomalous average. This is achieved by following the method of refs [184,185].

3.5.The static TDHFB equations in three dimensions

To proceed further and to investigate the behavior of the various density profiles both for homogeneous and trapped gases. We consider in this work the diagonal densities obtained by taking the local limit since these are the most physically accessible.

The static TDHFB equations are obtained by setting to zero the right hand sides of Eqs (3.19) in their local form. When one sets $r = r'$, we obtain:

$$i\hbar\dot{\Phi} = \left(-\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(r) - \mu + gn_c + 2g\tilde{n} \right)\Phi + g\,\tilde{m}\,\Phi^{*}, \tag{3.21.a}$$

$$i\hbar\dot{\tilde{m}} = 4\left(-\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(r) - \mu + 2gn \right)\tilde{m} + g\left(1 + \frac{\tilde{m}}{\Phi^2} \right)\Phi^2\left(2\tilde{n} + 1\right), \tag{3.21.b}$$

$$i\hbar\dot{\tilde{n}} = g\left(\tilde{m} * \Phi^2 - \tilde{m}\,\Phi *^2\right), \tag{3.21.c}$$

where $g = 4\pi\hbar^2 a / m$ is the coupling constant in 3D and a is the s-wave scattering amplitude. The most important remark in Eq.(3.21) is that the term $g\left(1+\frac{\tilde{m}}{\Phi^2}\right)$ which obtained without any renormalization scheme, is similar to the many-body *T*-matrix introduced at finite temperature in the so-called HFB-G2 approximation [70,184] and in the variational approach of [185].

It is important to note that the equations (3.21) are not totally independent. Indeed, in the local case equation (3.14) provides a useful relation between $\tilde{n}$ and $\tilde{m}$

$$\left(1+2\tilde{n}\right)^2-\left|2\tilde{m}\right|^2=I\,. \tag{3.22}$$

This equation helps us to eliminate the noncondensed density from the set (3.21), which simplifies the numerical solution.

3.6.Numerical results

For numerical purposes, it is convenient to start our treatment with the dimensionless form of the set (3.21). Let us consider a spherical trap with frequency ω, $V_{\text{ext}}(r)=\frac{1}{2}m\omega^2r^2$ and use the harmonic oscillator length $a_{H0}=\sqrt{\hbar/m\omega}$, as well as a_{H0}^{-3} and ħω as units of length, density and energy respectively. The dimensionless radial distance is $q=r/a_{H0}$. The dimensionless condensed, non-condensed and anomalous densities are respectively $\hat{n}_c=a_{H0}^3n_c$, $\hat{\tilde{n}}=a_{H0}^3\tilde{n}$ and $\hat{\tilde{m}}=a_{H0}^3\tilde{m}$. Therefore, $\hat{n}=\hat{n}_c+\hat{\tilde{n}}$ is the dimensionless total density. With these definitions, the static equations corresponding to (3.21) write as:

$$\begin{aligned}
&\left(-\frac{d^2}{dq^2}+q^2-\nu+8\pi\frac{a}{a_{HO}}\left(\frac{\hat{\Psi}^2}{q^2}+2\hat{\tilde{n}}+\frac{\hat{\chi}}{q}\right)\right)\hat{\Psi}=0,\\
&\left(-\frac{d^2}{dq^2}+q^2-\nu+8\pi\frac{a}{a_{HO}}\left(2\hat{n}+\frac{2\hat{\tilde{n}}+\hat{V}^{-1}}{4}\right)\right)\hat{\chi}+8\pi\frac{a}{a_{HO}}\left(\frac{2\hat{\tilde{n}}+\hat{V}^{-1}}{4}\right)\frac{\hat{\Psi}^2}{q}=0,
\end{aligned} \tag{3.23}$$

where $\hat{V}=V/a_{HO}^3$ is the normalized volume and we have introduced the dimensionless chemical potential $\nu=2\mu/\hbar\omega$ and the s-wave scattering length *a*. We have deliberately omitted the third equation in (3.21) since it is of no interest for the following. The quantity $\hat{\tilde{n}}$ is determined via the relation (3.22) which becomes in our units

$$\hat{\tilde{n}}=\frac{1}{2\hat{V}}\left[\left(I+4\hat{V}^2\,\frac{\hat{\chi}^2}{q^2}\right)^{1/2}-1\right]. \tag{3.24}$$

The atom-atom interaction is now completely specified by the parameter a/a_{HO}. The normalization condition writes in these new units as $\int d^3q\,\hat{n}(q)=N$, where *N* is the total particles number.

The static TDHFB equations can be solved numerically. The numerical method divides into two steps. The first one consists to finding the solutions of the static TDHFB equations that satisfies the boundary conditions summarized as follows: since the full wave function, the normal and the anomalous averages must vanish as $q \to \infty$, the nonlinear term inside the equation (3.21.a) becomes negligible compared to the other terms. Therefore, the two equations of $\hat{\Phi}$ and $\hat{\tilde{m}}$ have the same asymptotic behavior $\hat{\Phi} \approx \hat{\tilde{m}} \approx q^{-3/2} e^{\frac{-q^2}{4}}$ for $q \to \infty$. The second step is used to propagate the solutions of the static TDHFB equations using a finite-difference method.

To illustrate our finite temperature formalism, we consider the ^{87}Rb gas with the following parameters [59, 187]: $a = 5.82\,10^{-9}$ m, $a_{H0} = 7.62\,10^{-7}$ m and $\hbar\omega = 1.32\,10^{-31}$ J. A convenient dimensionless parameter describing the effective strength of the interactions is $\gamma = Na / a_{H0}$ [188, 189]. We begin by plotting the condensed, the noncondensed and the anomalous densities as functions of the radial distance for several values of the condensate fraction N_c / N and hence of the temperature. Densities and lengths are measured in units of a_{HO}^{-3} and a_{HO} respectively.

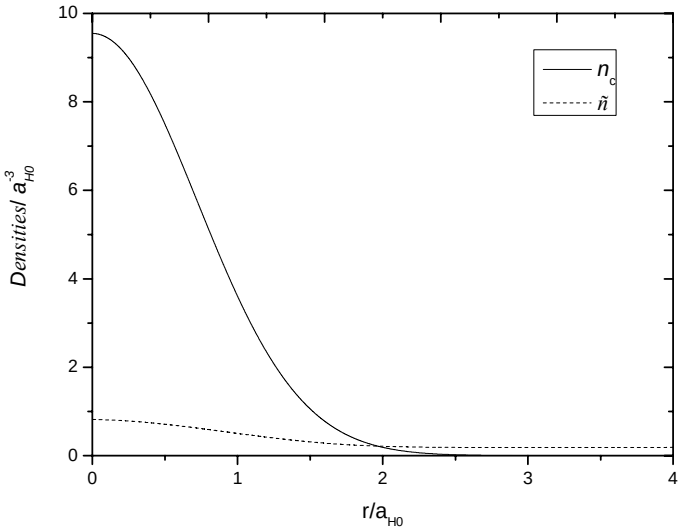


Figure 3. 1. The non-condensate (solid line) and the condensate (dashed line) densities as function of the radial distance (in units of a_{H0}) for $\tilde{N}/N$ =14%.

In figure 3.1 (for *T*=1.2 nK), almost all the atoms are condensed in the center of the trap. Consequently, the thermal cloud is negligibly small compared to the condensate density which almost coincides with the total density.

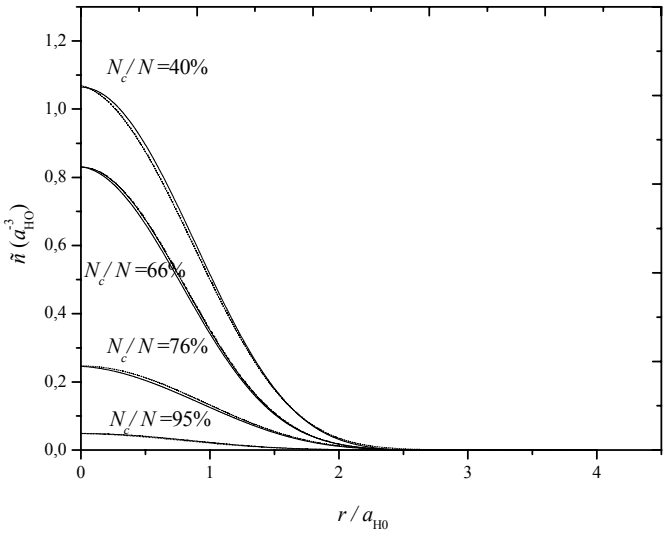


Figure 3.2. The non-condensate density versus the radial distance for various condensate fractions, $a/a_{H0} = 7.6410^{-3}$ and $N = 2000$ atoms. Solid: our result, dashed: the ideal gas result.

In the figure 3.2, we see that the non-condensate density is increasing significantly with decreasing condensate fraction. Furthermore, it is quite interesting to observe that the ideal gas model (dashed line) is still a good approximation.

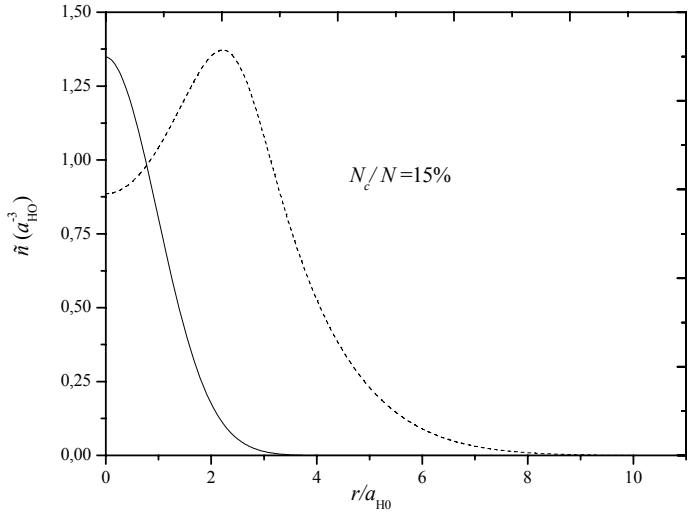


Figure 3.3. The non-condensate density versus the radial distance for $N_c/N = 15\%$, $a/a_{H0} = 7.6410^{-3}$ and $N = 2000$ atoms. Solid: our result, dashed: HFB-BdG.

In figure 3.3, we compare our non condensate density with that predicted by the HFB-BdG equations. As we clearly see here is that our results are in disagreement with the HFB-BdG calculations [69]. The discrepancies are more pronounced near the center of the trap, where

the HFB-BdG approximation predicts a hole. On the other hand, our result is in accordance with the experiments of Ref. [190-192], where no special structure is observed near the center and where the Gaussian shape of the thermal cloud seems to be maintained. These observations may be extended to the anomalous average.

3.7.Vortex at finite temperature

In this section, we will try to extract something useful about superfluidity in 3D Bose system. The idea is to relate our predictions with appropriate numerical simulations for some realistic experiments in traps to study the vortex stability without rotating fluid.

One of most important features of ultracold atoms is that they can be easily controlled and imaged directly, and are relatively simple to treat theoretically, so are very good systems in which to study superfluid behavior. The proposed section will theoretically study the properties of this superfluid in ultracold gases. Of particular interest are vortices, which are a familiar feature in fluids where they sometimes appear as whirlpools or tornados. They appear in superfluids when they are rotated or forced to flow past an obstacle too quickly. The vortices can then interact with atoms that are not part of the superfluid, creating a frictional force and therefore a resistance to the flow. So, the vortices are an important component in the breakdown of superfluidity. A strong motivation for research into this problem is that similar behavior is found in other systems, such as liquid helium or inside neutron stars, but isn't fully understood theoretically.

Using again our formalism and considering a condensate penetrated by a single vortex line, we search for solutions of the form $e^{i\ell\varphi}$, where ℓ denotes the number of circulation quanta of the vortex. In this section we restrict ourselves to the case $\ell = 1$ due to the instability of multiquantum vortices [193-197]. By employing the spherical symmetry, the static equations. (3.23) can be reduced to radial equations, in which we add the centrifugal term $1/q^2$, and then we discretize them using the same numerical method as above. Let us begin by plotting condensed and the thermal cloud for $N = 10^5$.

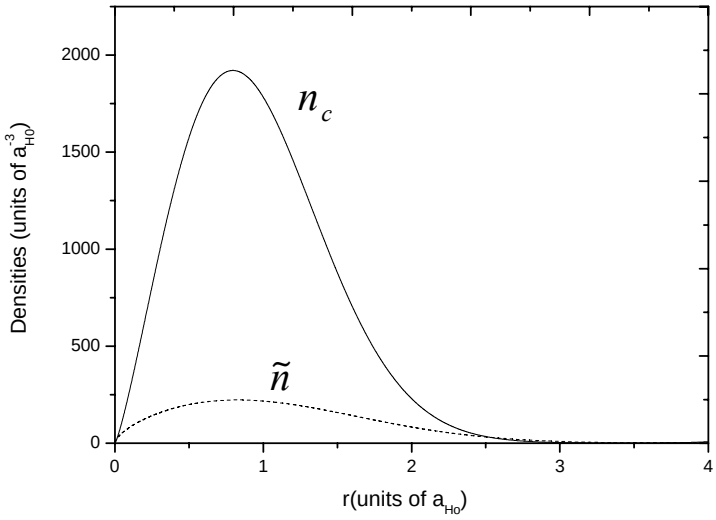


Figure.3.4. Condensate and thermal gas density profiles for $\gamma = 10$ and $N_c / N = 13\%$.

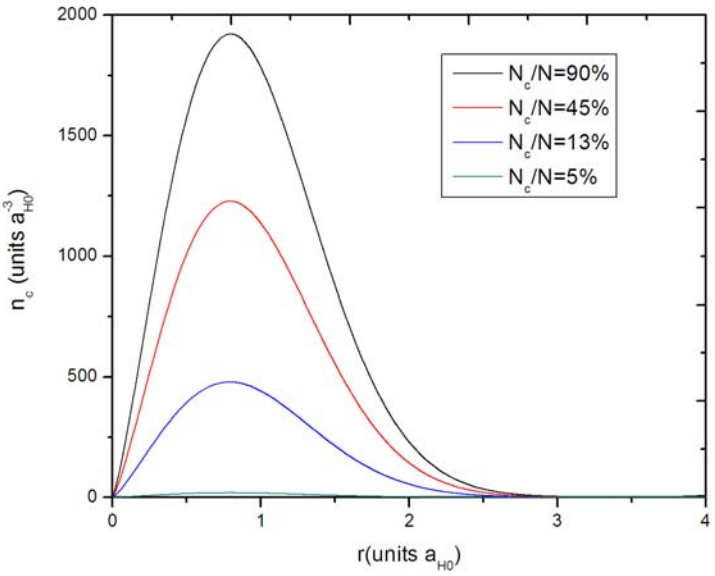


Figure.3.5. Condensate density profiles for various condensate fractions

Figure 3.4 represents the density profiles of the condensed and the noncondensed densities at low temperatures. We observe that the thermal gas forms a local minimum in the center of trap and appears as a tornado surrounds the condensate which leads to a coreless vortex (empty core). This new image is in disagreement with that predicted in [71, 198] where the thermal gas is concentrated in the vortex core, where it fills the space left by the condensate and exerts an outward pressure on it, preventing the condensate from collapsing into the core

which ultimately leads to a stable vortex. As far as we know, the stabilization of the vortex by the thermal cloud suggested in [199] is not observed experimentally yet. It arises when the thermal cloud is treated as static [200], but does not occur when the dynamics of the thermal cloud is taken into account as in our case.

Figure 3.5 depicts the vortex states for varying condensed fraction and for $\gamma = 10$. We see that by decreasing N_c/N, n_c begins to decrease and start to disappear when N_c/N approaches 5%. This overall behavior has been obtained in [191, 200]. Furthermore, it is clearly seen that the core size becomes larger when the vortex line reaches the boarder of the condensate, where the condensed density decreases.

Chapter 4

Anomalous Density for Bose Gas at Finite Temperature

4.1. Introduction

The pair anomalous average $\tilde{m}(\vec{r},\vec{r}') = <\overline{\Psi}(\vec{r})\overline{\Psi}(\vec{r}')>$ bears its name from the fact that there is an unequal number of creation and annihilation operators being averaged over. An analogous correlation plays a dominant role in the BCS theory of superconductivity [27], where fermionic atoms pair up to form the so-called Cooper pairs. In the case of Bose-Einstein condensation of neutral bosonic atoms, where the condensate mean field $\Phi(r)$ is the dominant parameter. It is well known that the anomalous density is proportional to the s-wave scattering length i.e. the interactions between atoms and $\tilde{m} = 0$ for the ideal Bose gas. Theoretically, the anomalous average arises in all calculations for Bose system with broken gauge symmetry [138, 178, 201, 202]. It quantifies the correlations of pairs of non- condensate atoms with pairs of condensate atoms due to the Bogoliubov pair promotion process in which two condensate atoms scatter each other out of the condensate which is responsible for the well-known Bogoliubov particle hole structure of excitations in the system [202]. The anomalous density can also be interpreted as a measure of the squeezing of the non-condensate field fluctuations [203]. Certainly, the presence of this quantity adds new features to the well-known problems and attracts our attention to the three and two-dimensional systems.

It is interesting to discuss the role of the so-called pair anomalous average arising in the theoretical description of partially-condensed Bose gases. In the scientific community, one often makes the simplified assumption that this quantity can be "safely" neglected. Although results based on such an approximation indeed appear to yield (somewhat puzzlingly?) often very good agreement with experimental findings, from a fundamental perspective this quantity should not be neglected. In this chapter we provide further evidence on this issue, discussing the relative role of this quantity under various relevant conditions in three dimensional Bose gas.

Among the theoretical investigations of the anomalous density, we can cite in particular those of Hutchinson *et al* [69] and Giorgini [204] based on the mean field HFB-BdG approximation. To go beyond the mean field, Fedichev *et al* [205] and Proukakis *et al* [202, 207] developed a finite temperature perturbation theory using a HFB basis. Another kind of approaches has been developed by Griffin [68] based on the Green's function method to derive an equation for the condensate and its fluctuations. Yukalov [208-210] adopted a quite different approach by using the notion of representative statistical ensembles. Recently, Wright *et al*. [201, 202] have used the classical-field trajectories of the Projected Gross-Pitaevskii equation.

In fact, for almost all practical purposes, the anomalous density is always neglected. This is based in the general owing to the fact that its contributions are negligibly small. However, Yukalov [208-210] pointed out that even if it is the case, it is an essential ingredient for the consistency of the formalism. We will go further by using our TDHFB formalism to show that the contribution of the anomalous density is not as small as claimed. On the other hand, the anomalous density profiles seem to have no structure at the centre of the trap for weak interactions. This is completely disagreement with what was found in the literature [68, 69, 201] where the HFB-BdG approximation and the classical-field trajectories of the Projected Gross-Pitaevskii equation were used, and where these densities are found to have a "dip". Let us now start our analysis by treating the homogeneous case for this reason it is convenient to write our TDHB equation in the momentum space.

4.2.Uniform TDHFB equation in *d*-dimensions:

In the uniform case ($V_{\text{ext}}(r)=0$) and for a thermal distribution at equilibrium, by working in the momentum space, the matrix density can be written as

$$\rho_{ij}(\vec{r},\vec{r}')=\int \frac{d^d k}{(2\pi)^d} e^{i\vec{k}.(\vec{r}-\vec{r}')}\rho_{ij}(k), \tag{4.1}$$

where $\rho_{ij}(k)$ is the Fourier transform of $\rho_{ij}(\vec{r},\vec{r}')$. We can then easily rewrite Eq. (3.14) of the Heisenberg invariant as

$$I_k = \tilde{n}_k(\tilde{n}_k+1)-|\tilde{m}_k|^2 = \frac{1}{4\sinh^2(\varepsilon_k/2T)}, \tag{4.2}$$

with ε_k is the Bogoliubov energy spectrum given below.

The physical meaning of Eq.(4.2) is that it allows us to calculate in a very useful way the dissipated heat for *d*-dimensional Bose gas as [183]

$$Q_d = \frac{1}{n}\int E_k I_k \frac{d^d k}{(2\pi)^d}, \tag{4.3}$$

where $E_k = \hbar^2 k^2 / 2m$ is the energy of a free particle.

Furthermore, at zero temperature, Eq. (4.2) reduces to $|\tilde{m}_k|^2 = \tilde{n}_k(\tilde{n}_k + 1)$, which constitutes an explicit relation between the normal and the anomalous densities at zero temperature and indicates that these two quantities are of the same order of magnitude at low temperatures which leads to the fact that neglecting $\tilde{m}$ while maintaining $\tilde{n}$ is a quite unsafe approximation.

The excitation energy ε_k is determined in our formalism via the random-phase approximation (RPA) [168] which can be found by expanding all quantities around their equilibrium solution. The RPA appears as a direct application of the general Balian-Vénéroni formalism to the Lie algebra of single boson operators [168, 175, 176].

Thus we write

$$\begin{aligned} \Phi(k,t) &= \Phi(k) + \delta\Phi(k,t) \\ \tilde{n}(k,t) &= \tilde{n}(k) + \delta\tilde{n}(k,t) \\ \tilde{m}(k,t) &= \tilde{m}(k) + \delta\tilde{m}(k,t) \end{aligned}. \tag{4.4}$$

Then, we have written these quantities on a diagonal basis (RPA matrix) which derived from the set (3), and kept only the first-order terms. After a long, but straightforward calculation, we arrive at the gapless expression of the Bogoliubov spectrum [68, 183]

$$\varepsilon_k = \sqrt{(\mathrm{E_k} - \mu + \Sigma_{11})^2 - \Sigma_{12}^2}, \tag{4.5}$$

where $\Sigma_{11} = 2\mathrm{g_d} n$ and $\Sigma_{12} = \mathrm{g_d}(n_c + \tilde{m})$ are respectively the first order normal and anomalous self-energies with $n = n_c + \tilde{n}$ is the total density.

Note that Eq.(4.5) can be also obtained using the Green's functions (see e.g.[68]). It provides a useful finite-temperature version of the healing length and the sound velocity c_s as

$$\xi = \hbar / \sqrt{m\Sigma_{12}} = \hbar / \sqrt{m n_c g_d \left(1 + \frac{\tilde{m}}{n_c}\right)} = \hbar / m c_s , \tag{4.6}$$

In order to get explicit formulas for the non-condensed and the anomalous averages in *d*-dimensions we may use Eq. (4.5). Simple calculation yields [178, 183]

$$\tilde{n} = \frac{1}{2}\int \frac{d^d k}{(2\pi)^d}\left[\frac{E_k + g_d(n_c + \tilde{m})}{\varepsilon_k}\sqrt{I_k} - 1\right], \tag{4.7.a}$$

$$\tilde{m} = -\frac{1}{2}\int \frac{d^d k}{(2\pi)^d}\left[\frac{g_d(n_c + \tilde{m})}{\varepsilon_k}\sqrt{I_k}\right]. \tag{4.7.b}$$

It is worth noting that the set (3.21.a) and (4.7) together form the generalized HFB equations. This shows that, in the static case, our formalism recovers easily the full HFB equations at both zero and finite temperatures.

4.3.Anomalous density in homogeneous three dimensional Bose gas

It is convenient now to analyze the asymptotic behavior of equations (4.6) with respect to the temperature.

At low temperature $\tilde{n}$ and $\tilde{m}$ behave as

$$\begin{aligned} \tilde{n} &= \frac{1}{2}\int \frac{d^3 k}{(2\pi)^3}\left[\frac{E_k + g_d(n_c + \tilde{m})}{\varepsilon_k} - 1\right] \\ \tilde{m} &= -\frac{1}{2}\int \frac{d^3 k}{(2\pi)^3}\left[\frac{g_d(n_c + \tilde{m})}{\varepsilon_k}\right] \end{aligned} \quad . \qquad (T \to 0) \tag{4.8}$$

At high temperature we can use the asymptotic form $\sqrt{I_k} \cong \frac{2T}{\varepsilon_k}$. Then, $\tilde{n}_k$ and $\tilde{m}_k$ take the form

$$\begin{aligned} \tilde{n} &= \int \frac{d^3 k}{(2\pi)^3}\frac{E_k + g(n_c + \tilde{m})}{\varepsilon_k}\left(\frac{T}{\varepsilon_k}\right) - \frac{1}{2} \\ \tilde{m} &= -\int \frac{d^3 k}{(2\pi)^3}\frac{g(n_c + \tilde{m})}{\varepsilon_k}\left(\frac{T}{\varepsilon_k}\right) \end{aligned} \qquad (T \to T_c). \tag{4.9}$$

To illustrate comparatively the behavior of the normal and anomalous densities, as functions of temperature for a uniform Bose gas, it is useful to introduce the dimensionless variables $\eta = \frac{\varepsilon_k}{g(n_c + \tilde{m})}$ and $\tau = \frac{T}{g(n_c + \tilde{m})}$. Therefore, equations (4.7) become

$$\begin{aligned} \tilde{n}(\eta) &= \frac{\sqrt{1+\eta^2}}{2\eta}\sqrt{I(\eta)} - \frac{1}{2} \\ \tilde{m}(\eta) &= -\frac{1}{2\eta}\sqrt{I(\eta)} \end{aligned}, \tag{4.10}$$

where $\sqrt{I(\eta)} = \coth\left(\frac{\eta}{2\tau}\right)$

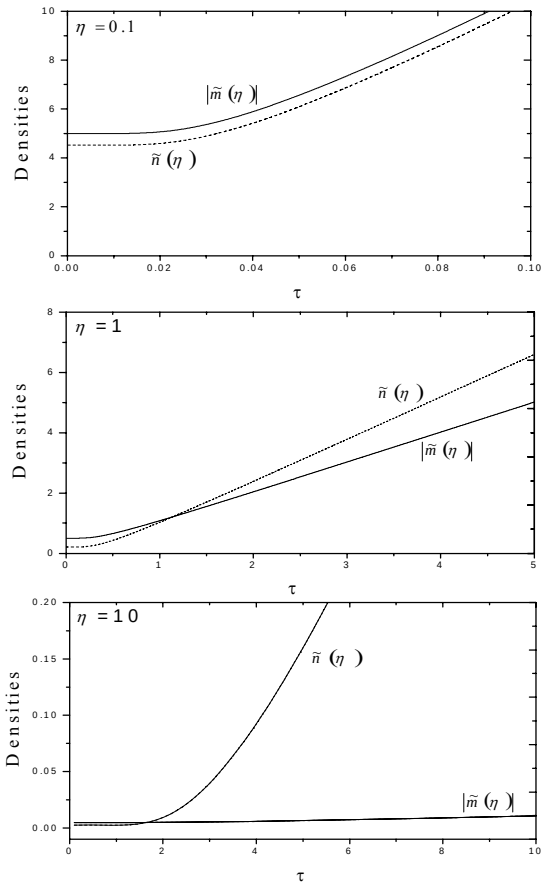


Figure4. 1. The absolute value of the anomalous density $\tilde{m}(\eta)$ (Solid line) and the non condensate density $\tilde{n}(\eta)$ (dashed line) vs. the temperature τ for different values of η .

In figure 4.1 we show that the absolute value of the anomalous density is always larger than the noncondensed density for small value of $\eta = 0.1$ at low temperature. Moreover, the absolute value of the anomalous density is comparable with the noncondensed density for $\eta = 1$ ($|\tilde{m}| \approx \tilde{n}$ for $\tau \approx 1.2$). However, at high temperatures, the anomalous density becomes much smaller than the non condensed density. As can be seen from these figures, the behavior of the normal and anomalous densities found here is in good agreement with the recent theoretical results of refs [209-213].

Finally, we can check that omitting the anomalous density, while keeping the normal one, is mathematically inappropriate this is clearly shown in (4.6) [178]. From these facts, it is understandable now that neglecting the anomalous density at low temperature for homogeneous Bose gas as one habitually does in the literature is principally unjustified approximation. Let us turn to analyze the situation for trapped Bose gas.

4.3.1. Solution at zero temperature

The integral (4.7.b) has both an infrared and ultraviolet convergence in 3 D. This divergence is well-known and arises due to the use of the contact potential. So the integral (4.7.b) can be calculated by means of the dimensional regularization [208, 214-216], which gives for the integral

$$\int_0^\infty \frac{xdx}{\sqrt{1+x^2}} = -1, \tag{4.11}$$

and therefore the anomalous density can be written as

$$\tilde{m}_{T=0} = \frac{1}{\pi^2 \xi^3} = \frac{(mc_s)^2}{\pi^2}\sqrt{mgn_c} = \frac{8}{\sqrt{\pi}}\left(n_c a^3\right)^{1/2} = 3\tilde{n}, \tag{4.12}$$

where $c_s = \sqrt{(n_c + \tilde{m})g/m}$ is the sound velocity.

The dimensional regularization follows from perturbation theory of scattering and it gives asymptotically exact results at weak interactions i.e. $g \to 0$. So the extrapolation to finite interactions requires that the limiting condition $\tilde{m}/n_c << 1$ be satisfied. Therefore, using this technique presupposes that value of the healing length takes the form $\xi = \hbar/\sqrt{mn_c g}$. Equation (4.12) clearly shows that the anomalous density is larger than the noncondensed

density at $T=0$. Such a result confirms both our formula (4.2) and our qualitative analysis exposed in the previous section.

4.3.2. Solution at low temperature

To find the low temperature behavior of $\tilde{m}$, we may rewrite eq. (4.7.b) as

$$\begin{aligned}\tilde{m} &= -\frac{1}{2}\int \frac{d^3k}{(2\pi)^3}\frac{g_d(n_c+\tilde{m})}{\varepsilon_k} - \frac{1}{2}\int \frac{d^3k}{(2\pi)^3}\left[\frac{g_d(n_c+\tilde{m})}{\varepsilon_k}\left(\sqrt{I_k}-1\right)\right] \\ &= \tilde{m}_{T=0} - \frac{1}{2}\int \frac{d^3k}{(2\pi)^3}\left[\frac{g_d(n_c+\tilde{m})}{\varepsilon_k}\left(\sqrt{I_k}-1\right)\right] \\ &= \tilde{m}_{T=0} - \tilde{m}_T\end{aligned} \quad , \tag{4.13}$$

where $\tilde{m}_T$ is the thermal contribution of the anomalous density.

At low temperatures, the main contribution of this integral comes from the region of small momentum. Then the use of the integral

$$\int_0^\infty x^{2j-1}\left[\coth(\alpha x)-1\right]dx = \frac{\pi^{2j}\left|B_{2j}\right|}{2j\alpha^{2j}}, \tag{4.14}$$

where B_{2j} are the Bernoulli number, leads to the following expression for the thermal contribution of the anomalous density:

$$\tilde{m}_T = \frac{mT^2}{12\hbar^3 c_s} \ . \tag{4.15}$$

Recalling that in limit $\tilde{m}/n_c << 1$, the sound velocity is $c_s = \sqrt{n_c g/m}$ and the coupling constant g is expressed through the scattering length and density as $g = 4\pi\hbar^2 a/m$, we find

$$\tilde{m}_T = \frac{2}{3\sqrt{\pi}}\left(n_c a^3\right)^{1/2}\left(\frac{\pi T}{ng}\right)^2 = \tilde{n} \ ; \quad T << ng \tag{4.16}$$

Comparing the result of Eq. (4.16) with the zero-temperature anomalous density $\tilde{m}_{T=0}$ following from Eq. (4.12) we see that at temperatures $T << ng$ the thermal contribution is small and can be omitted when calculating the total anomalous density (4.13).

The situation is quite different at temperatures $T >> ng$, where the main contribution to $\tilde{m}$ (4.13) comes from single-particle excitations which leads immediately to a vanishing anomalous density.

4.3.3. Link with the *T*-matrix

As we have mentioned in section 4.2, the anomalous average is calculated simply by putting population into the quasi-particle modes (see Eq. (4.7.b))

$$\tilde{m} = -\sum_k \left[\frac{g(n_c + \tilde{m})}{\varepsilon_k} \coth(\varepsilon_k / 2T) \right]. \tag{4.17}$$

We now have the full method in place for gapless self-consistent calculations at finite temperature. There is, however, a snag. If we use this expression directly, by summing over all states, we come up against the main problem associated with using a contact form of the interaction. We find that the expression for $\tilde{m}$ diverges as we take the sum over higher and higher states i.e. the so called ultraviolet divergence.

We recall that $\tilde{m}$ represents the pair correlations between particles in the presence of the condensate and excited atoms. Part of this correlation, however, has already been included in the contact interaction which represents the effect of the pair correlation. These pair correlations modify the scattering of two condensate atoms, producing an effective interatomic potential [70,184]. To understand better the link to the effective interaction, it is easiest to use the first equation of our TDHFB equation (3.21.a)

$$\left(-\frac{\hbar^2}{2m}\Delta + V_{ext}(\vec{r}) - \mu \right)\Phi(\vec{r}) + g\left(|\Phi(\vec{r})|^2 + 2\tilde{n}(\vec{r})\right)\Phi(\vec{r}) + g\,\tilde{m}(\vec{r})\Phi^*(\vec{r}) = 0\,, \tag{4.18}$$

with $\Phi(\vec{r})$ is normalized to the total number of condensed particles. The form of the effective interaction in this case can be seen by grouping the final term with the expression $g|\Phi|^2\Phi$ to give

$$g\left(|\Phi(\vec{r})|^2\Phi(\vec{r}) + \tilde{m}(\vec{r})\Phi^*(\vec{r})\right) = g\left[1 + \frac{\tilde{m}(\vec{r})}{\Phi^2(\vec{r})}\right]|\Phi(\vec{r})|^2\Phi(\vec{r}) = \tilde{U}(r)|\Phi(\vec{r})|^2\Phi(\vec{r})\,. \tag{4.19}$$

Hence, $\tilde{U}(r)$ can be thought of as an approximation to the full many body interaction potential between two condensate atoms in the presence of the excited atoms mean field.

We now want to confirm that this definition of the effective potential is equivalent to the many body *T*-matrix to confirm the definition.

4.3.4. The many body *T*-matrix in the homogeneous limit

The full many body *T*-matrix contains all the effects of the medium on the pair interactions in a gas. It has been shown [70] that T^{MB} is related to the low-momentum limit of the vacuum scattering amplitude g via the following equation

$$T^{MB} = \frac{g}{1+\int \frac{d^3k}{(2\pi)^3}\left[\frac{1}{2\varepsilon_k}(2N_k+1)-\frac{1}{2E_k}\right]}, \tag{4.20}$$

where $N_k = [e^{\varepsilon_{k/T}} - 1]^{-1}$.

The term with $(-1/2E_k)$, therefore, corresponds to scattering in vacuo. So,

$$T^{MB} = g\left\{1 - T^{MB}\int \frac{d^3k}{(2\pi)^3}\left[\frac{(2N_k+1)}{2\varepsilon_k} - \frac{1}{2E_k}\right]\right\}. \tag{4.21}$$

We now have to show that this expression is equivalent to $\tilde{U}(r)$ in uniform gas. To see this, we need the expression for $\tilde{m}$ which after the subtraction of the ultra-violet divergent part is given

$$\tilde{m} = -n_c T^{MB}\int \frac{d^3k}{(2\pi)^3}\left[\frac{(2N_k+1)}{2\varepsilon_k} - \frac{1}{2E_k}\right]. \tag{4.22}$$

Since $n_c = \Phi^2$, comparisons with the expression for clearly shows that

$$T^{MB} = g\left[1 + \frac{\tilde{m}}{\Phi^2}\right]. \tag{4.23}$$

We have shown, therefore, that the effective interaction corresponds to the zero-energy, zero momentum limit of the homogeneous many body *T*-matrix.

To obtain an estimate value of $\tilde{m}$ we note that the quasi-particle energy goes over to the free particle energy for $\varepsilon_k > gn_c$. So at $T = 0$ we find

$$\tilde{m} = -n_c g\int_0^{k=\frac{1}{\xi}} \frac{d^3k}{(2\pi)^3}\left[\frac{1}{2\varepsilon_k} - \frac{1}{2E_k}\right] = 3\left[n_c\frac{8}{3}\left(\frac{n_c a^3}{\pi}\right)^{1/2}\right] = 3\tilde{n}\ , \tag{4.24}$$

where $\xi = \hbar^2/\sqrt{mng}$ is the healing length.

This result is in good agreement with that obtained in Eq.(4.12) using the dimensional regularization which constitutes in this sense a simplest version of mean field at $T = 0$. It is important to see that this procedure can only work if the effective cutoff due to the quasi-

particle energy goes over to the free particle one. This procedure also prove that the anomalous density still bigger than the noncondensed density at zero temperature which is in good agreement with our result [178, 208].

4.4.Anomalous density for a trapped Bose gas

We adopt the same numerical method used in the previous chapter and then we consider the ^{87}Rb gas with the following parameters [187,188]: $a = 5.8210^{-9}$ m, $a_{H0} = 7.6210^{-7}$ m and $\hbar\omega = 1.3210^{-31}$ J. A convenient dimensionless parameter describing the effective strength of the interactions is $\gamma = Na / a_{H0}$ [59,189]. We begin by plotting the anomalous density as functions of the radial distance for several values of the temperature and for $N = 20000$ atoms i.e. $\gamma = 153$.

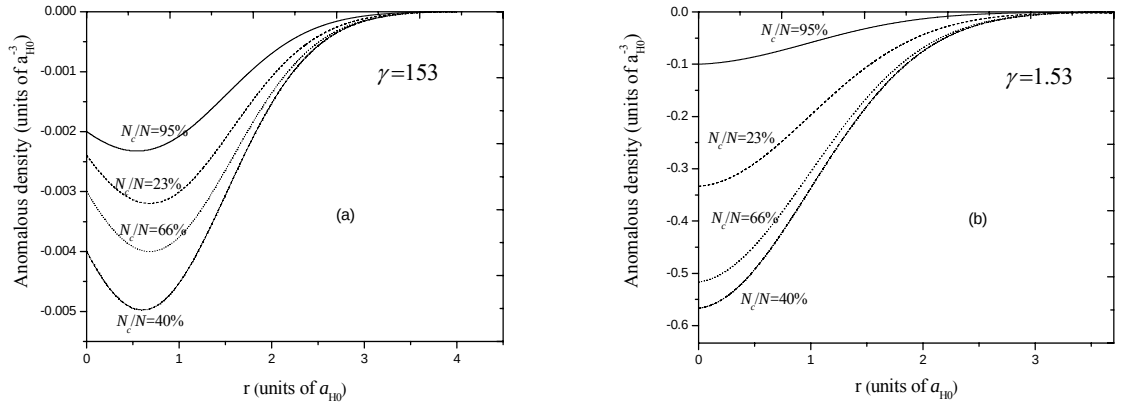


Figure4. 2. The anomalous density profiles for various condensate fractions.

Figure 4.2 (a) depicts the anomalous density for varying condensation fraction and for $\gamma = 153$. We notice that by decreasing N_c / N , $\tilde{m}$ begins to increase in absolute value then decreases when N_c / N approaches 50%. This overall behavior has also been obtained in [69,201]. The anomalous density remains real and negative value whatever the temperature and the position. The presence of effective repulsive atomic interactions between the atoms, and thus also between the condensate and the thermal cloud, leads to the appearance of a local dip in the anomalous density at the centre of the trap.

In figure 4.2 (b) we show that for a small value of the interaction parameter ($\gamma = 1.53$) the shape of the anomalous density is surprisingly modified in particular we observe that the dip in the neighbourhood of the centre of the trap disappears and the curve takes a Gaussian form.

The central anomalous density is lowered for weak interactions. Such a result can be justified by the effect of interactions i.e. for a small number of particles or small value of γ, the interactions between the atoms of the condensate and the thermal cloud are lowered which means that the correlations become weak and that's why the anomalous density remains small and takes a Gaussian shape together with the thermal and the condensate density. We note that the effect of interactions on the anomalous density was studied theoretically earlier by many authors but no one looks how the shape of this quantity varies depending on interactions.

We now turn our attention to analyze more obviously the temperature dependence behavior of the non condensate and the anomalous fractions defined respectively as $\tilde{N}/N$ and $\left|\tilde{M}/N\right|$ where $\tilde{N}=\int d\vec{r}\tilde{n}(r)$ and $\tilde{M}=\int d\vec{r}\left|\tilde{m}(r)\right|$ are the integrated values of the non condensate and the anomalous densities.

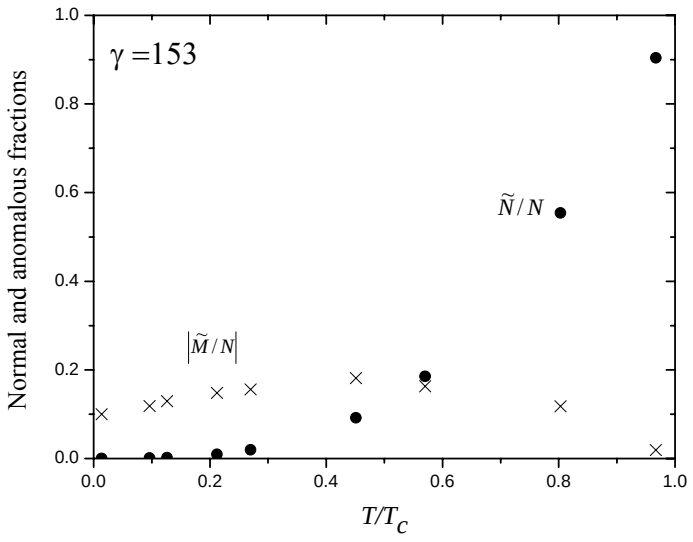


Figure 4.3. The normal and anomalous fractions versus reduced temperature for $\gamma = 153$.

In figure 4.3, we plot the non-condensate and the absolute value of anomalous fractions as function of the reduced temperature T/T_c for $\gamma = 153$ (where we follow the method outlined in [69]). It can be seen that $\tilde{N}/N$ is increasing significantly with increasing temperature and that is why $\tilde{N}$ reaches to a maximum value close to the Bose-Einstein condensation transition temperature. Furthermore, it is quite interesting to observe that the absolute value of the

anomalous fraction $\left|\tilde{M}/N\right|$ becomes small as the temperature approaches zero or T_c. It reaches a maximum at intermediate temperatures ($T \approx 0.5T_c$).

On the other hand, a careful look at figure 4.3 shows that $\left|\tilde{M}/N\right|$ is larger than $\tilde{N}/N$ at low temperature ($T \leq 0.5T_c$) which is visible in our relation (4.4). This result is in disagreement with what is given in literature [69] where the authors still based on the idea that the anomalous fraction is always smaller than the normal one for any range of temperature even at low temperatures without any physical or mathematical justifications. Secondly, when the temperature approaches to its critical value the fraction of non-condensed particles becomes close to the unity. That is why at $T \cong T_c$ the anomalous fraction simultaneously with the condensate one become much smaller than the normal fraction. Such feature is well explained in the literature [69, 201, 208-212]. Most importantly, the anomalous and normal fractions are of the same order of magnitude at intermediate temperatures. It is worth noticing that this behavior persists even for $\gamma = 1.53$ with a small change in the amplitudes of these fractions. Hence, we may infer from these results that the anomalous fraction plays a central role at low temperatures. It is therefore highly unlikely to neglect it for $T < T_c$.

The importance of the anomalous density can be highlighted if we compare the expressions, derived with and without taking into account the anomalous averages, with measured quantities, thus measuring the contributions from the anomalous averages. In some cases, the difference is drastic. For instance, the BEC transition is of first order when the anomalous average is not taken into account, while it is second order when we take it into account. Another example is the fact that the compressibility becomes infinite, implying that the system is unstable if the anomalous averages are absent. Moreover, the superfluid transition does not occur, if the anomalous averages are omitted [208,209].

Chapter 5

Anomalous correlation function in two dimensional Bose gas

5.1.Introduction

The subject of low-dimensional quantum gases has a long pre-history. The influence of dimensionality of the system of bosons on the presence and character of Bose-Einstein condensation and superfluid phase transition has been a subject of extensive studies in the spatially homogeneous case. From a general point of view, the absence of a true condensate in two-dimensions (2D) and one-dimension (1D) at finite temperatures follows from the Bogoliubov k^{-2} theorem and originates from long-wave fluctuations of the phase (see, e.g. [41,42]). This has been expounded by Mermin and Wagner [217] and by Hohenberg [218], and formed a basis for later investigations.

The case of 2D Bose fluid is particularly fascinating because of its “marginal” behavior. In an infinite uniform 2D fluid thermal fluctuations at any nonzero temperature are strong enough to destroy the fully ordered state associated with Bose-Einstein condensation, but are not strong enough to suppress superfluidity in an interacting system at low, but non-zero temperatures. Further, the presence of residual "quasi-long-range" order at low temperatures leads to an interesting interplay between superfluidity and condensation in all experimentally relevant finite-size systems. It was Popov who originally introduced the idea of a quasicondensate to explain the superfluidity of a two-dimensional Bose gas [45, 219]. The difference to a true BEC is that phase fluctuations destroy the coherence of the global phase throughout the condensate, and phase coherence governs only regimes of a size smaller than the size of the condensate, characterized by the coherence length l_ϕ .

Moreover, the microscopic theory of the 2D superfluid transition was developed by Berezinskii [220] and Kosterlitz and Thouless [221] (see [222] for a more recent review). The transition takes place in the degenerate regime, where the density fluctuations in an interacting gas are significantly suppressed. How does it occur?

It occurs through the formation of bound vortex-antivortex pairs; vortices can exist only in the form of bound pairs of vortices with opposite circulations $\pm 2\pi$. Since they do not have any net charge, such pairs do not create any net circulation along closed contours larger than the pair size, which for a tightly bound pair is also of order. Such pairs therefore have only a short-range effect on the phase and the velocity field, and do not have a large effect on the behavior of the correlation function $g_1(r)=\tilde{n}(r)=\langle\Psi^+(r)\Psi(0)\rangle$ at large distances. In addition, at any non-zero temperature, pairs are continuously created and annihilated through thermal fluctuations. On the other hand, above $T_{BKT}=\pi\hbar^2 n_s/2m$ where n_s is the superfluid density, unbinding of vortex pairs and proliferation of free vortices becomes energetically favorable. Free vortices then form a disordered gas of phase defects and completely "scramble" the phase (see figure 1). This destroys the quasi-long-range order and suppresses superfluidity. At even higher temperature where density fluctuations are strong, the notion of individual vortices becomes physically irrelevant.

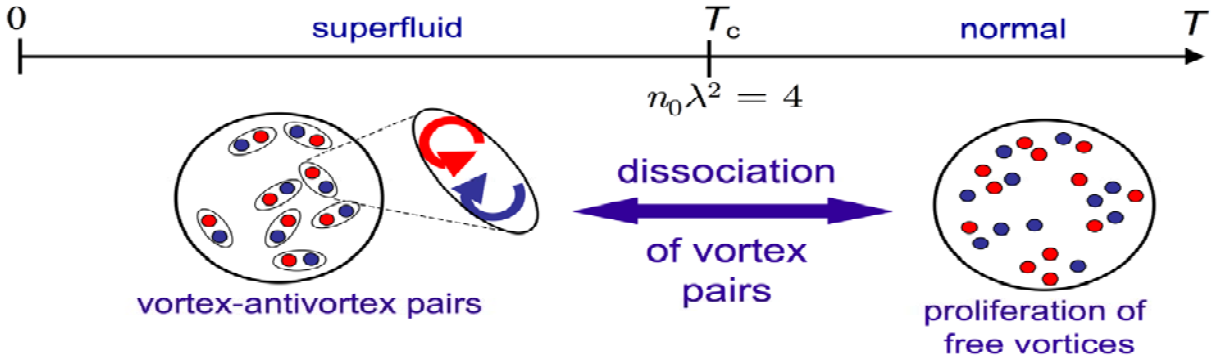


Figure 5.1. The BKT mechanism at the origin of the superfluid transition. Below the transition temperature (left figure), vortices exist only in the form of bound pairs formed with vortices with opposite circulation. When approaching the transition point the density of pairs grows and the average size of a pair diverges. Just above the transition point (right figure), a plasma of free vortices is formed and the superfluid density vanishes.

As stated above, the two-dimensional case is a very special case, and sound contributions only started in the early seventies by Schick (1971) [223] and Popov (1972) [219], after the 3D and 1D cases were pretty much well established, at least for the uniform case. After the remarkable experimental progress of the ultracold gases in two dimensions [224-232] which recently attracted great attention, several theoretical studies of fluctuations, scattering properties and the appropriate thermodynamics have been carried out in [233-238]. In fact, in most of the previous references, the anomalous density is neglected under the claim that it is a divergent and unmeasured quantity as well as its contribution is very small compared to the other terms. Otherwise, the importance of the anomalous density in three-

dimensional Bose gas has been well highlighted in the previous chapter (see also our recent papers [177, 178]).

Due to the complexity and the particularity of dilute 2D Bose gases, many analytical investigations have been performed recently to find corrections beyond mean-field at zero temperature. One should cite at this stage that Pricoupenko [186,239] employs the pseudo potential with a Gaussian variational approach. Mora and Castin [240], on the other hand, used their lattice model which is a sort of regularization scheme to treat ultraviolet divergences. Cherny *et al* [241] used a reduced-density matrix of second order and a variational procedure to derive results identical to those of Refs [239, 240] for equation of state (EoS) and ground-state energy. The above analytical results have been checked using Monte Carlo calculations to find numerical agreement with beyond mean-field terms in 2d [242, 243]. Recently, Mora and Castin [244] have been also extended their approach [240] one step beyond Bogoliubov theory which gives good accuracy with the simulations of [243].

A summary of the most important works till 2005 are presented in Table I, where we report the expression for the energy per particle. Almost all beyond mean field (MF) theories agree on the presence of the $\ln|\ln na^2|$ term but differs in the constant, or explicitly discuss that the constant term cannot be obtained within the used approach.

year	first author	type	terms
1971	Schick	MF	$E^{\mathrm{MF}}/N = 2\pi\hbar^2 n/(m\lvert\ln na^2\rvert)$
1971	Popov	BMF	$\ln\lvert\ln na^2\rvert - \ln 4\pi - 1/2$
1978	Lozovik	BMF	$\ln\lvert\ln na^2\rvert - \ln 4\pi + 1/2$
1978	Hines	BFM	$\ln\lvert\ln(na^2/\pi)\rvert - \ln 2\pi^3 - 2\gamma + 3/2$
1988	Fisher	BFM	$\ln\lvert\ln na^2\rvert - \ln 4\pi - 1/2$
1992	Kolomeisky	BFM	$\ln\lvert\ln(4\pi na^2)\rvert - \ln 4\pi$
1993	Ovchinnikov	BMF	$\ln\lvert\ln na^2\rvert$
2001	Lieb	MF	$E^{\mathrm{MF}}/N = 2\pi\hbar^2 n/(m\lvert\ln na^2\rvert)$
2001	Cherny	BMF	$\ln\lvert\ln na^2\rvert - \ln\pi - 2\gamma - 1/2$
2002	Andersen	BMF	$\ln\lvert\ln na^2\rvert - \ln 4\pi - 1/2$
2003	Mora	BMF	$\ln\lvert\ln na^2\rvert - \ln\pi - 2\gamma - 1/2$
2004	Pricoupenko	BMF	$\ln\lvert\ln na^2\rvert - \ln\pi - 2\gamma - 1/2$
2005	Pilati	BMF	$0.86\ln\lvert\ln na^2\rvert - 2.26$

Table 1 . Literature overview: equation of state of a dilute two-dimensional Bose gas. Fifth column, terms of the low density expansion appearing as straight lines in Fig. 1 in the limit of large ln | ln na2|.

Another kind of extensions has been developed recently by Sinner *et al* [245] which based on using the functional renormalization group to study dynamical properties of the 2D Bose gas at $T = 0$. The approach is free from infrared divergences and satisfies both the Hungeholtz-Pines (HP) [31] relation and the Nepomnyashchy identity [246], which states that the anomalous self-energy vanishes at zero frequency and momentum. The spectrum energy thus satisfies a Bogoliubov-type expression with a renormalized sound velocity. Although the above approaches provide good predictions for the thermodynamic of 2D Bose gas in the universal regime, they are limited only at zero temperature.

The present chapter deals with extending our variational Time Dependent Hartree-Fock-Bogoliubov (TDHFB) theory to the case of 2D Bose systems. Therefore, a number of questions arise naturally: Does the anomalous density exist even at finite temperature in 2d Bose gas? How does its behavior compare with the normal density at zero temperature? What are the effects of this quantity on the thermodynamics of the system?

In what follows, we restrict ourselves to study the two dimensional behavior of the anomalous density and its effects on the depletion, the chemical potential and the ground-state energy. We therefore, compare our results with recent Monte Carlo simulations and analytic predictions. The validity of the HP theorem and Nepomnyashchy identity are also discussed within the present formalism. In addition we will extend our results at finite temperature where we calculate in particular the one-body anomalous correlation function. Furthermore, we will apply our formalism to analyze the behavior of the superfluid fraction. We then emphasize the importance of the anomalous density for the occurrence of superfluid transition and sound velocity.

5.2.Noncondensed and anomalous densities at zero temperature

Let us now discuss the behavior of the normal and anomalous densities in homogeneous 2D Bose gas at both zero and finite temperatures. From this point we consider the regime in weakly repulsive interaction at zero temperature where $\sqrt{I_k} = 1$. In two-dimensional Bose gas, the interaction parameter ($g_d = g_2$) depends logarithmically on the chemical potential as

$$g_2 = \left[\frac{4\pi\hbar^2}{m} \frac{1}{\ln\left(2\hbar^2 / m\mu a^2\right)} \right], \tag{5.1}$$

where a is the two-dimensional scattering length among the particles and g_2 is the two-body T-matrix (see e.g. [236-240]).

The calculation of the integral in Eq. (4.7.a) of the previous chapter leads us to the following expression of the non-condensed density [247]

$$\tilde{n} = \frac{1}{2}\int \frac{d^2k}{(2\pi)^2}\left[\frac{E_k + g_2(n_c + \tilde{m})}{\varepsilon_k} - 1\right] = \frac{1}{4\pi\xi^2}. \tag{5.2}$$

This equation is in good agreement with that obtained in [239,248].

At zero temperature 2D case, the integral in Eq.(4.7.b) becomes

$$\tilde{m} = -\frac{1}{2}\int \frac{d^2k}{(2\pi)^2}\left[\frac{g_2(n_c + \tilde{m})}{\varepsilon_k}\right]. \tag{5.3}$$

Clearly, this integral has an ultraviolet divergence in both two and three dimensions. This divergence is well-known and arises due to the use of the contact potential. To regulate the ultraviolet divergences, we may use the dimensional regularization [249]. In such a technique one calculates the loop integrals in $d = 2 - 2\eta$ dimensions for values of η where the integrals converge. One then analytically continues back to $d = 2$ dimensions. With dimensional regularization, an arbitrary renormalization scale M is introduced. This scale can be identified with the simple momentum cutoff. An advantage of dimensional regularization is that in two dimensions systems it automatically sets power divergences to zero, while logarithmic divergences show up as poles in η [249]. Using this technique one gets for the anomalous density

$$\tilde{m}^{\Lambda}_{T=0} = -\frac{\Lambda^2}{4} J_{0,1}, \tag{5.4}$$

where Λ is the regularized-part which is related to the size of particles and interactions as $\Lambda = 2/\xi$. This parameter is similar to that used in [239,244, 249].

And $J_{0,1} = \frac{1}{4\pi}\left[\frac{1}{\eta} - L + O(\eta)\right]$ with $L = \ln\left(\Lambda^2 / 4M^2\right)$.

Thus the convergent part of the anomalous density provides

$$\tilde{m}_{T=0}^{\Lambda} = \frac{\Lambda^2}{16\pi}\ln\left(\Lambda^2/4M^2\right). \tag{5.5}$$

A useful remark at this level, the non-condensed density of Eq.(5.2) can be rewritten also in terms of Λ as $\tilde{n} = \Lambda^2/16\pi$.

At $T = 0$, the condensed density has a significant value and hence constitutes the dominant quantity in the system, while both the non-condensed and the anomalous densities vanish for $\Lambda \to 0$ which ensures that $\Sigma_{11}^{\Lambda=0} = 2\mu$ and $\Sigma_{12}^{\Lambda=0} = \mu$ in good accordance with the Hugenholtz-Pines theorem $\Sigma_{11}^{\Lambda=0} - \Sigma_{12}^{\Lambda=0} = \mu$ [31]. On the other hand, once we find $\Sigma_{12}^{\Lambda=0} \neq 0$, this means that the actual version of our extended variational TDHFB including a dimensional regularization does not satisfy the Nepomnyashchy identity [246] as it should be for any limited approximation order (see for example Griffin *et al* [68,110], Yukalov [208-210], Pricoupenko [239] and Andersen [248]). Indeed, in a Bose-condensed system, the anomalous self-energy must be nonzero in order to define a meaningful nonzero sound velocity and healing length. In addition, a zero sound velocity leads evidently to an unstable system (see Eq.(9)).

Indeed, our approach can be an effective way to verify the Nepomnyashchy identity, but on the condition that we sum over all terms of perturbation theory for the self-energy with renormalization of the sound velocity [183] to ensure the stabilization of the system as it has been demonstrated in [245].

Conversely, at finite-temperature three-dimensional Bose gas, the chemical potential satisfies the generalized version of HP theorem given by Hohenberg and Martin [250] $\Sigma_{11}^{\Lambda} - \Sigma_{12}^{\Lambda} = \mu$. In such a situation, when $T \geq T_c$, both the condensate and the anomalous densities vanish [177,178, 208] whatever the value of Λ, which implies directly that $\Sigma_{12}^{\Lambda} = 0$ and $\Sigma_{11}^{\Lambda} = 2g\tilde{n} \approx 2\mu$. Consequently, a vanishing anomalous self-energy is further guaranteed at high temperature and momentum in 3D systems. Physically, this result is reasonable because the gas becomes completely thermalized and therefore there is neither superfluid nor acoustic waves when the temperature reaches its critical value.

On the other side, the dimensional regularization gives an asymptotically exact result at weak interactions ($g_2 \to 0$). The extrapolation to finite interactions requires that the limiting condition $\tilde{m}/n_c << 1$ be verified. In real systems, however, the interactions have a finite

range a and so $1/a$ provides a natural ultraviolet cutoff M [249]. Hence, using this technique presupposes that value of the healing length in Eqs.(5.2) and (5.5) takes the form $\xi = \hbar / \sqrt{m n_c g_2}$. In the case where $n_c \approx n$, we recover easily the well-known result of Schick [223] for the depletion, while Eq.(5.5) has no analog in the literature. Under these conditions, the anomalous average turns out to be given as [183,247]

$$\widetilde{m}_{T=0} = \frac{m\mu_0}{4\pi\hbar^2} \ln\left(\frac{m\mu_0 a^2}{\hbar^2}\right), \tag{5.6}$$

where $\mu_0 = g_{2d} n$.

Figure 5.2 shows that the non-condensed and the anomalous densities, as function of the dimensionless parameter $x = m\mu_0 a^2 / \hbar^2$, are competitive contributions at zero temperature. For small values of x, we observe that the non-condensed density is greater than the anomalous one while this later becomes the dominant quantity for the whole range of x ($x > 10$). $\widetilde{n}$ and $\widetilde{m}$ are comparable only for $x \approx 10$. Therefore, we deduce that omitting the anomalous density, while keeping the normal one is physically and mathematically inappropriate. It is noticed that this behavior holds also in three dimensional Bose gas [177, 178, 208].

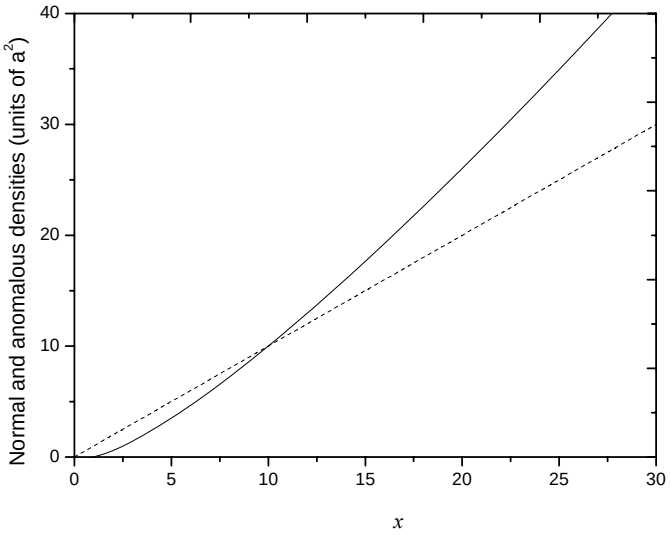


Figure 5. 2. Non-condensed (dashed line) and anomalous (solid line) densities as function of x

It is important now to discuss how the anomalous density can modify the chemical potential and hence the other thermodynamic quantities of dilute Bose gas. The first order

quantum corrections to the chemical potential are given by $\delta\mu = g_d(\tilde{n}+\tilde{m})$ [35]. Therefore, using the results obtained in Eqs.(5.2) and (5.6) with the assumption $n \approx n_c$ at $T=0$. One obtains for the chemical potential

$$\mu = \mu_0\left[1+\frac{m\mu_0}{4\pi\hbar^2 n}\ln\left(\frac{m\mu_0 a^2 e}{\hbar^2}\right)\right]. \tag{5.7}$$

The ground-state energy is obtained through [183]

$$E/N = \int_0^n \mu dn = \frac{\mu_0}{2}\left[1+\frac{mg_2}{8\pi\hbar^2}\ln\left(\frac{m\mu_0 a^2\sqrt{e}}{\hbar^2}\right)\right]. \tag{5.8}$$

The leading term in Eq.(5.7) was first obtained by Schick [223] while the second represents our correction to the chemical potential [184]. Clearly this correction is *universal*, depending only on the interactions and scattering length. It is worth mentioning that the additional logarithm term in Eq.(5.7) is analogous to that found recently in [244]. Moreover, what is interesting in Eq. (5.7) is that if we invert it and take the limit of vanishing density, we thereby recover the well-known Popov's EoS [219].

Before plotting figures (5.3) and (5.4), we use the dimensionless relation $na^2 = x^2\left[\frac{1}{2}-\ln\left(\frac{xe^{\gamma}}{2}\right)\right]$ where γ is the Euler's constant [239, 244]. Here we mention that the Euler's gamma constant appearing in some of the theoretical results is related to the dependence in the ladder approximation of the chemical potential on the scattering amplitude [35], which in turn contains in its short-range expansion [250].

One can see from figure 5.3 that for the value of the gas parameter around 5×10^{-5} there is a difference of 10% between the equations of state while for na^2 larger than 5×10^{-3} all EoS are practically identical.

Figure.4 shows that our expression of the ground sate energy (Eq.(17)) gives also an estimate compatibility within error bars of Monte-Carlo simulations [242, 243] and analytic results of [239-241, 244]. Furthermore, it is clearly seen from figures 5.3 and 5.4 that there is an upward shift of our curve relative to that of ref [244], which is indeed due to a prefactor which appears in the expansion of the later reference.

Another important feature revealed in figure 5.3 is that there is no difference between dipolar and short-range interaction for densities lower than 10^{-10} [243].

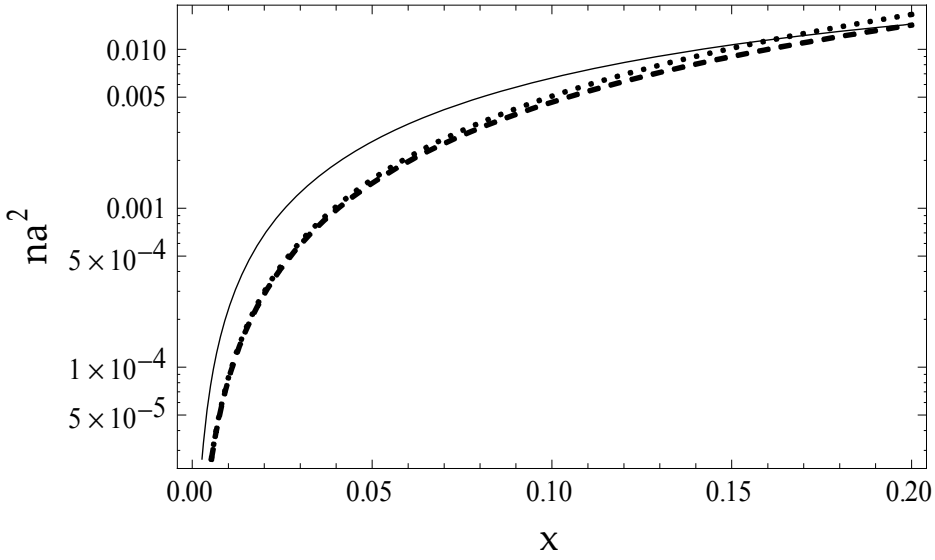


Figure 5.3. Equation of State of 2D homogeneous Bose gas. Solid line: our extended variational approach. Dashed line: EoS predicted in [186,239, 240]. Dotted line: first correction beyond Bogoliubov theory [244].

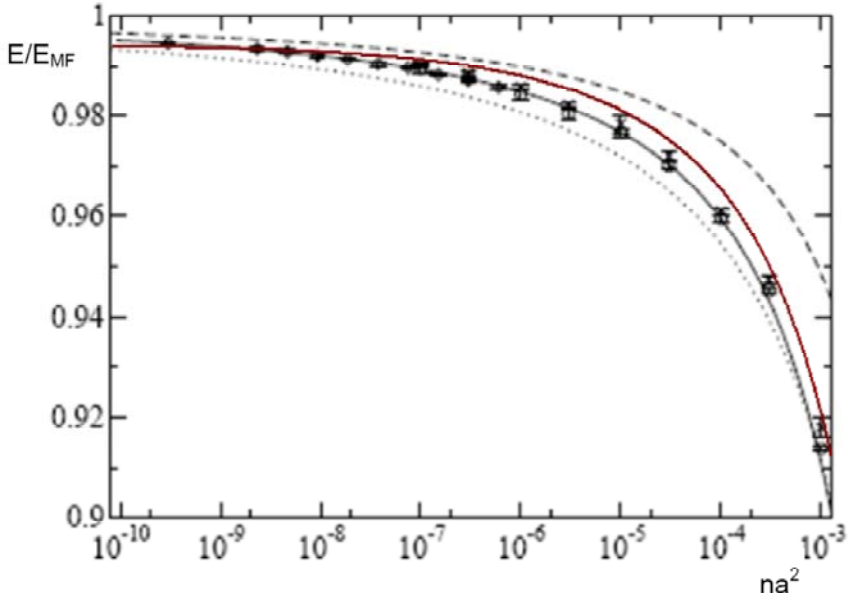


Figure 5.4. Ground state energy of a two dimensional Bose gas, as a function of the gas density, in units of the mean field prediction E_{MF}. Brown solid line: our calculations. Dark solid line: energy obtained from the beyond Bogoliubov [244]. Dashed line: analytical prediction of [241]. Dotted line: analytical calculations of [239]. Plotting symbols with error bars: numerical results of [242], for interactions given by hard disks (crosses) and by soft disks (circles); numerical results of [243], for dipolar interactions (diamonds).

5.3.Single-particle (one body) anomalous correlation function at finite temperature

Now we turn to analyze the finite temperature case. As we already mentioned in the introduction, the finite temperature uniform 2D Bose gas is characterized by the absence of a true Bose-Einstein condensate and long range order [217, 218].

For $k \to 0$, the integrals (5.2) and (5.3) are divergent at small momenta, which rules out the assumption of the presence of both a true condensate and anomalous density. The origin of this infrared divergence is related to long-wave fluctuations of the phase of the condensate wavefunction. So the physics of 2D Bose gas at finite-T can be understood in the context of the density-phase representation. Thus, the single-particle anomalous correlation function is found by using the field operator in the form:

$$\hat{\psi}(r) = e^{i\varphi}\sqrt{\hat{n}} \text{ and } \hat{\psi}^{+}(r) = \sqrt{\hat{n}}e^{-i\phi}. \tag{5.9}$$

Following the hydrodynamic approach described in [235,248,252] with the assumptions $\tilde{m}/n_c << 1$ and $n_c \approx n$ for $T \to 0$. In a such situation the spectrum (4.5) turns to given by

$$\varepsilon_k = \sqrt{E_k\left(E_k + 2\mu_0\right)}. \tag{5.10}$$

Then, substituting Eqs. (5.9) into the GPE (2.10) and separating real and imaginary parts, we get the coupled continuity and Euler hydrodynamic equations for the density and velocity $\hat{V} = (\hbar/m)\nabla\hat{\phi}$.

$$-\hbar\frac{\partial\sqrt{\hat{n}}}{\partial t} = \frac{\hbar^2}{2m}\left(\Delta\hat{\varphi}\sqrt{\hat{n}} + 2\nabla\hat{\varphi}.\nabla\sqrt{\hat{n}}\right), \tag{5.11}$$

$$-\hbar\frac{\partial\hat{\phi}}{\partial t} = \frac{\hbar^2}{2m}\left(\nabla\hat{\phi}\right)^2 - \frac{\hbar^2}{2m}\frac{\Delta\sqrt{\hat{n}}}{\sqrt{\hat{n}}} + V_{ext}(r) + gn. \tag{5.12}$$

For small density fluctuations, Eq.(5.11) shows that fluctuations of the phase gradient are also small. Writing the density operator as $\hat{n} = n + \delta\hat{n}$ and shifting the phase by $-\mu t/\hbar$, we then linearize Eqs.(5.11-5.12) with respect to $\delta\hat{n}$ and $\nabla\hat{\phi}$ around the stationary solution. The zero order terms give the Gross-Pitaevskii equation for the mean density:

$$\mu = -\frac{\hbar^2}{2m}\frac{\Delta\sqrt{\hat{n}}}{\sqrt{\hat{n}}} + V_{ext}(r) + ng, \tag{5.13}$$

and the first order terms provide equations for the density and phase fluctuations:

$$\hbar\frac{\partial}{\partial t}\left(\frac{\delta\hat{n}}{\sqrt{n}}\right)=\left(-\frac{\hbar^2}{2m}\Delta+V_{ext}(r)+ng-\mu\right)\left(2\sqrt{n}\hat{\phi}\right), \tag{5.14}$$

$$-\hbar\frac{\partial}{\partial t}\left(2\sqrt{n}\hat{\phi}\right)=\left(-\frac{\hbar^2}{2m}\Delta+V_{ext}(r)+3ng-\mu\right)\left(\frac{\delta\hat{n}}{\sqrt{n}}\right). \tag{5.15}$$

Solutions of Eqs. (5.14-5.15) for $\delta\hat{n}$ and $\nabla\hat{\phi}$ are obtained in terms of elementary excitations:

$$\delta\hat{n}=\sqrt{n}\sum_{\upsilon}f_{\upsilon}^{-}e^{-i\varepsilon_{\upsilon}t/\hbar}\hat{a}_{\upsilon}+hc\ , \tag{5.16}$$

$$\hat{\phi}=\frac{1}{\sqrt{4n}}\sum_{\upsilon}-if_{\upsilon}^{+}e^{-i\varepsilon_{\upsilon}t/\hbar}\hat{a}_{\upsilon}+hc\ , \tag{5.17}$$

where

$$f_{\upsilon}^{\pm}=u_k\pm v_k=\frac{1}{\Omega}\left(\frac{\varepsilon_k}{E_k}\right)^{\pm1/2}\exp\left(i\vec{k}.\vec{r}\right). \tag{5.18}$$

In the uniform case the chemical potential is $\mu_0=ng_2$, and the excitation spectrum is given by Eq. (5.10). The characteristic excitation energies at which the character of the spectrum transforms from the phonon into the single-particle one are of the order of μ. We, therefore, separate the energy space into two regions: low-energy (phonon) part with $k<\mu$, and high-energy (free-particle) part where $k>\mu$.

The single-particle anomalous correlation function is defined as $\tilde{m}(\boldsymbol{r},\acute{\boldsymbol{r}})=\langle\psi(\boldsymbol{r})\psi(\acute{\boldsymbol{r}})\rangle$. On the basis of Eqs. (5.9), we obtain

$$\tilde{m}(\boldsymbol{r},\acute{\boldsymbol{r}})=n\langle e^{i[\phi(\boldsymbol{r})+\phi(\acute{\boldsymbol{r}})]}\rangle\ . \tag{5.19}$$

Using the Taylor expansion of the exponent one power $\langle e^{x}\rangle=e^{-\frac{1}{2}\langle x^2\rangle}$. Hence the anomalous correlator becomes

$$\tilde{m}(\boldsymbol{r},\acute{\boldsymbol{r}})=ne^{\frac{1}{2}\langle[\phi(\boldsymbol{r})+\phi(\acute{\boldsymbol{r}})]^2\rangle}, \tag{5.20}$$

by means of the definition (5.17) and (5.18), one finds

$$\langle[\phi(\boldsymbol{r})+\phi(\boldsymbol{0})]^2\rangle=\frac{1}{2\Omega n}\sum_k\left\{\frac{\varepsilon_k}{E_k}[1+2N(k)]\left(1+\cos\left(\vec{k}.\vec{r}\right)\right)\right\}. \tag{5.21}$$

After transforming the sum to an integral and introducing $1+2N(k)=\coth(\varepsilon_k/2T)$ and $1+\cos\left(\vec{k}.\vec{r}\right)=\cos^2\left(\frac{\vec{k}.\vec{r}}{2}\right)$. We thus get

$$\langle[\phi(\boldsymbol{r})+\phi(\boldsymbol{0})]^2\rangle=\frac{1}{2n}\int\frac{d^2k}{(2\pi)^2}\left\{\frac{\varepsilon_k}{E_k}\coth(\varepsilon_k/2T)\cos^2\left(\frac{\vec{k}.\vec{r}}{2}\right)\right\}. \tag{5.22}$$

Then, inserting Eq. (5.22) into (5.20), we obtain for the single-particle anomalous correlation function

$$\tilde{m}(\vec{r}) = n\exp\left[-\frac{1}{2n}\int \frac{\varepsilon_k}{E_k}\coth(\varepsilon_k / 2T)\cos^2\left(\frac{\vec{k}.\vec{r}}{2}\right)\frac{d^2k}{(2\pi)^2}\right]; \quad (T << T_d). \tag{5.23}$$

At low temperatures ($T << \mu$) the main contribution to the integral of Eq.(5.23) comes from the region of small momentum then the single-particle anomalous correlation function undergoes a slow law decay at large distances:

$$\tilde{m}(r) = n\left(\frac{\xi}{r}\right)^{T/2T_d}, \tag{5.24}$$

where $T_d = 2\pi\hbar^2 n/m$ is the temperature of quantum degeneracy in 2D.

We can infer from these results that the anomalous average does not exist at finite temperature. This is strictly confirmed by Eq.(5.24) one finds that $\tilde{m}(r)$ vanishes for $r \to \infty$. Similarly to the situation in 2D at finite temperature regarding the normal correlator $\tilde{n}(\vec{r},\vec{r}') = g^{(1)}(\vec{r},\vec{r}') = <\Psi^+(\vec{r})\Psi(\vec{r}')> - \Phi^*(\vec{r})\Phi(\vec{r}')$, which tends to zero as $r \to \infty$, so that there is no true condensate, but one identifies instead the existence of a quasicondensate. However, this result also implies that there is no symmetry breaking, and consequently the anomalous average shouldn't exist at all at finite temperature. So the butter of this result is that the anomalous density accompanies in a manner analogous the true condensate in system of 2D homogeneous Bose gas.

5.4. Superfluid fraction

Usually, Bose-Einstein condensation is accompanied by superfluidity. However, in a two-dimensional system at finite temperature, there is no BEC, but there still exists superfluidity. The relation between them depends on the Bogoliubov-type nature of the spectrum Eq.(4.5) [233]. Also, what is important is that our formalism provides a useful relation between the superfluid fraction and the dissipated heat which is equivalent to that obtained in Refs [233, 208].

$$f_s = \frac{n_s}{n} = 1 - \frac{\hbar^2}{2mnT}\int \frac{d^2k}{(2\pi)^2}k^2 \frac{e^{\varepsilon_k/T}}{\left(e^{\varepsilon_k/T}-1\right)^2} = 1 - \frac{Q_{d=2}}{T}, \tag{5.25}$$

where n_s is the superfluid density.

It is very important to mention that the superfluid fraction f_s will be a divergent quantity and thus the superfluid transition does not occur when the anomalous average is omitted in Eq.(5.25).

At low temperature and weak interaction, we get

$$f_s = 1 - \frac{3\varsigma(3)}{2\pi\hbar^2 mnc_s^4} T^3, \tag{5.26}$$

where $\varsigma(3)$ is a Riemann zeta function and the sound velocity turns out to be given

$$c_s = c_s^{(0)} \sqrt{\left(1 - \frac{\tilde{n}}{n} + \frac{\tilde{m}}{n}\right)}, \tag{5.27}$$

with $c_s^{(0)} = \sqrt{\mu_0 / m}$ is the zero order sound velocity.

Upon neglecting the normal and the anomalous fractions we recover straightforwardly the superfluid fraction obtained earlier by Popov [219] and by Fisher and Hohenberg [233].

5.5. How to measure the anomalous correlation function?

As we have seen previously, the anomalous correlations functions have very unusual behavior in the systems with quasi-long order like zero-temperature one-dimensional and finite temperature two-dimensional systems.

One of the recent techniques describing the measurement of the anomalous correlation function for Bose gas is the so-called the interference experiments proposed by Polkovnikov *et al* [253,254]. It consists to consider two independent identical quasi-condensates allowed to expand in the transverse direction. After sufficient expansion, the atom distribution is measured using the imaging beam where the measuring beam is oriented along the axis of the original cloud. This beam integrates over local interference patterns and the fringes that we see on a detector are a result of averaging over the entire imaging length. In the presence of thermal or quantum fluctuations, interference patterns are not in phase at different points and the resulting interference fringes have a reduced contrast. Such reduction carries information about fluctuations in the original clouds.

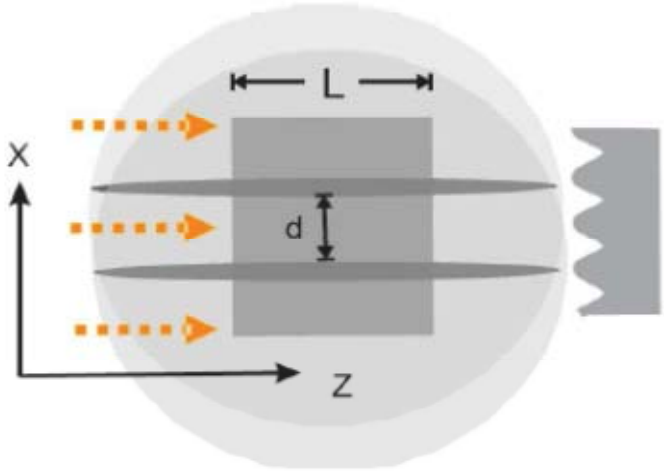


Figure 5.5. Experimental setup [253,254]

The quantum observable corresponding to the interference amplitude of the two condensates [254] is given by

$$\left\langle \left| A_Q \right|^2 \right\rangle = L \int_0^L \langle a(z)a(0) \rangle^2 \quad . \tag{5.28}$$

Thus the average intensity of the interference pattern depends on the two point correlation function along the individual one-dimensional condensates.

Note that this technique can be generalized to the case of different (non-identical) condensates and in any geometry.

Nevertheless, from our point of view, this technique is not able to measure the anomalous density for a single Bose condensate where there are correlations between pairs of atoms of the condensate and the thermal cloud. Until nowadays, as far as we know, there is no experimental technique which allows for a direct measurement of the anomalous density itself. Experimental data about the anomalous density remain a great challenge for the experimentalists.

Conclusions and perspectives

In this part of our thesis, we have analyzed the equilibrium properties of a weakly interacting, trapped three-dimensional Bose gas at finite temperatures.

By using a Gaussian density operator, we derive from the time-dependent variational principle of Balian-Vénéroni a set of coupled equations of motion for a self-interacting trapped Bose gas. These equations govern in a self-consistent way the dynamics of the condensate, the thermal cloud and the anomalous average. Our time dependent Hartree-Fock-Bogoliubov (TDHFB) equations generalize in a natural way many of the famous approximations found in the literature such as the Bogoliubov, the Gross-Pitaevskii, the HFB, the ZNG equations and others.

In order to apprehend better the advantages of our approach, we solve numerically the static TDHFB equations in the local limit for a contact potential and a harmonic trap. The outcomes of our numerical explorations are the following. First of all, the numerical resolution of our equations is relatively easy and is not as time-consuming as the HFB-BdG calculations especially for large atom numbers. For instance, the latter cannot be handled correctly as soon as $N \sim 10^4 - 10^5$. By contrast, there are no such limitations in our case. Secondly, although we obtain for the condensate density a quite good agreement with the literature and with the experiments, our predicted thermal cloud and anomalous average differ substantially from the HFB-BdG results especially near the center of the trap. Indeed, we obtain Gaussian shapes for both densities while the HFB-BdG calculations predict ''holes'' (that is local minima) near the center. These holes are absent (at least concerning $\tilde{n}$) in the experiments of Gerbier *et al*. and Caracanhas *et al*. We recall that the HFB-BdG numerical calculations have been performed for a reduced atom number $(N \sim 2000)$. The question that naturally arises is whether these holes may disappear for large atom numbers. In fact, a preliminary HFB-BdG calculation seems to confirm this conclusion.

On the other hand, owing to its importance to account for many-body effects, we have analyzed the behavior of the anomalous density. We recover a well-known prediction of HFB-BdG since $\tilde{m}$ increases with the temperature and then decreases as one approaches the transition. Moreover, we show that at low temperatures, the anomalous density is greater than the non condensate density, although both are very small.

The comparison between the noncondensed and anomalous densities at different temperatures is analyzed for homogeneous Bose gas. This analysis shows the significance of the anomalous density compared to the noncondensed density at low temperature.

In the trapped case, we recover the well-known theoretical prediction of HFB-BdG since $\tilde{m}$ increases with the temperature and then decreases as one approaches the transition. Furthermore, we found that the dip of the anomalous density is destroyed for sufficiently weak interactions. Moreover, we show that at low temperatures, the anomalous fraction is larger than the non condensate one. The former necessarily plays a major role in the Bose-Einstein condensation phenomenon. Any approach neglecting the anomalous fraction at low temperatures will inevitably lead to inconsistencies.

We have studied also the finite temperature behavior of a single vortex in a partially condensed ultra-cold Bose gas by means of the TDHFB formalism, in which the condensate is modeled by a generalized Gross-Pitaevskii equation. Our numerical calculations provide a new image for the vortex shape at finite temperature. Therefore, we have found that the thermal gas forms a local minimum in the center of trap and appears as a tornado surrounds the condensate which leads to a coreless vortex (empty core) in disagreement with predictions of ref [198] where the thermal gas is concentrated in the vortex core, where it fills the space left by the condensate and exerts an outward pressure on it. Otherwise, we showed that the core size becomes larger when the vortex line reaches the boarder of the condensate, where the condensed density decreases.

We have used again our TDHFB formalism to investigate the finite-temperature physics of a Bose-Einstein condensate confined to a two-dimensional geometry. This formalism has been proven successful in the three-dimensional case. However, in the lower dimensional system phase fluctuations must be taken into consideration at comparatively lower temperatures. In a regime below the critical temperature they destroy the global coherence of the condensate and the superfluid state is best described as a quasicondensate. In our formalism phase fluctuations are included via the contribution to the non-condensate density from low-energy quasiparticles. We showed that the formalism is not only applicable in the two-dimensional case, but also that the quantities obtained, such as the single-particle anomalous correlation function (the off-diagonal density matrix), allow for a quantitative analysis even in the phase fluctuating regime.

We have studied, in particular, the behavior of the anomalous density in two-dimensional homogeneous Bose gases. We find that this quantity has a finite value in the limit of weak interactions. We have discussed also the effects of the anomalous average on some

thermodynamic quantities. As an example, we have given formulas for the chemical potential, ground-state energy, the depletion and superfluid fraction. The later does not occur if the anomalous density is neglected. In the ultra-dilute limit, the known results are reproduced. This feature makes our predictions in accordance with Monte-Carlo simulations and analytical calculations. Also, we have shown that our approach satisfies the HP theorem at zero temperature while it does not verify the Nepomnyashchy identity as it should be for any limited approximation. Moreover, the importance of the anomalous density compared to the normal one at low temperature has been also highlighted. In addition, by using the density phase fluctuation we found that the single-particle anomalous correlation function undergoes a slow law decay at large distances such a result implies that the anomalous average does not exist at finite temperature. Finally, an interesting question to ask is whether some quantity can exist in this system which accompanies the quasicondensate density in a manner analogous to that in which the anomalous density accompanies a true condensate?

As for any variational approach, one has to discuss the relevance of the trial space for the problem at hand and how to extend it in order to take into account many important effects which we did not deal with in this paper. Among the most important phenomena, we can cite in particular the effect of the inclusion of the triplets, the damping of the excitations (Landau and Beliaev) and the particle exchange. While the former may be easily handled by the ''post-Gaussian'' approximation, the two latter require dissipative effects which are totally absent in the present formalism since the von-Neumann entropy is conserved.

The dynamics of the anomalous density will be the goal of our next work with the aim to understand how this quantity evolves in time when the trap is switched off suddenly. Furthermore, to examine more carefully our TDHFB formalism, we will focus in the future on the behavior of the anomalous density in dipolar Bose-Einstein condensates at finite temperature both in the static and the dynamic cases.

Appendices

Appendix A

Density of state of the *d*-dimensional harmonic oscillator

The density of state of the D-dimensional harmonic oscillator can be calculated from the integral

$$g_d(E) = \frac{1}{(2\pi\hbar)^d} \int d^d r \int d^d p \, \delta\left[E - \left(p^2/2m + V_{ext}(r)\right)\right]. \tag{A1}$$

Both the momentum and the spatial integral are transformed due to their rotational symmetry as

$$\int_{-\infty}^{+\infty} d^d x = S^d \int_0^{\infty} dx \, x^{d-1} \, . \tag{A2}$$

So, we get after substituting $E_p = p^2/2m$

$$g_d(E) = 2\left(\frac{m}{2\hbar^2}\right)^{d/2} \frac{1}{\Gamma(d/2)^2} \int_0^{\infty} dr r^{d-1} \int_0^{\infty} dE E^{\frac{d}{2}-1} \delta\left(E - E_p - V_{ext}(r)\right). \tag{A3}$$

The evaluation of the energy integral yields

$$g_d(E) = 2\left(\frac{m}{2\hbar^2}\right)^{d/2} \frac{1}{\Gamma(d/2)^2} \int_0^{\infty} dr r^{d-1} \left(E - V_{ext}(r)\right)^{\frac{d}{2}-1} \Theta\left(E - V_{ext}(r)\right), \tag{A4}$$

where the Heaviside function arises from the integration over the delta distribution. We now insert the isotropic trapping potential $V_{ext}(r) = m\omega^2 r^2/2$ and substitute $x = r^2$, so that we get

$$g_d(E) = 2\left(\frac{m}{2\hbar^2}\right)^{d/2} \frac{E^{\frac{d}{2}-1}}{\Gamma(d/2)^2} \int_0^{\infty} dx x^{\frac{d}{2}-1} \left(1 - \frac{m\omega^2}{2E} x\right)^{\frac{d}{2}-1} \Theta\left(1 - \frac{m\omega^2}{2E} x\right). \tag{A5}$$

Evaluation the Heaviside function we obtain

$$g_d(E) = \frac{E^{\frac{d}{2}-1}}{(\hbar\omega)^D \Gamma(d/2)^2} \int_0^1 dx x^{\frac{d}{2}-1} (1-x)^{\frac{d}{2}-1}, \tag{A6}$$

with the definition of beta function,

$$B(x,y)=\int_0^1 dtt^{x-1}(1-t)^{y-1}=\frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}. \tag{A7}$$

Finally we get the density of state for isotropic harmonic oscillator in *d*-dimensions

$$g_d(E)=\frac{E^{d-1}}{(\hbar\omega)^d\Gamma(d)}. \tag{A8}$$

Appendix B

TDHFB equations in the functional Schrödinger representation

We derive in this appendix the general expressions for the TDHFB equation in the functional Schrödinger representation where the density operator is viewed as describing a multidimensional Gaussian wave packet. The boson creation and destruction operators are introduced by means of the following transformations

$$\psi(x) = \frac{1}{\sqrt{2}}\big(\varphi(x) + i\pi(x)\big) \text{ and } \psi(x)^{+} = \frac{1}{\sqrt{2}}\big(\varphi(x) - i\pi(x)\big), \tag{B1}$$

where $\varphi(x)$is field operator and $\pi(x)$ is the canonical field momentum.

The vector αtakes the form

$$\propto (x,t) = \begin{pmatrix} \varphi(x,t) \\ -i\pi(x,t) \end{pmatrix}, \tag{B2}$$

which leads to the classical structure of the two first equations of the TDHFB system

$$\frac{d\varphi(x)}{dt} = \frac{\partial E}{\partial \pi(y)}, \ \frac{d\pi(x)}{dt} = -\frac{\partial E}{\partial \varphi(y)}. \tag{B3}$$

Note that the set (B3) is not closed since it depends on the evolution of the matrixρ, which we recall contains the normal and anomalous correlation functions.

$$\Xi(x,y,t) = \begin{pmatrix} 2G(x,y,t) & -iT(x,y,t) \\ -iT(y,x,t) & -S(x,y,t) \end{pmatrix}, \tag{B4}$$

where

$$\varphi(x,t) = \frac{Tr\big(\mathcal{D}(t)\bar{\Phi}(\mathrm{x})\big)}{Tr\mathcal{D}(t)}, \tag{B5.a}$$

$$\pi(x,t) = \frac{Tr\big(\mathcal{D}(t)\bar{\Pi}(\mathrm{x})\big)}{Tr\mathcal{D}(t)}, \tag{B5.b}$$

$$G(x,y,t) = \frac{Tr\left(\mathcal{D}(t)\bar{\Phi}(\mathrm{x})\bar{\Phi}(\mathrm{y})\right)}{Tr\mathcal{D}(t)}, \tag{B5.c}$$

$$S(x,y,t) = \frac{Tr\left(\mathcal{D}(t)\bar{\Pi}(\mathrm{x})\bar{\Pi}(\mathrm{y})\right)}{Tr\mathcal{D}(t)}, \tag{B5.d}$$

$$T(x,y,t) = \frac{Tr\left(\mathcal{D}(t)\left(\bar{\Phi}(\mathrm{x})\bar{\Pi}(\mathrm{y})+\bar{\Pi}(\mathrm{y})\bar{\Phi}(\mathrm{x})\right)\right)}{Tr\mathcal{D}(t)}, \tag{B5.e}$$

and for any operator$O$: $\bar{O} = O - Tr(\mathcal{D}(t)\mathrm{O})$ i.e. $\bar{\Phi} = \Phi - \varphi$ and $\bar{\Pi} = \Pi - \pi$. The hermiticity of $\mathcal{D}(t)$ implies that the matrices $G, S$and $T$are real and that G and $S$are symmetric in the space indices.

The Heisenberg invariant is equal to

$$I(x,y) = \int d^3z[\langle\bar{\Phi}(\mathrm{x})\bar{\Phi}(\mathrm{z})\rangle\langle\bar{\Pi}\mathrm{z}\bar{\Pi}(\mathrm{y})\rangle - \langle\bar{\Phi}(\mathrm{x})\bar{\Pi}(\mathrm{z}) + \bar{\Pi}(\mathrm{z})\bar{\Phi}(\mathrm{x})\rangle\langle\bar{\Phi}(\mathrm{z})\bar{\Pi}(\mathrm{y}) + \bar{\Pi}(\mathrm{y})\bar{\Phi}(\mathrm{z})\rangle] \tag{B6}$$

For the pure state

$$I(x,y) = \delta^3(x-y)\ . \tag{B7}$$

For completeness, let us close the set (B3) by writing the TDHFB evolution of the matrices (B5). Using the equation (3.9.c), one obtains

$$\frac{dG(x,y,t)}{dt} = 2\left(2\frac{\partial E}{\partial T}G + T\frac{\partial E}{\partial S}\right)(x,y), \tag{B8.a}$$

$$\frac{dS(x,y,t)}{dt} = -2\left(2S\frac{\partial E}{\partial T} + \frac{\partial E}{\partial G}T\right)(x,y)\ , \tag{B8.b}$$

$$\frac{dT(x,y,t)}{dt} = -2\left[T, \frac{\partial E}{\partial T}\right](x,y) - 4\left(G\frac{\partial E}{\partial G} - \frac{\partial E}{\partial S}S\right)(x,y). \tag{B8.c}$$

Equations (B3) and (B8) constitute the TDHFB equations in the functional form.

Appendix C

Dimensional regularization

1. Dimensional regularization in three dimensions

Dimensional regularization can be used to regularize both the ultraviolet and infrared divergences in three-dimensional integrals over momenta. The spatial dimension is generalized to $d = 3 - 2\epsilon$ dimensions. The continuum limit is taken by replacing sums over wave vectors by integrals in $d = 3 - 2\epsilon$ dimensions: $1/V \sum_p \longrightarrow \mathrm{M}^{2\epsilon} \int \frac{d^d p}{(2\pi)^d}$.

Here, M is a renormalization scale that ensures that the integral has the canonical dimension also ford $\neq 3$. In the following, we absorb the factor$\mathrm{M}^{2\epsilon}$ in the measure and so it will not appear explicitly. Integrals are evaluated at a value of d, for which they converge and then analytically continued to $\mathrm{d} = 3$.

The integral $I_{m,n}$ is defined by

$$I_{m,n}(\Lambda) = \mathrm{M}^{2\epsilon} \int \frac{d^d p}{(2\pi)^d} \frac{p^{2m}}{p^n \left(p^2+\Lambda^2\right)^{2/n}}. \tag{C1}$$

With dimensional regularization, $I_{m,n}$ is given by the formula

$$I_{m,n}(\Lambda) = \frac{\Omega_\mathrm{d}}{(2\pi)^d} \mathrm{M}^{2\epsilon} \Lambda^{\mathrm{d}+2\mathrm{m}-2\mathrm{n}} \times \frac{\Gamma\left(\frac{\mathrm{d}-\mathrm{n}}{2}+\mathrm{m}\right)\Gamma\left(\mathrm{n}-\mathrm{m}+\frac{\mathrm{d}}{2}\right)}{2\Gamma\left(\frac{\mathrm{n}}{2}\right)}, \tag{C2}$$

where $\Omega_\mathrm{d} = 2\pi^{\mathrm{d}/2}/\Gamma\left(\frac{\mathrm{d}}{2}\right)$ is the area of a d-dimensional sphere.

The integrals$I_{m,n}$ satisfy the relations

$$\frac{d}{d\Lambda^2} I_{m,n} = -\frac{\mathrm{n}}{2} I_{m+1,n+2} \tag{C3.a}$$

$$(d + 2m - n) I_{m,n} = n I_{m+2,n+2}, \tag{C3.b}$$

$$\Lambda^2 I_{m,n} = I_{m-1,,n-2} - I_{m+1,,n}. \tag{C3.c}$$

The first relation follows directly from the definition of $I_{m,n}$. The second relation follows from integration by parts, while the last is simply an algebraic relation.

The specific integrals we need in the calculations are listed below. In the limit $d \longrightarrow 3$ they become

$$I_{0,-1} = \frac{\Lambda^5}{15\pi^2}, I_{1,1} = \frac{\Lambda^3}{3\pi^2}, I_{-1,-1} = -\frac{\Lambda^3}{6\pi^2}, I_{4,5} = -\frac{4\Lambda}{3\pi^2}, I_{2,3} = -\frac{\Lambda}{\pi^2}, I_{0,1} = -\frac{\Lambda}{2\pi^2}, \tag{C4}$$

$$I_{-2,-1} = -\frac{\Lambda}{4\pi^2}\left[\frac{1}{\epsilon} + 4 - L - \gamma + log(\pi)\right], \tag{C5}$$

$$I_{-1,-1} = -\frac{1}{4\Lambda\pi^2}\left[\frac{1}{\epsilon} + 2 - L - \gamma + log(\pi)\right], \tag{C6}$$

where $L = log\left(\Lambda^2/\mathrm{M}^2\right)$. The integrals $I_{-1,-1}$ and $I_{-2,-1}$ are both logarithmically divergent in the infrared and this shows up as a pole in ϵ.

2. Dimensional regularization in two dimensions

Some of the one-loop momentum integrals are infrared divergent or ultraviolet divergent or both. They can be written in terms of the integral$I_{m,n}$, which is defined by

$$I_{m,n}(\Lambda) = \left(\frac{\mathrm{e}^{\gamma}\mathrm{M}^2}{4\pi}\right)^{\epsilon} \int \frac{d^d p}{(2\pi)^d} \frac{p^{2m}}{p^n\left(p^2+\Lambda^2\right)^{2/n}}. \tag{C7}$$

Here, M is a renormalization scale that ensures that $I_{m,n}$ has the canonical dimension also for $d \neq 2$. $\gamma \approx 0.5772$ is the Euler-Mascheroni constant. With dimensional regularization, $I_{m,n}$is given by the formula

$$I_{m,n}(\Lambda) = \frac{\Omega_{\mathrm{d}}}{(2\pi)^d}\left(\frac{\mathrm{e}^{\gamma}\mathrm{M}^2}{4\pi}\right)^{\epsilon} \Lambda^{\mathrm{d+2m-2n}} \times \frac{\Gamma\left(\frac{\mathrm{d-n}}{2}+\mathrm{m}\right)\Gamma\left(\mathrm{n-m}+\frac{\mathrm{d}}{2}\right)}{2\Gamma\left(\frac{\mathrm{n}}{2}\right)}. \tag{C8}$$

In two dimensions, these integrals have logarithmic and power ultraviolet divergences. The power divergences are set to zero in dimensional regularization, while the logarithmic divergences appear as poles inϵ. The specific integrals are

$$J_{0,-1} = -\frac{\Lambda^4}{32\pi}\left[\frac{1}{\epsilon} - L - \frac{1}{2} + \frac{1}{2}\left[L^2 + L - \frac{5}{2} + \frac{\pi^2}{2}\right]\epsilon + \mathcal{O}(\epsilon^2)\right], \tag{C9}$$

$$J_{-1,-1} = \frac{\Lambda^2}{8\pi}\left[\frac{1}{\epsilon} - L + 1 + \frac{1}{2}\left[(L-1)^2 + 1 + \frac{\pi^2}{2}\right]\epsilon + \mathcal{O}(\epsilon^2)\right], \tag{C10}$$

$$J_{1,1} = -\frac{\Lambda^2}{8\pi}\left[\frac{1}{\epsilon} - L - 1 + \frac{1}{2}\left[(L+1)^2 - 4 + \frac{\pi^2}{2}\right]\epsilon + \mathcal{O}(\epsilon^2)\right], \tag{C11}$$

$$J_{0,1} = \frac{1}{4\pi}\left[\frac{1}{\epsilon} - L + \frac{1}{2}\left[L^2 + \frac{\pi^2}{2}\right]\epsilon + \mathcal{O}(\epsilon^2)\right], \tag{C12}$$

where $L = \log\left(\Lambda^2/4M^2\right)$ and $\Lambda = 2/\xi$.

Part II. Effects Of The Rotonization In Two Dimensional Dipolar Bose Gas

General introduction

1. Topic of the second part

In the last decade, ultracold gases of dipolar particles, which include atoms with a large magnetic moment and polar molecules, attracted a great deal of interest (see for review [255, 258]). Being electrically or magnetically polarized such particles interact with each other via long-range anistropic dipole-dipole forces, which drastically changes the nature of quantum degenerate regimes. Experiments with chromium atoms (magnetic moment $6\mu_B$) [256, 259], together with theoretical studies [260,261], have revealed the dependence of the shape and stability diagram of trapped dipolar Bose-Einstein condensates on the trapping geometry and interaction strength. They initiated spinor physics with quantum dipoles [262, 263], and now also dysprosium [264] and erbium [265] atoms (magnetic moment $10\mu_B$ and $7\mu_B$ respectively) have entered the game. Recently, fascinating prospect for the observation of novel quantum phases have been opened by the creation of ultracold clouds of polar molecules and cooling them to almost quantum degeneracy [257-266]. In this case, the dipole-dipole forces can be orders of magnitude larger, and one has a possibility to manipulate the molecules making use of their rotational degrees of freedom.

Recent experimental efforts are directed towards creating ultracold dipolar gases of heteronuclear molecules with large dipolar moments, where the dipolar effects should be more pronounced. The relative strength of the dipolar interaction for such a system is calculated by taking the ratio between the "dipolar length" and the s-wave scattering length [256]. For many polar molecules this ratio is 2 orders of magnitude larger than in the case of chromium atoms. The main problem encountered in the case of heteronuclear molecules lies in cooling them to low enough temperatures for dipolar effects to become noticeable. It was found that the best way to proceed is to create polar molecules from ultracold atoms through a process of photoassociation [267]. The molecules must then be brought to their lowest rovibrational state such that effects like dipolar relaxation are minimized [256]. A series of successes in recent years were reported in creating ultracold dipolar molecules, but to this moment the goal of achieving quantum degeneracy was not reached. For example, bosonic ultracold molecules were created in experiments with $^{85}Rb^{133}Cs$ [267] or $^{7}Li^{133}Cs$ [268]. Most recent breakthrough was registered in

creating fermionic polar molecules near quantum degeneracy; a long-lived ultracold gas of rubidium-potassium $^{40}K^{87}Rb$ with dipolar moment on the order of one Debye (1D=3.33564×10^{-30} cm) was reported in [269]. On the other hand, there has already been noticeable theoretical study of ultracold dipolar gases in the Fermi liquid state. Density distribution and stability of dipolar Fermi gases were investigated in [270]. Dipolar effects were predicted to give deformations of the Fermi sphere [271, 272]. Going to lower temperatures, pairing and formation of BCS superfluid phase was predicted and studied for ultracold dipolar gases [273]. One of the most exciting perspective open in these studies is the possible creation of fractional Quantum Hall States [274] and Wigner crystals [275].

The 2D system of fermionic polar molecules attracts also a great deal of interest, in particular when they are in the same internal state. Various aspects have been discussed regarding this system in literature, in particular the emergence and beyond mean field description of the topological $p_x + ip_y$ phase for microwave-dressed polar molecules [276, 277], interlayer superfluids in bilayer and multilayer systems [278-281], the emergence of density-wave phases for tilted dipoles [282-285]. The case of superfluid pairing for tilted dipoles in the quasi2D geometry beyond the simple BCS approach has been discussed in Ref. [282]. The Fermi liquid behavior of this system has been addressed by using the Fourier transform of the dipole-dipole interaction potential [282, 286-289] and the many-body theory (beyond mean field) has been constructed in [290].

Moreover, the partially attractive and partially repulsive nature of the dipolar interaction together with its long range character makes the question of stability for strong dipolar interactions more intricate [255-258]. Indeed, a homogeneous dipolar condensate is unstable when the dipolar interaction is stronger than the s-wave scattering interaction [255-258]. Furthermore, the dipolar interaction's anisotropy means that it can be attractive and thus making the BEC susceptible to collapse. The collapse is followed by an explosion of the condensate (Bose-nova). This effect was investigated theoretically and experimentally in chromium BEC and the expanding remnants of the condensate were revealed to share the same d-wave symmetry of the dipolar interaction [291]. Trapping bosonic gases on optical lattices promises to open new ways in studying quantum phase transitions: from superfluid to crystal [292], superfluid to Mott insulator [256]; also rich physics is expected when the lattice geometry is modified, when low-

dimensional systems are simulated by tuning the trapping frequencies, when gas mixtures are considered etc. [256].

2. Outline

Chapter 1 of this part reviews the theoretical and experimental properties of bosonic gases interacting via the long-range, anisotropic dipole-dipole interaction, in addition to the short-range and isotropic contact interaction usually considered in ultracold gases. The characteristic features emerging from the dipolar interaction are emphasized. We present in particular the basic techniques involving the study of the dipolar Bose-Einstein condensed gases in a general and concise form. Starting from the definition of the dipole-dipole interaction and its importance in BEC following the Bogoliubov energy spectrum, we investigate both the Gross-Pitaevskii mean-field theory from which we develop the corresponding hydrodynamic equations for dipolar Bose gas.

In chapter 2, we discuss fluctuations in a dilute two-dimensional Bose-condensed dipolar gas, which has a roton-maxon character of the excitation spectrum. We calculate the density-density correlation function, fluctuation corrections to the chemical potential, compressibility, and the normal (superfluid) fraction. It is shown that the presence of the roton strongly enhances fluctuations of the density, and we establish the validity criterion of the Bogoliubov approach. At zero temperature the condensate depletion becomes significant if the roton minimum is sufficiently close to zero. At finite temperatures in the dilute regime where $nr_*^2 \ll 1$, with $r_* = md^2/\hbar^2$ being the characteristic dipole-dipole distance, exceeding the roton energy and the interaction between particles, the effect of thermal fluctuations is stronger and it may lead to a large normal fraction of the gas which may significantly reduce the superfluid fraction even at temperatures well below the Kosterlitz-Thouless transition temperature.

Chapter 1

Overview on Dipolar Gases

1.1.Dipole-Dipole interaction:

Usually the dominant interatomic interactions separated by a distance **r** in an ordinary atomic Bose-Einstein condensate are asymptotically of the van der Waals type, which is short-range in comparison to the de Broglie wavelength of the atoms and isotropic [256-257,293]. However, in the case of dipolar gas, another type of interactions, namely the dipole-dipole interaction between particles plays an important role in the condensate, which is anisotropic (the strength and sign of the interaction depend on the angle θ between the polarization direction and the relative position of the particles) and long range (it decays like $1/r^3$ where r is the separation between the two dipoles).

Atoms or molecules having a permanent dipole moment (either magnetic or electric) interact not only via short range potentials, but also via the dipole-dipole interaction. The energy due to the DDI for two particles 1 and 2 reads [255]:

$$U_{dd}(r) = \frac{C_{dd}}{4\pi}\frac{(\vec{e}_1.\vec{e}_2)r^2-3(\vec{e}_1.\vec{r})(\vec{e}_2.\vec{r})}{r^5} \quad , \tag{1.1}$$

where $C_{dd} = \mu_0\mu^2$ is the coupling constant for particles having a permanent magnetic dipole moment μ (μ_0 is the permeability of vacuum), and d^2/ε_0 for the particles having a permanent electric dipole moment d (ε_0 is the permittivity of vacuum). For a polarized sample where all dipoles point in the same direction z, $\vec{e}_1$ and $\vec{e}_2$ are the unit vectors (see Fig. 2). We get the well kwon expression:

$$U_{dd}(r) = \frac{C_{dd}}{4\pi}\frac{1-3cos^2\theta}{r^3}. \tag{1.2}$$

where θ being the angle between the direction of polarization and the relative position of the particles.

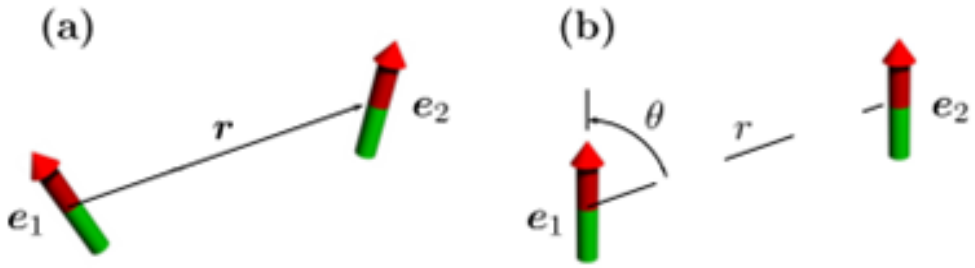


Figure 1.1. Two atoms interacting via dipole-dipole interaction, (a) non polarized case; (b) polarized case.

In practice one always has a competition between contact and dipolar interactions; it is therefore useful to define the following (dimensionless) ratio of the dipolar length to the s-wave scattering length:

$$\epsilon_{dd} = \frac{C_{dd}}{3g} = \frac{4\pi d^2}{3g} = \frac{1}{3}\frac{a_{dd}}{a} , \tag{1.3}$$

it compares the relative strength of the dipolar and contact interactions, which determines the physical properties of the system. For usual atomic magnetic moments μ (e.g. for the alkalis), ϵ_{dd} is very small (typically a few 10^{-3}, for example, for ^{87}Rb, one has dipole-dipole interaction among them is a factor of 36 smaller than in a chromium BEC. The corresponding strength parameters are $\epsilon_{dd} = 0.0064$ for ^{87}Rb and $\epsilon_{dd} = 0.0035$ for ^{23}Na) making the dipolar effects negligible [293]. A strong dipolar system (purely dipolar gas) can be created employing the so called Feshbach resonance.

Species	Dipole moment	a_{dd}	ε_{dd}
^{87}Rb	$1.0\,\mu_B$	$0.7\,a_0$	0.007
^{52}Cr	$6.0\,\mu_B$	$16\,a_0$	0.16
KRb	0.6 D	$2.0 \times 10^3 a_0$	20
ND_3	1.5 D	$3.6 \times 10^3\,a_0$	36
HCN	3.0 D	$2.4 \times 10^4\,a_0$	240

Table 1.1. Dipolar constants for various atomic and molecular species, for the molecular species (the yet unknown) scattering length is assumed to be $100a_0$ (as the c_6 coefficient of the dimer is comparable to the one of a single atom, the order of magnitude of the scattering length is similar, but obviously the actual value highly depends on the details of the potential

1.2. Why Dipolar gases are interesting?

Gaseous Bose-Einstein condensates with DDI have become a fast growing field of theoretical and experimental interest due to their nature; for most of the systems studies so far, one assumes the dipole moment to be polarized, i.e. oriented in the same direction via applying either magnetic or electric fields, the dipole-dipole interaction potential $U_{dd}(\mathbf{r})$ has two important properties: it is anisotropic, and is of long range character, these properties have important consequences.

1.2.1. Anisotropy:

The dipole-dipole interaction has the angular symmetry of the Legendre polynomial of second order $P_2(\cos\theta)$, as θ varied between 0 and $\frac{\pi}{2}$, the factor $1-3cos^2\theta$ varies between (-2) and (1). The interaction is anisotropic and partially attractive. In particular, if the two dipoles are aligned "head-to-tail" ($\theta = 0$), they attract themselves, and the interactions will be attractive. Therefore, the condensate becomes unstable similar to the ordinary case of attractive short-range interaction (negative s-wave scattering length), which leads to mainly attractive gas that should therefore exhibit collapse (see figure 3(b)). While the dipole-dipole interaction is repulsive when the dipoles placed side-to-side (parallel), then they repel each other in the case of horizontal pancake traps [255] ($\theta = \pi/2$), this case leads to a mainly repulsive gas and should allow at least partially stabilize the system (see Figure3 (a)). For the special value $\theta = \arccos(1/\sqrt{3}) \approx 54.7°$ which often called "magic angle'', the DDI vanishes [255-257]. Since the potential of dipoles placed at different positions is proportional to the spherical harmonic $Y_2^0(\theta,\varphi)$, one says that the interaction exhibits *d*-wave symmetry (angular momentum $l = 2$).

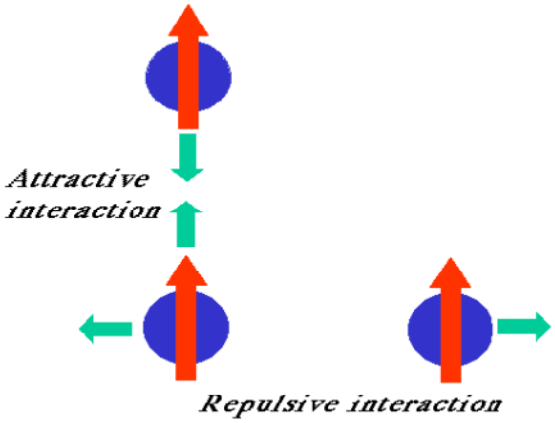


Figure 1. 2. The anisotropy of dipole-dipole interaction

By means of an appropriate rotating magnetic field, the anisotropy may be employed to tune the dipolar interactions [256], introducing a second control mechanism in addition to the tuning of the isotropic interactions by means of Feshbach resonances [256]. Additionally, the anisotropy of the magnetic dipolar interaction was shown to lead to a measurable anisotropic deformation of the expanding chromium BEC [256] (see Fig.1.3). The dipolar anisotropy should also cause sound to propagate with different speed in different directions providing an interesting tool to investigate dissipation mechanisms, e.g. the Landau criterion for superfluidity.

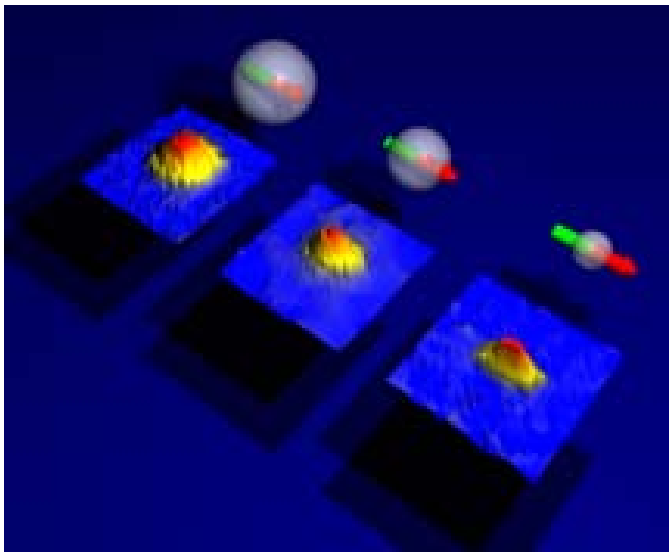


Figure 1.3. Effects of the dipolar interactions between the magnetic moments of the atoms. This manifests itself in an elongation of the condensate along the magnetization direction, yielding a clear change in the condensate ellipticity (from Pfau group, university of Stuttgart [256]).

1.2.2. Long range:

The long-range nature of dipolar interaction is manifest when one calculates the potential energy U_{dd} of a particle in a dipolar system

$$\int_{r_0}^{\infty} U_{dd} d^d r, \tag{1.4}$$

where d is the dimensionality of the system and r_0 some short-distance cutoff converges at large distances. For interaction decaying at large distances as $1/r^n$, this implies that one needs to have $d < n$ in order to consider the interaction to be short range. Therefore, the dipole-dipole interaction $n = 3$ is long-range in three dimensions, and short range in one and two dimensions.

1.3.Creation of Chromium BEC

In this section, we briefly review the main steps of the experimental realization of the BEC with dipole-dipole interaction in degenerate quantum gases.

We first address the various electronic and magnetic properties of chromium atoms (see Table 1.2). Due to the special characteristics of Cr atoms, standard methods cannot be applied to generate a Cr-BEC. Therefore, the path which leads to the generation of a chromium BEC is long and required a lot of experimental and theoretical work on all aspects of cooling and trapping.

Isotope	^{50}Cr	^{52}Cr	^{53}Cr	^{54}Cr
Abundance	4.35%	83.79%	9.50%	2.37%
Nuclear spin	I=0	I=0	I=3/2	I=0
Statistic	boson	boson	fermion	boson

Table 1.2. The properties of the four naturally occurring isotopes of chromium For the bosonic isotopes which have no nuclear spin, this means that it hasn't hyperfine structure, which gives rise to total electronic spin quantum number of 3 (S=3) in their ground state $^7S_3$.

Owing to its high magnetic moment in the ground state, chromium is a good candidate for the study of dipolar interactions in a degenerate gas [256]. The successful operation of a chromium magneto-optical trap (MOT) and repumping on the inter-combination lines as well as the development of a continuous loading scheme of chromium atoms into a magnetic trap are important steps towards the production of a Cr-BEC.

First, chromium can be laser cooled using the $^7S_3 \leftrightarrow {}^7P_4$ transition at 425.6 nm. However, strong excited state collisions limit the density in a MOT to relatively low values [256]. Therefore, in a typical MOT configuration, the steady state atom number in a Cr MOT is limited to a few 10^6. In addition the cooling transition is not closed, as there is a decay channel from the $^7P_4$ state to the metastable state $^5D_4$ (via an inter-combination transition). These facts seem to rule out any hope to achieve Bose condensation of Chromium by standard methods. However, the atoms in the metastable state have a magnetic dipole moment of 6 μ_B which is strong enough so that they remain magnetically trapped in the inhomogeneous magnetic field configuration of the MOT. One can thus accumulate large atom numbers in the metastable state $^5D_4$ (where they are decoupled from the MOT light and thus do not suffer from excited state collisions), and then, at the end of the MOT phase, repump them using light at 663.2 nm. In this way, one ends up with more than 10^8 ground state atoms magnetically trapped. The magnetic field configuration of the MOT should be modified to the one of a Ioffe-Pritchard trap, allowing a continuous loading of a magnetic trap, in which evaporative cooling could be performed.

However, when the density in the magnetic trap becomes too high, one cannot gain anymore in phase-space density due to increasing *dipolar relaxation*. This two-body loss mechanism, in which the spin of one of the colliding atoms is flipped (this is allowed as the dipole-dipole interaction does not conserve the spin, but only the total angular momentum), is especially important for Chromium, compared to the case of alkalis, as its cross section scales as the cube of the magnetic dipole moment.

The way to circumvent dipolar relaxation is to optically pump the atoms into the absolute ground state $m_S = -3$ (via the $^7S_3 \leftrightarrow {}^7P_3$ transition at 427.6 nm) and hold them in an optical dipole trap. Then, in the presence of a magnetic field such that the Zeeman splitting between adjacent spin states is much higher than the thermal energy, dipolar relaxation is energetically forbidden. One can then perform evaporative cooling in the dipole trap and obtain a Chromium condensate [256]. Recently, an alternative method has been used to obtain ^{52}Cr condensates, using direct loading of the optical dipole trap [294].

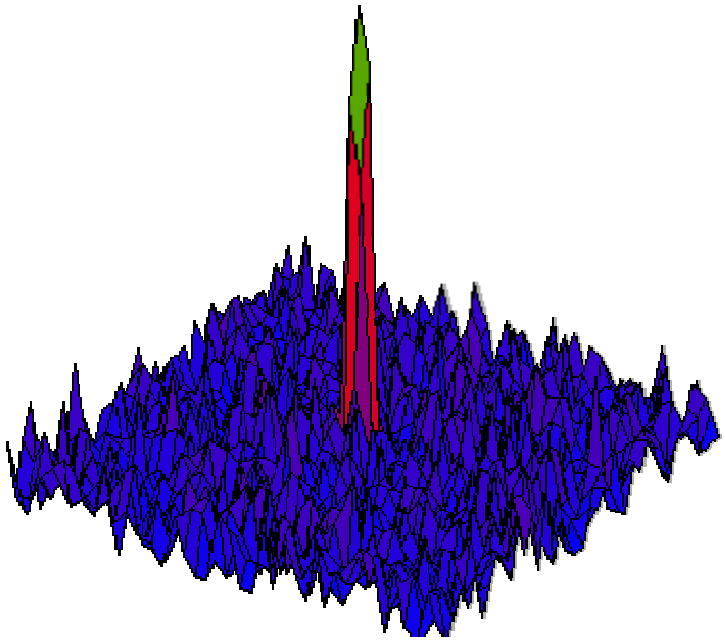


Figure 1.4. Observation of Cr-BEC from LPL group, Paris13 University [266].

1.4.Scattering properties

The long range anisotropic character of the DDI leads to peculiar low-energy scattering properties: not only the s-wave, but all partial waves contribute to the scattering, in contrast with the case of short-range interaction, where only the s-wave scattering only plays a role. Here we should recall the general theory of low-energy scattering for a central potential failing off at large distance as $1/r^n$, the elastic scattering phase shifts $\delta_l(k)$ [295]

$$\tan \delta_l(k) = \mathrm{A}k^{2l+1} + Bk^{n-2}. \qquad (1.5)$$

The elastic cross-section is proportional to $\sin \delta_l / k^2$.

The phase shifts of (1.5) can be scaled for $k \to 0$, as k^{2l+1} if $l < (n-3)/2$, and k^{n-2} otherwise [295]. For a van der Waals potential ($n = 6$), only $l = 0$ (s-wave) contribute at low energy. In the ultracold regime, the scattering is thus fully characterized by the scattering length a. In the study of quantum gases, the true interaction potential between the atoms can

then be replaced by a pseudo-potential having the same scattering length, the so-called contact interaction given by Eq.(2.3) of Part I.

The situation is quite different if, in addition to short range interactions, there is a significant dipole-dipole interaction. The slow decay as $1/r^3$ at large distances implies that for all l waves (the first term of (1.5) vanishes at zero energy while the second term is constant) i.e. $\delta_l \sim k$ at low momentum, and all partial waves contribute to the scattering amplitude. Moreover, due to the anisotropy of the DDI, the angular momentum is no conserved during the scattering amplitude. Consequently, the DDI mixes all partial waves with even angular momentum for bosons and odd l in the case of fermions.

The main conclusion of this theory is that we may replace the actual interparticle interaction with an effective potential of the form

$$U(r) = g\delta(r) + U_{dd}(r), \tag{1.6}$$

where g is defined as before but in principle the s-wave scattering length a is now dipole dependent $a(d)$.

The scattering of bosonic dipoles is determined by both long-range and short range interactions which play a crucial role, as we shall see in next sections, in physics of dipolar Bose gases. While for fermionic dipoles, the s-wave channel is absent and hence the low energy scattering is determined only by long-range part.

1.5.Time dependent GP equation with dipole-dipole interaction:

Let us consider a gas of dipolar bosons. The second quantized Hamiltonian of the system reads:

$$\hat{H} = \int d\mathbf{r}\hat{\psi}^{+}(\mathbf{r})\left[\frac{-\hbar^2}{2m}\Delta + V(\mathbf{r}) - \mu + \frac{g}{2}\left|\hat{\psi}(\mathbf{r})\right|^2\right]\hat{\psi}(\mathbf{r}) + \frac{1}{2}\iint d\mathbf{r}d\mathbf{r}'\hat{\psi}^{+}(\mathbf{r})\hat{\psi}^{+}(\mathbf{r}')U_{dd}(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\,\hat{\psi}(\mathbf{r})\,. \tag{1.7}$$

We may thus easily obtain the Heisenberg equations for the dynamics of the field operator, by employing the bosonic commutation rules. Since we are interested in the case of BECs in the limit of $T = 0$, we may use then $\hat{\psi}(\mathbf{r}) \to \Phi(\mathbf{r})$ (see chapter 2of Part I). We find straightforwardly the following equation for the dynamics of the wave function $\Phi(\mathbf{r}, t)$ of dipolar Bose-Einstein condensate

$$\hbar\frac{\partial\Phi(\mathbf{r},t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}) + g|\Phi(\mathbf{r},t)|^2 + \Phi_{dd}(r')\right]\Phi(\mathbf{r},t), \tag{1.8}$$

where

$$\Phi_{dd}(r') = \frac{C_{dd}}{4\pi}\int d\mathbf{r}' \frac{1-3cos^2\theta}{r^2}|\Phi(\mathbf{r}',\mathrm{t})|^2, \quad (1.9)$$

is the dipole-dipole interacting potential.

Here $\Phi(\mathbf{r},t)$ is normalized to the total number of particles $\int dr|\Phi(\mathbf{r},\mathrm{t})|^2 = N$.

Note that this is a modified version of the well-known GP equation. In the absence of DDI the nonlinearity is given by local term $g|\Phi(\mathbf{r},t)|^2$. On the contrary, the nonlinearity introduced by the DDI is non local. The applicability of the GP equation was tested in Ref. [296, 297] by using many-body diffusion Monte-Carlo calculations with the result that a GP equation with the pseudo potential is adequate to describe the gas provided it is dilute: $na^3 \ll 1$. Such a dilute dipolar gas is described by a non-local GP, which was first derived for dipolar gases by Yi and You [298,299], and then developed in a series of papers.

1.6.Excitations in homogeneous dipolar Bose gas: Phonon instability

1.6.1. Fourier transform

In view of studying the elementary excitations in a dipolar condensate, as well as for numerical calculations, it is convenient to use the Fourier transform of the dipole-dipole interaction. Fourier transform is

$$\widetilde{U}_{dd}(p) = \int d^3r\, U_{dd}(r)e^{-ikr}\,. \quad (1.10)$$

In the analysis of dipolar gases, the Fourier transform of the DDI turns out to be very helpful. This Fourier transform may be easily retrieved by rewriting:

$$U_{dd}(r) = \frac{C_{dd}}{4\pi r^3}\left(-4\sqrt{\frac{5}{\pi}}\right)Y_{20}(\theta), \quad (1.11)$$

where Y_{lm} are the spherical harmonics. We employ the expansion of a wave in spherical harmonics:

$$e^{ikr} = 4\pi\sum_{l=0}^{\infty} i^l\, j_l(kr)\sum_{m=-l}^{l} Y_{lm}^*(\theta_k,\varphi_k)Y_{lm}(\theta_k,\varphi_k), \quad (1.12)$$

using the integral:

$$\int dr\,\frac{j_2(kr)}{r} = \frac{1}{3}, \quad (1.13)$$

and orthonormality condition of the spherical harmonics:

$$\int Y_{20}^*(\theta,\varphi)\,Y_{20}(\theta)\sin\theta d\theta d\varphi = \delta_{ll'}\delta_{mm'}, \quad (1.14)$$

and introducing Eqs. (1.11)-(1.14) into Eq. (1.10), one gets

$$\widetilde{U}_{dd}(k) = -\frac{C_{dd}}{3}\left(-4\sqrt{\frac{5}{\pi}}\right)\sum_{l=0}^{2}\sum_{m=-2}^{2}\delta_{ll'}\delta_{mm'}\,Y_{20}(\theta_k,\varphi_k)$$

$$= -\frac{C_{dd}}{3}\left(-4\sqrt{\frac{5}{\pi}}\right)Y_{20}(\theta_k,\varphi_k), \quad (1.15)$$

the Fourier transform of the dipole-dipole interaction turns to be given by

$$\widetilde{U}_{dd}(k) = \frac{C_{dd}}{3}(3\cos^2\theta_k - 1), \tag{1.16}$$

where θ_k is the angle between the excitation momentum k and the direction of dipoles.

Therefore, in spirit of this Fourier transform and with the definition (1.3) for ϵ_{dd}, the momentum-space interaction (1.6) for the homogeneous system yields

$$\widetilde{U}(k) = g + \frac{C_{dd}}{3}(3\cos^2\theta_k - 1) = g[1 + \epsilon_{dd}(3\cos^2\theta_k - 1)]. \tag{1.17}$$

Remarkably, in three dimensions, the Fourier transform of the dipole-dipole interaction does not depend on the modulus of the wavevector $\boldsymbol{k}$, a feature which is shared by the contact interaction, whose Fourier transform is simply g.

1.6.2. Phonon instability

Because of the partially attractive character of the dipole-dipole interaction, the stability of a dipolar BEC is a problem that needs to be addressed. We consider a 3D homogeneous dipolar condensate, having an equilibrium density n. We then perform the standard Bogoliubov method described in chapter 2 of Part I, one can show easily that the excitation spectrum is given by

$$\varepsilon_k = \sqrt{E_k^2 + 2E_k n\widetilde{U}(k)}\,. \tag{1.18}$$

Including the interaction (1.17) into (1.18), the spectrum becomes

$$\varepsilon_k = \sqrt{E_k^2 + E_k\mu[1 + \epsilon_{dd}(3\cos^2\theta_k - 1)]}. \tag{1.19}$$

where $\mu = ng$ being the chemical potential.

According to our knowledge, the spectrum (1.19) has been first calculated by Santos *et al*. [260].

For large momenta ($k \to \infty$), the Bogoliubov dispersion law is reduced to the free-particle form:

$$\epsilon_k = E_k\,. \tag{1.20}$$

In the opposite limit for small momenta ($k \to 0$) the Bogoliubov dispersion law (1.19) is well approximated by the phonon-like linear dispersion form

$$\epsilon_k = \hbar C_s k\,, \tag{1.21}$$

with the dipolar sound velocity is

$$C_s = c_{s0}\sqrt{1 + \epsilon_{dd}(3\cos^2\theta_k - 1)}, \tag{1.22}$$

where $c_{s0} = \sqrt{ng/m}$ is the sound velocity of purely contact interaction.

Note that for $\theta_k = \pi/2$, $C_s = c_{s0}\sqrt{1-\epsilon_{dd}}$ and $\varepsilon_k = \sqrt{E_k^2 + E_k\mu(1-\epsilon_{dd})}$. As a result, the properties of the Bogoliubov spectrum depend crucially on the parameter ϵ_{dd}.

i) For $\epsilon_{dd} < 1$, the short-range part of the interparticle interaction dominates and dipole-dipole interaction provides only corrections. This case corresponds to a stable BEC and was studies in earlier experiments [255].

ii) For $\epsilon_{dd} > 1$, some excitation modes are purely imaginary and thus the homogenous 3D dipolar gas is dynamically unstable against very long wavelength excitations. Such feature often denotes as "phonon instability".

1.7.Hydrodynamic equations:

Solving the time-dependent Gross-Pitaevskii Eq. (1.8) is not always the most adequate way to study the properties of Bose-Einstein condensates. When it comes to the low-lying excitations, for example, it is often useful to switch to an equivalent treatment which is provided by the hydrodynamic equations.

Building on the fact that the order parameter is a complex field, we factorize the condensate wave function according to the Madelung transformation $\psi(r,t) = \sqrt{n(\mathbf{r},t)}e^{i\phi(\mathbf{r},t)}$, with n the atomic density and ϕ the phase of the order parameter and it is a real quantity, related to the superfluid velocity field by $v(r,t) = \frac{\hbar}{m}\nabla\phi(r,t)$. Substituting this expression in Eq. (1.8) and separating real and imaginary parts, one gets the continuity equation

$$\frac{dn(\mathbf{r},t)}{dt} = -\frac{\hbar}{m}\nabla\big(n(\mathbf{r},t)\nabla\phi(\mathbf{r},t)\big), \tag{1.23}$$

Correspondingly, the real part yields the Euler equation

$$-\hbar\frac{d\phi(\mathbf{r},t)}{dt} = \frac{-\hbar^2}{2m}\frac{\Delta\sqrt{n(\mathbf{r},t)}}{\sqrt{n(\mathbf{r},t)}} + \frac{\hbar^2}{2m}\left(\frac{\partial\phi(\mathbf{r},t)}{\partial\mathbf{r}}\right)^2 + V(\mathbf{r}) + gn(\mathbf{r},t) + \Phi_{dd}(\mathbf{r}'), \tag{1.24}$$

which together form a closed system of equations for n and ϕ which is completely equivalent to the Gross-Pitaevskii Eq. (1.8).

Indeed, the static properties of the condensate can be investigated by setting $dn/dt = 0$ and $v = 0$ in Eqs. (1.23) and (1.24). Despite the fact that they can be used to study static properties, the best application of the hydrodynamic equations is the investigation of the low-lying excitations. Since these are low energetic excitations, their study can be carried out by considering small density fluctuation around the equilibrium. In such situation one can linearize Eqs.(1.23, 1.24) with respect to $\delta\hat{n}$ and $\nabla\hat{\phi}$ around the stationary solution. One gets both for the zero and the first orders:

$$\mu = \frac{-\hbar^2}{2m}\frac{\Delta\sqrt{n(\mathbf{r},t)}}{\sqrt{n(\mathbf{r},t)}} + \frac{\hbar^2}{2m}\left(\frac{\partial\phi(\mathbf{r},t)}{\partial\mathbf{r}}\right)^2 + V(\mathbf{r}) + gn(\mathbf{r},t) + \Phi_{dd}(\mathbf{r}'), \tag{1.25}$$

$$\hbar \frac{\partial}{\partial t}\left(\frac{\delta \hat{n}}{\sqrt{n}}\right) = \left[\frac{-\hbar^2}{2m} \Delta_{\mathbf{r}} + V(\mathbf{r}) + gn - \mu + \Phi_{dd}(r')\right]\left(2\sqrt{n}\hat{\phi}\right), \quad (1.26)$$

$$-\hbar \frac{\partial}{\partial t}\left(2\sqrt{n}\hat{\phi}\right) = \left[\frac{-\hbar^2}{2m} \Delta_{\mathbf{r}} + V(\mathbf{r}) + 3gn - \mu + \Phi_{dd}(r')\right]\left(\frac{\delta \hat{n}}{\sqrt{n}}\right). \quad (1.27)$$

These equations constitute the most important results in this chapter. Solutions of such equations in terms of elementary excitations allow us to calculate the one body correlation function and the density-density fluctuations in homogeneous dipolar Bose gases.

In the following chapters, we demonstrate the power of these hydrodynamic equation and we discuss fluctuations in a dilute two-dimensional Bose-condensed dipolar gas, which has a roton-maxon character of the excitation spectrum. It will be interesting to see how the rotonization enhances these fluctuations? and therefore when the criterion of the Bogoliubov approach will be valid?

Chapter 2

Two-dimensional dipolar Bose gas with the roton-maxon excitation spectrum

2.1.Introduction

One of the key issues for dipolar Bose-condensed gases is the presence of the roton-maxon character of the excitation spectrum and the possibility of obtaining supersolid states in which the condensate wavefunction is a superposition of a uniform background and a lattice structure. The roton-maxon structure of the spectrum has been first predicted for strongly pancaked Bose-Einstein condensates [300]. However, the idea to obtain a supersolid state when the roton touches zero and uniform BEC becomes unstable, did not succeed because of the collapse of the system [301, 302]. Since that time, several proposals have been made for the creation of supersolid states with bosons [303]. They rely on the potential of interatomic interaction which is flat at short distances and decays at large separations, and the results then indicate the presence of dense supersolid clusters [304].

This activity brought in analogies with liquid helium, where the studies of the roton-maxon spectrum and the attempts to observe experimentally the supersolid state have spanned for decades [305, 306] after the early theoretical prediction [307]. However, the most credible claim for the observation of the supersolid [308] is now withdrawn [309]. It is worth mentioning that the old idea of obtaining a stable density-modulated state (supersolid) in superfluid helium moving with a supercritical velocity [310] is now being discussed in a general context of superfluidity in Bose gases flowing with velocities larger than the Landau critical velocity [311].

The roton-maxon character of the excitation spectrum was also attracting large attention by itself. In relation to liquid helium, it has been discussed how the position of the roton minimum influences the phenomenon of superfluidity [312]. In the context of dipolar bosons in two dimensions, numerical calculations of zero temperature phase diagram [313–314] found that the reduction of the condensed fraction with an increase in the density can be attributed to the appearance of the roton minimum. Finite temperature Monte Carlo calculations [315] have

revealed that the rotonization of the spectrum can decrease the Kosterlitz-Thouless superfluid transition temperature. Although the calculations [31-315] were focused on fairly high densities, they raised the question of applicability of the Bogoliubov approach for dipolar bosons [314]. At the same time, there was an extended activity on the static and dynamical properties of dilute trapped dipolar Bose-Einstein condensates on the basis of the Bogoliubov approach [316–319]. It is therefore instructive to identify the validity criterion of the Bogoliubov approach for Bose-condensed dipolar gases with the roton-maxon excitation spectrum, and this is the subject of the present chapter. We show that at zero temperature the density fluctuations originating from the presence of the roton minimum, lead to a significant depletion of the condensate and modify thermodynamic quantities if the roton minimum is sufficiently close to zero. At finite temperatures exceeding the roton energy, thermal density fluctuations may have a much stronger influence, leading to a large increase of the normal fraction.

2.2.Dipolar bosons in the quasi2D geometry

We consider dipolar bosons (tightly) confined in one direction (z) to zero point oscillations and assume that in the *x, y* plane the translational motion is free. The dipole moments are oriented perpendicularly to the *x, y* plane, so that at large interparticle separations r, the interaction potential is (for sake of simplicity we write in the rest of the thesis $U_{dd}(r) = V(r)$)

$$V(r) = \frac{d^2}{r^3}, \tag{2.1}$$

with d being the dipole moment. For electric dipoles (polar molecules) this can be done by applying a strong electric field and for magnetic dipoles by using a magnetic field.

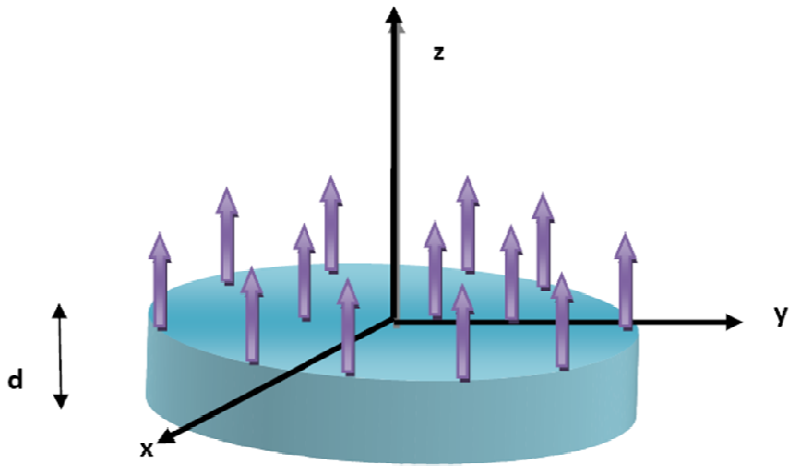


Figure 2. 1. Dipolar Bose-Einstein condensate tightly confined in the z-direction.

The short-range part of the potential is assumed to be such that there is a roton-maxon excitation spectrum. In the ultracold limit where the particle momemta satisfy the inequality $kr_* \ll 1$ with $r_* = md^2/\hbar^2$ being the characteristic dipole-dipole distance, the so-called anomalous term coming from distances of the order of the de Broglie wavelength of particles [295] and obtained using a perturbative approach in $V(r)$. The off-shell scattering amplitude is defined (see [277])

$$f(\boldsymbol{k'}, \boldsymbol{k}) = \frac{4\hbar^2}{m} \int d^2 r e^{-i\boldsymbol{k'}.\boldsymbol{r}} \psi_k(\boldsymbol{r}) V(\boldsymbol{r}). \tag{2.2}$$

where $\psi_k(\boldsymbol{r})$ is the true wavefunction of the relative motion with momentum $\boldsymbol{k}$, is given by :

$$f(\boldsymbol{k'}, \boldsymbol{k}) = \frac{2\pi\hbar^2}{m} \left[\frac{1}{\ln\left(\frac{\kappa}{k}\right) + \frac{i\pi}{2}} - r_* |\boldsymbol{k} - \boldsymbol{k'}| \right], \tag{2.3}$$

A detailed derivation of the scattering amplitude (2.3) will be given in appendix A.

where we omit higher order terms in k. The second term in the right hand side represents the anomalous contribution and it takes into account all partial waves. The first term in the right hand side of Eq.(2.3) describes the short-range contribution. It is obtained by putting $k' = 0$ and proceeding along the lines of the 2D scattering theory [295]. The parameter κ depends on the behavior of $V(\boldsymbol{r})$ at short distances. In the quasi2D geometry it also depends on the confinement length in the z-direction, $l_0 = \sqrt{\hbar/m\omega_z}$, where ω_z is the confinement frequency. One then can express κ through the 3D coupling constantg_{3D}. If the analog of the 3D s-wave scattering length $a = mg_{3D}/4\pi\hbar^2 \ll l_0$, then κ is exponentially small [234, 235] and we may omit the k-dependence under logarithm in Eq.(2.3), as well as $i\pi/2$ in denominator of the first term. This gives

$$f(\boldsymbol{k'}, \boldsymbol{k}) = g(1 - C|\boldsymbol{k} - \boldsymbol{k'}|), \tag{2.4}$$

where the 2D short-range coupling constant is $g = g_{3D}/\sqrt{2}l_0$ and $C = 2\pi\hbar^2 r_*/mg$. Employing the result of Eq.(2.4) in the secondly quantized Hamiltonian [301, 302], we obtain

$$\hat{H} = \sum_{\boldsymbol{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\boldsymbol{k}}^+ \hat{a}_{\boldsymbol{k}} + \frac{g}{2S} \sum_{\boldsymbol{k},\boldsymbol{q},\boldsymbol{p}} (1 - C|\boldsymbol{q} - \boldsymbol{p}|) \hat{a}_{\boldsymbol{k}+\boldsymbol{q}}^+ \hat{a}_{\boldsymbol{k}-\boldsymbol{q}}^+ \hat{a}_{\boldsymbol{k}+\boldsymbol{p}} \hat{a}_{\boldsymbol{k}-\boldsymbol{p}}, \tag{2.5}$$

where S is surface area, and $\hat{a}_{\boldsymbol{k}}^+$, $\hat{a}_{\boldsymbol{k}}$ are the creation and annihilation operators of particles. At zero temperature there is a true Bose-Einstein condensate in 2D, and we may use the standard Bogoliubov approach. Assuming the weakly interacting regime where $mg/2\pi\hbar^2 \ll 1$ (and $r_* \ll \xi$, with $\xi = \hbar/\sqrt{mng}$ being the healing length), we reduce the Hamiltonian to a bilinear

form, employ the usual Bogoliubov transformation $\hat{a}_{\boldsymbol{k}} = u_k \hat{b}_{\boldsymbol{k}} - v_k \hat{b}^+_{-\boldsymbol{k}}$, we then obtain the diagonal form of $\hat{H}$ in terms of operators $\hat{b}^+_{\boldsymbol{k}} \hat{b}_{\boldsymbol{k}}$ of elementary excitations as

$$\hat{H} = E_0 + \sum_{\boldsymbol{k}} \varepsilon_k \hat{b}^+_{\boldsymbol{k}} \hat{b}_{\boldsymbol{k}}. \tag{2.6}$$

The Bogoliubov functions u_k, v_k are expressed in a standard way as in chapter 2 of part I (see Eqs. (2.36)), where $E_k = \hbar^2 k^2/2m$, and the Bogoluibov excitation energy is given by:

$$\varepsilon_k = \sqrt{E_k^2 + 2\mu E_k (1 - Ck)}, \tag{2.7}$$

where $\mu = ng$ is the chemical potential and $N = nS$ is the number of particles. To zero order the ground state energy is $E_0 = \mu N/2$. For small momenta the excitations are sound waves, $\varepsilon_k = \sqrt{\mu/m}k$. The dependence of ε_k on k remains monotonic with increasing k if $C \leq \sqrt{8}\xi/3$ (see figure.2.2). For the constant C in the interval

$$\frac{\sqrt{8}}{3}\xi \leq C \leq \xi, \tag{2.8}$$

the excitation spectrum has a roton-maxon structure known from the physics of liquid helium. It is then convenient to represent ε_k in the form [320]:

$$\varepsilon_k = \frac{\hbar^2 k}{m}\sqrt{(k - k_r)^2 + k_\Delta^2}, \tag{2.9}$$

where $k_r = 2C/\xi^2$ and $k_\Delta = \sqrt{4/\xi^2 - k_r^2}$. If the roton is close to zero, then k_r is the position of the roton, and

$$\Delta = \frac{\hbar^2 k_\Delta k_r}{2m} = 2ngC\sqrt{\frac{mgn}{\hbar^2} - C^2\left(\frac{mgn}{\hbar^2}\right)^2}, \tag{2.10}$$

is the height of the roton minimum (see figure 2.2).

For $C = \xi$ the roton minimum touches zero, and at larger C the uniform Bose-Einstein condensate becomes dynamically unstable. This is reflected in the appearance of imaginary excitation energies ε_k. It should be noted that the coupling constant g can be tuned by using Feshbach resonances or by modifying the frequency of the tight confinement ω_0. Therefore, although the range of C given by Eq.(2.8) is rather narrow, it can be reached without serious difficulties. This opens wide possibilities to study the influence of the rotonization of the excitation spectrum on the properties of the system. The condition $C = 2\pi d^2/g = \xi$ is reduced to $mg/2\pi\hbar^2 = a_{3D/\sqrt{2}l_0} = 2\pi n r_*^2$. For dysprosium atoms we have the dipole-dipole distance $r_* \simeq 200$ °A and at 2D densities ~10^9 cm^{-2} the roton-maxon spectrum is realized for the 3D

scattering length a_{3D} of several tens of angstroms at the frequency of the tight confinement of 30 kHz leading to the confinement length l_0 above 1000 ˚A.

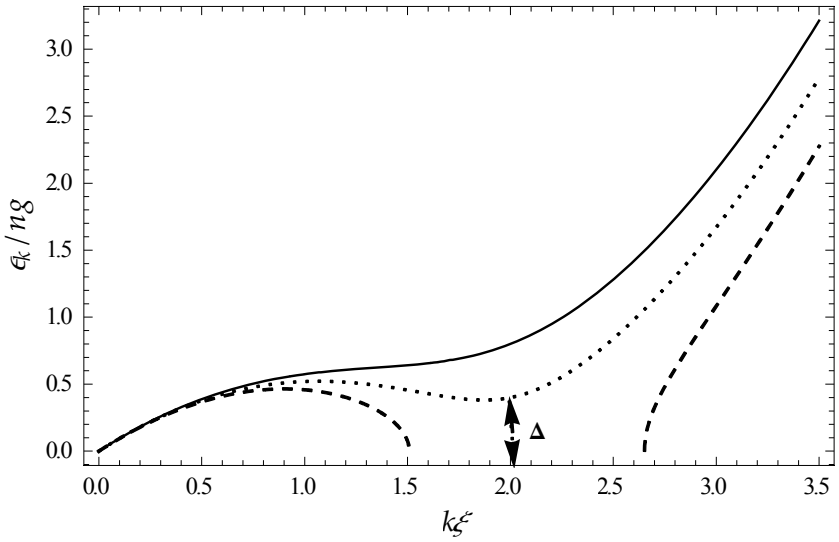


Figure 2.2. Excitation energy ε_k of the quasi-2D dipolar BEC as a function of momentum k for several values of $k_r\xi$. The solid curve ($k_r\xi$ = 1.84) shows a monotonic dependence ε_k, the dotted curve ($k_r\xi$= 1.96) is ε_k with the roton-maxon structure, and the dashed curve ($k_r\xi$= 2.08) corresponds to dynamically unstable BEC.

2.3. Density Fluctuation and condensate depletion at $T = 0$

The Bogoliubov approach assumes that the density and phase fluctuations are small. In our 2D case at $T = 0$, the presence of the roton does not significantly change the phase fluctuations and they remain small. However, the situation with the density fluctuations is different. Using the operator of the density fluctuations defined in Eq.(5.16) of chapter 5 of Part I (or see Eqs (1.25-1.27 of Chapter 1, Part II), we obtain for the density-density correlation function:

$$\frac{\langle \delta\hat{n}(r)\delta\hat{n}(0)\rangle}{n^2} = \frac{1}{n}\int \frac{d^2k}{(2\pi)^2}\frac{E_k}{\varepsilon_k}(1+2N_k)e^{i\boldsymbol{k}.\boldsymbol{r}}, \tag{2.11}$$

where $N_k = \left[e^{\varepsilon_k/T} - 1\right]^{-1}$ are occupation numbers for the excitations. It is instructive to single out the roton contribution to the correlation function (2.10). At $T = 0$ we have $N_k = 0$ and using Eq.(2.9) we obtain for the contribution of momenta near the roton minimum:

$$\frac{\langle \delta\hat{n}(r)\delta\hat{n}(0)\rangle_r}{n^2} = \frac{k_r^2}{2\pi n}\ln\left(\frac{k_r}{k_\Delta}\right)J_0(k_r r)\ ; \qquad k_\Delta r \ll 1 \tag{2.12}$$

If the roton is close to zero, we have C close to ξ and $k_r \simeq 2/\xi$. Then Eq.(2.12) yields:

$$\frac{\langle \delta\hat{n}(r)\delta\hat{n}(0)\rangle_r}{n^2} = \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right)J_0(2r/\xi), \tag{2.13}$$

We thus see that the density fluctuations grow logarithmically when the roton minimum is approaching zero and they can become strong for very small Δ [320]. In this case they lead to a significant depletion of the condensate.

The non-condensed fraction of particles is given by:

$$\frac{\tilde{n}}{n} = \frac{1}{n}\sum_k v_k^2 = \frac{1}{4n}\int \frac{d^2k}{(2\pi)^2}\left(\frac{E_k}{\varepsilon_k} + \frac{\varepsilon_k}{E_k} + 2\right), \tag{2.14}$$

The integral over dk is logarithmically divergent at large momenta because of the dipole-dipole contribution to the interaction strength, $-gCk$. However, this form of the dipole-dipole contribution is valid only for $k \ll 1/r_*$. We thus may put a high momentum cut-off $1/r_*$which leads to

$$\frac{\tilde{n}}{n} = \frac{mg}{4\pi\hbar^2}\left[1 - k_r\xi - \frac{3(k_r\xi)^2}{4} - \frac{(k_r\xi)^2}{2}\ln\left(\frac{\xi}{r_*(2-k_r\xi)}\right)\right], \tag{2.15}$$

In the absence of the dipole-dipole interaction (r_* = 0 and $k_r = 0$) we recover the usual result for for the 2D BEC with short-range interparticle repulsion, $\tilde{n}/n = mg/4\pi\hbar^2$. For $\Delta \to 0$ we have $2 - k_r\xi \approx (k_\Delta\xi/2)^2$and Eq.(2.15) transforms to [320]

$$\frac{\tilde{n}}{n} \simeq \frac{mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\varsigma\right), \tag{2.16}$$

where $\varsigma = \sqrt{2\pi\hbar^2/e^2mg}$.

As we see from Eqs. (2.13) and (2.16), if the roton minimum is close to zero ($C \simeq \xi$ and $k_r = 2/\xi$) small condensate depletion and small fluctuations of the density require the inequality

$$\frac{mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right) \ll 1, \tag{2.17}$$

It differs only by a logarithmic factor $\ln(2ng/\Delta)$ from the small parameter of the theory, $(mg/2\pi\hbar^2 \ll 1)$, in the absence of the roton.

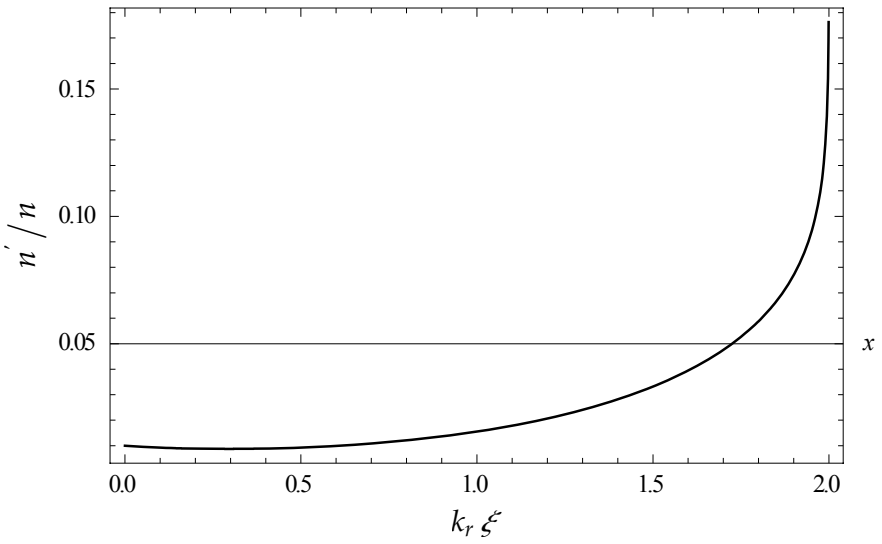


Figure2. 3. Noncondensed fraction as a function of $k_r\xi$ for $mg/4\pi\hbar^2 = 0.01$ ($\xi/r_* = 100/k_r\xi$).

This figure shows that the non-condensed fraction increases when the roton energy decreases, such a behavior has been found in numerical calculations of Ref. [316].

The same parameter logarithmic factor (2.17) appears in the fluctuation correction to the chemical potential and in the one-body density matrix.

$$g_1(r) = \langle\hat{\psi}^+(r)\hat{\psi}(0)\rangle = n_0 + \int \frac{d^2k}{(2\pi)^2} v_k^2\, e^{i\boldsymbol{k}.\boldsymbol{r}}, \tag{2.18}$$

where $\hat{\psi}^+(r) = 1/\sqrt{S}\sum_k \hat{a}_{\boldsymbol{k}}\, e^{i\boldsymbol{k}.\boldsymbol{r}}$ is the field operator.

Assuming that the roton minimum is close to zero and taking into account only the contribution of momenta near this minimum, we get [320]:

$$g_1(r) = n_0\left[1 + \frac{mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right)J_0(2r/\xi)\right], \tag{2.19}$$

The correction to the chemical potential due to quantum fluctuations is given by:

$$\frac{\delta\mu}{\mu} \simeq \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right), \tag{2.20}$$

However, the situation changes in the calculation of the compressibility. At $T = 0$ the inverse compressibility is equal to $n^2\partial\mu/\partial n$. Then, using Eqs.(2.20) and (2.10), for the roton minimum close to zero we obtain [320]:

$$\frac{\partial\mu}{\partial n} = g\left[1 + \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng\,e}{\Delta}\right) + \frac{gm}{\pi\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\right], \tag{2.21}$$

In the case when $2ng/\Delta \gg 1$, it is useful to omit the logarithm term from Eq.(2.21)

$$\frac{\partial \mu}{\partial n} = g\left[1 + \frac{mg}{\pi\hbar^2}\left(\frac{2gn}{\Delta}\right)^2\right], \tag{2.22}$$

where g is the mean field contribution, and the second and third terms originate from quantum fluctuations. Small deviations of the compressibility from the mean field result require the inequality [320]

$$\frac{mg}{\pi\hbar^2}\left(\frac{2ng}{\Delta}\right)^2 \ll 1, \tag{2.23}$$

We thus conclude that at $T = 0$ the validity of the Bogoliubov approach is guaranteed by the presence of the small parameter (2.23). For the dysprosium example given in the end of section 2.2, the chemical potential is about 5 nK, and the criterion (2.23) is satisfied for the roton energy above 2 nK.

2.4. Fluctuation at finite temperatures

In 2D at finite temperatures, long-wave fluctuations of the phase destroy the condensate [217-219]. There is the so-called quasicondensate, or condensate with fluctuating phase. In this state fluctuations of the density are suppressed but the phase still fluctuates. The transition from a non-condensed state to quasiBEC is of the Kosterlitz-Thouless type and it occurs through the formation of bound vortex-antivortex pairs [220,221]. Somewhat below the Kosterlitz-Thouless transition temperature the vortices are no longer important, and in the weakly interacting regime that we consider the phase coherence length l_ϕ is exponentially large. Thermodynamic properties, excitations, and correlation properties on a distance scale smaller than l_ϕ are the same as in the case of a true BEC. Moreover, for realistic parameters of quantum gases, l_ϕ exceeds the size of the system [248], so that one can employ the ordinary BEC theory.

Irrespective of the relation between l_ϕ and the size of the system, one may act in terms of the density and phase variables (hydrodynamic approach). We now show that the rotonization of the spectrum can strongly increase thermal fluctuations of the density and therefore destroy the Bose condensed state even at very low T. Using equation (2.11) we calculate the density-density correlation functions. Assuming that the roton energy Δ is very small (at least $\Delta \ll T$), the main contribution to the integral in Eq.(2.11) comes from momenta near k_r, and we obtain:

$$\frac{\langle \delta\hat{n}(r)\delta\hat{n}(0)\rangle_r}{n^2} = \frac{4mg}{\hbar^2}\frac{T}{\Delta}J_0(2r/\xi), \tag{2.24}$$

where it is also assumed that $k_\Delta r \ll 1$.

Comparing this result with Eq.(2.12) we see that instead of the logarithmic factor we have the factor $2\pi T/\Delta \gg 1$.

The same large factor appears in the correction to the chemical potential due to thermal fluctuations. For $\Delta \ll$ T we have:

$$\frac{\delta\mu}{\mu_0} = \sum_{\boldsymbol{k}}(u_k - v_k)N_k \simeq \frac{2mg}{\hbar^2}\frac{T}{\Delta}, \tag{2.25}$$

We now calculate the density of the normal component in the presence of the roton. In 2D the expression for this quantity is obtained in the same way as in 3D [321], and it reads:

$$n_T = -\int \frac{\hbar^2 k^2}{2m}\frac{\partial N_k}{\partial \varepsilon_k}\frac{d^2k}{(2\pi)^2}, \tag{2.26}$$

If the roton minimum is close to zero and $\Delta \ll$ T, then the momenta near the roton minimum are the most important, and the integration over dk yields:

$$\frac{n_T}{n} = \frac{2mg}{\hbar^2}\frac{T}{\Delta} \tag{2.27}$$

The employed approach requires the condition $n_T \ll n$ because we used the spectrum of excitations obtained by the Bogoliubov method. Again at temperatures T $\gtrsim \Delta$, we should have the same inequality [320]

$$\frac{2mg}{\hbar^2}\frac{T}{\Delta} \ll 1. \tag{2.28}$$

A different small parameter appears in the calculation of the compressibility. The inverse isothermal compressibility is proportional to$(\partial P/\partial n)_T$, where the pressure is $= (\partial F/\partial S)_T$, with the free energy given by $F = E_0 + T\sum_k \ln[1 - Exp(-\varepsilon_k/T)]$. For the roton minimum close to zero and $\{T, ng\} \gg \Delta$, we obtain [320]:

$$\left(\frac{\partial P}{\partial n}\right)_T = ng\left[1 - \frac{mg}{\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\frac{T}{\Delta} + \cdots\right], \tag{2.29}$$

where we omitted less important finite-temperature contributions and the zero temperature contribution proportional to the small parameter (2.23). Eq.(2.29) shows that at temperatures T $\gg \Delta$, the Bogoliubov approach requires the inequality [319]

$$\frac{mg}{\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\frac{T}{\Delta} \ll 1, \tag{2.30}$$

whereas for T $\lesssim \Delta$ it is sufficient to have criterion (2.23).

For certain quantities the Bogoliubov approach may give good results at T $\gg \Delta$ if $(mg/\hbar^2)T/\Delta \ll 1$, and at T $\lesssim \Delta$ in the presence of the ordinary small parameter $mg/2\pi\hbar^2$ amplified by a

logarithmic factor $\ln(2ng/\Delta)$ for $ng \gg \Delta$. However, the validity of this approach is guaranteed only if the inequalities (2.30) and (14) are satisfied. For $T \gg \Delta$ the compressibility following from Eq.(2.29) and the normal fraction given by equation (2.27) can become significant, by far exceeding similar quantities in an ordinary 2D Bose gas with short-range interactions at the same temperature, coupling constant g and density.

2.5.Conclusion

We have shown that the roton-maxon structure of the excitation spectrum, which can be achieved in dipolar Bose-condensed gases in the 2D geometry, strongly enhances fluctuations of the density. We obtained the validity criterion of the Bogoliubov approach and found that at finite temperatures in the dilute regime where $nr_*^2 \ll 1$, thermal fluctuations may significantly reduce the superfluid fraction even at temperatures well below the Kosterlitz-Thouless transition temperature.

General conclusion

The second part of this thesis was dedicated to dipolar Bose-Einstein condensates. Starting from the definition of dipole-dipole interaction and its relevance in Bose-Einstein condensation. Proceeding in that way, we briefly discussed in Chapter 1 the main ingredients of the forthcoming experimental investigations of Cr-BEC. During this journey we took the opportunity to review some theoretical properties of Bose gas with DDI such as the Bogoliubov excitation spectrum and the sound velocity. Moreover, we derived from the Gross-Pitaevskii equation the hydrodynamic formalism which allows us to study the density and phase fluctuations for dipolar Bose gases.

On the other hand, we have discussed fluctuations in a dilute two-dimensional Bose-condensed dipolar gas, which has a roton-maxon character of the excitation spectrum. We calculate the density-density correlation function, fluctuation corrections to the chemical potential, compressibility, and the normal (superfluid) fraction. It is shown that the presence of the roton strongly enhances fluctuations of the density, and we establish the validity criterion of the Bogoliubov approach. At zero temperature the condensate depletion becomes significant if the roton minimum is sufficiently close to zero. At finite temperatures exceeding the roton energy and the interaction between particles, the effect of thermal fluctuations is stronger and it may lead to a large normal fraction of the gas which may significantly reduce the superfluid fraction even at temperatures well below the Kosterlitz-Thouless transition temperature.

Finally, as a logical pursuing of our work, it would be interesting to know how to describe the emerging state with strong fluctuations? and how to manipulate the short-range physics for obtaining a stable supersoliod?

Appendix A

Scattering theory in two dimensions

1. Hard-Disc Scattering in 2D

The advantages of studying the hard sphere scattering are: it is a limit to radial Schrödinger equation at large radii and, it is solvable using the "least amount" of approximations. It also shows how phase shifts and the scattering amplitude are obtained. Then it can be immediately written down.

$$V = \begin{cases} \infty, & r \leq a \\ 0, & r > a \end{cases}, \tag{A1}$$

with a the radius of the hard sphere.

1.1.Schrödinger equation

The Schrödinger equation for the hard sphere scattering in 2D is

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{\hbar^2 k^2}{2m}\right]\psi(\boldsymbol{r}) = 0, \tag{A2}$$

Then turning to the polar coordinates and using the ansatz

$$\psi(\boldsymbol{r}) = \chi(r)\Theta(\theta), \tag{A3}$$

one has for

$$\left[\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + k^2\right]\chi(r)\Theta(\theta) = 0, \tag{A4}$$

which is equivalent to

$$\left[\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)\right) + k^2\right]\chi(r)\Theta(\theta) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\chi(r)\Theta(\theta) = 0. \tag{A5}$$

In two dimensions one has

$$\Theta(\theta) \sim e^{-il\theta}, \tag{A6}$$

where l is the orbital angular momentum ranging from $-\infty$ to $+\infty$. It then remains to deal with the radial Schrödinger equation

$$\left[\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)\right) + k^2 - \frac{l^2}{r^2}\right]\chi(r) = 0. \tag{A7}$$

Now it is useful to introduce the scaled radial wave function, representing as $\chi(r) = R(r)/\sqrt{r}$ such that the first derivative in r vanishes. This requirement yields

$$\left[\frac{d^2}{dr^2} + k^2 + \frac{1}{r^2}\left(\frac{1}{4} - l^2\right)\right] R(r) = 0, \tag{A8}$$

1.2.s-wave scattering amplitude

Now we deal with solution for zero angular momentum ($l = 0$). If the radius r is much larger than disc radius a i.e. ($r > a$), the Schrödinger equation (A8) reduces to

$$\left[\frac{d^2}{dr^2} + \frac{1}{4r^2} + k^2\right] R(r) = 0, \tag{A9}$$

which has the wave function solution

$$\chi(r) = AJ_0\,(kr) + BY_0\,(kr), \tag{A10}$$

where $J_0\,(kr)$and $Y_0\,(kr)$ are Bessel functions, A and B are k-dependent coefficients.

At $r = a$, when the potential becomes infinite, the wave function must vanish ($\chi(a) = 0$). This boundary condition allows to determine a relation between the coefficients of the wave function. If one works in the low energy limit, such that $ka \ll 1$, then the two Bessel functions at a take the asymptotic form [322]:

$$\begin{cases} Y_0\,(kr) \simeq \frac{2}{\pi}\left[\ln\left(\frac{kae^{\gamma}}{2}\right)\right], \\ J_0\,(kr) \simeq 1 \end{cases} \tag{A11}$$

where $\gamma \simeq 0.557$ is the Euler constant.

Then using the boundary condition

$$AJ_0\,(ka) + BY_0\,(ka) = 0, \tag{A12}$$

yields the coefficients ratio

$$-\frac{A}{B} = \frac{Y_0\,(ka)}{J_0\,(ka)}. \tag{A13}$$

For $ka \ll 1$, the ratio (A13) becomes

$$-\frac{A}{B} \simeq \frac{2}{\pi}\left[\ln\left(\frac{kae^{\gamma}}{2}\right)\right]. \tag{A14}$$

Now let us look at large distances i.e. far away from the disc, the energy is still low $k \ll 1$, but $ka \gg 1$, the Bessel functions have the form

$$\begin{cases} Y_0\,(kr) \simeq \sqrt{\frac{2}{\pi kr}}\sin\left(kr - \frac{\pi}{4}\right) \\ J_0\,(kr) \simeq \sqrt{\frac{2}{\pi kr}}\cos\left(kr - \frac{\pi}{4}\right) \end{cases}. \tag{A15}$$

From the small $r$expansion of Bessel functions, one notices that Y_0 is divergent when $r \to 0$. At large r the potential is zero and it is expected that the solution would be similar in form with the one obtained when there is no potential in the Schrödinger equation, namely a Bessel J_0 function. At large distance, the influence of the hard-disc potential manifests itself only in a phase shift δ_0 appearing in the argument of J_0. Then the wave function at large r has the form

$$\chi(r) = \sqrt{\frac{2}{\pi kr}}\left[A\cos\left(kr - \frac{\pi}{4}\right) + B\sin\left(kr - \frac{\pi}{4}\right)\right] \simeq \beta J_0\,(kr + \delta_0)$$

$$\simeq \beta\sqrt{\frac{2}{\pi kr}}\cos\left(kr - \frac{\pi}{4} + \delta_0\right)$$

$$= \beta\sqrt{\tfrac{2}{\pi kr}}\left[\cos(\delta_0)\cos\left(kr - \tfrac{\pi}{4}\right) + \sin(\delta_0)\sin\left(kr - \tfrac{\pi}{4}\right)\right], \tag{A16}$$

where β is a constant.

The coefficients A and B are determined as a function of the phase shift by comparing the first and last form of the wave function in the above sequence of equation

$$\begin{cases} A = \beta\cos(\delta_0) \\ B = -\beta\sin(\delta_0) \end{cases} \tag{A17}$$

Therefore, Eqs. (A16) and (A17) lead to following expression of the phase shift

$$-\frac{A}{B} = \cot(\delta_0) = \frac{2}{\pi}\left[\ln\left(\frac{kae^{\gamma}}{2}\right)\right]. \tag{A18}$$

Then using the relation between scattering amplitude and the phase shift, we find

$$f(k) = \frac{4\hbar^2}{m}\frac{1}{i - \cot(\delta_0)} = -\frac{4\hbar^2}{m}\frac{\tan(\delta_0)}{1 - i\tan(\delta_0)} = \frac{2\pi\hbar^2}{m}\frac{1}{\frac{i\pi}{2} - \ln\left(\frac{kae^{\gamma}}{2}\right)}. \tag{A19}$$

2. Dipole-Dipole Scattering

2.1. s-wave scattering

In this section we will discuss low-energy two-body scattering of identical particles undergoing the 2D translational motion and interacting with each other at large separations via the potential

$$V(r) = \frac{d^2}{r^3} = \frac{\hbar^2 r_*}{mr^3}. \tag{A20}$$

where $r_* = md^2/\hbar^2$ is the characteristic dipole-dipole distance. The value of d depends on the external electric field. The term low-energy means that their momenta satisfy the inequality $kr_* \ll 1$.

The on-shell scattering amplitude defined as

$$f_l(k) = \int_0^\infty J_l(kr)V(\boldsymbol{r})\psi_k(\boldsymbol{r})\, dr^2. \tag{A21}$$

where $\psi_l(\boldsymbol{r})$ is the true wave function of the relative motion with momentum **k**. It is governed by the Schrödinger equation

$$\left[-\frac{\hbar^2}{m}\nabla^2 + \frac{d^2}{r^3}\right]\psi_k(\boldsymbol{r}) = \frac{\hbar^2 k^2}{m}\psi_k(\boldsymbol{r}), \tag{A22}$$

here m is the reduced mass.

For the solution of the scattering problem, it is more convenient to normalize the wave function of the radial relative motion with orbital angular momentum l in such a way that it is real and, for $r \to \infty$, one has

$$\psi_l(r) = J_l(kr) - \tan\delta_l\, N_l(kr) \propto \cos\left(kr - \frac{l\pi}{2} - \frac{\pi}{4} + \delta_l(k)\right), \tag{A23}$$

where N_l is the Neumann function. One checks straightforwardly that

$$\tan\delta_l(k) = -\frac{\mathrm{m}}{4\hbar^2} f_l(k), \tag{A24}$$

In region I where $r < r_0$, the *s*-wave ($l = 0$) relative motion of two particles is governed by the Schrödinger equation with zero kinetic energy:

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{r_*}{r^3}\right]\psi_I(r) = 0, \tag{A25}$$

At distances where the interaction potential is behaving as $V(r) = r_*\hbar^2/mr^3$, the solution of Eq. (A25) reads

$$\psi_I(r) \propto \left[AK_0\left(2\sqrt{\frac{r_*}{r}}\right) + I_0\left(2\sqrt{\frac{r_*}{r}}\right)\right], \tag{A26}$$

where $K_0$and $I_0$are the modified Bessel functions and the constant A is determined by the behavior of $V(r)$ at shorter distances.

In region II where $r > r_0$, the relative motion is practically free and the potential $V(r)$ can be considered as perturbation. To zero order we then have for the relative wave function,

$$\psi_{II}^{(0)}(r) = J_0(kr) - \tan\delta_0\, N_0(kr), \tag{A27}$$

where the scattering phase shift δ_0 is due to the interaction between particles in region I.

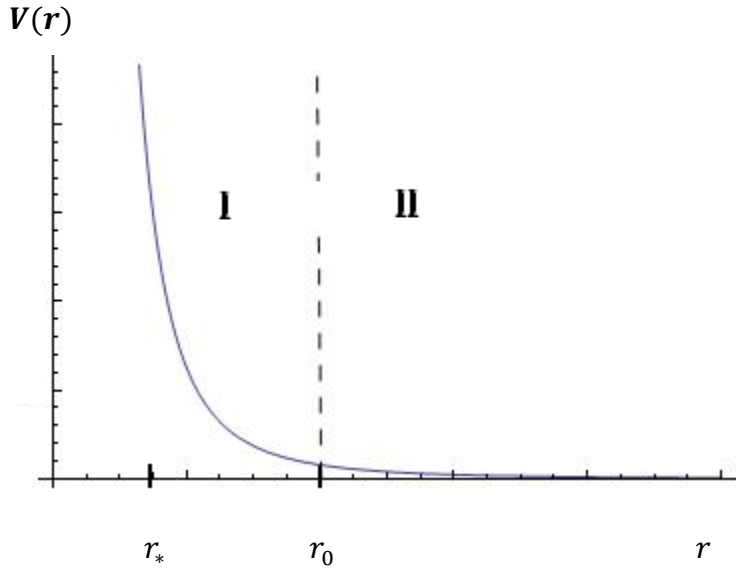


Figure A1. The division of ranges into regions I ($r < r_0$) and II ($r > r_0$).

The two solutions are matched at the artificial distance r_0 which is selected such that $r_* \ll r_0 \ll k^{-1}$. At $r = r_0$, the wave functions and the respective first derivatives must agree

$$\begin{cases} \psi_I(r_0) = \psi_{II}^{(0)}(r_0) \\ \psi_I'(r_0) = \psi_{II}^{(0)\prime}(r_0) \end{cases}, \tag{A28.a}$$

or equivalently by equalizing the logarithmic derivatives at $r = r_0$

$$\frac{\psi_I'(r_0)}{\psi_I(r_0)} = \frac{\psi_{II}^{(0)\prime}(r_0)}{\psi_{II}^{(0)}(r_0)}. \tag{A28.b}$$

Then, using the fact that for $x \ll 1$, we have [322]:

$$\begin{cases} I_0(x) = 1 + \frac{x^2}{4} \\ J_0(x) = 1 - \frac{x^2}{4} \\ N_0(x) = \frac{2}{\pi}\left\{\left(1 - \frac{x^2}{4}\right)\ln\left(\frac{x}{2}\right) + \gamma + \frac{x^2}{4}\right\} \\ K_0(x) = -\left(1 + \frac{x^2}{4}\right)\ln\left(\frac{x}{2}\right) - \gamma + (1-\gamma)\frac{x^2}{4} \end{cases}. \tag{D29}$$

Confining ourselves to the terms up to $\sim r_*$ when using Eq. (A28.b). Then, omitting terms proportional to k^2, we obtain:

$$\tan\widetilde{\delta_0} = \frac{\pi}{2Q} + \frac{\pi}{2Q^2}\frac{r_*}{r_0}\varkappa, \tag{A30}$$

where

$$Q = \ln\left(\frac{kr_d}{2}e^{\gamma}\right)$$

and

$$\varkappa = 2 + 2\ln\left(\frac{r_0}{r_d}\right) + \ln^2\left(\frac{r_0}{r_d}\right)$$

with $r_d = r_* e^{2\gamma - 2A}$.

On the other hand, the contributions to the s-wave scattering phase shift from distance $r > r_0$ should be included perturbatively. In this region, to first order in $V(r)$, the relative wave function is given by

$$\psi_{II}^{(1)} = \psi_{II}^{(0)} - \int_{r_0}^{\infty} G(r,\acute{r})\, V(\acute{r})\psi_{II}^{(0)}(\acute{r})d^2\acute{r}, \tag{A31}$$

where the Green's function for the free s-wave motion obeys the radial equation:

$$-\frac{\hbar^2}{m}\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} + k^2\right] G(r,\acute{r}) = \frac{\delta(r-\acute{r})}{2\pi r}. \tag{A32}$$

For the normalization of the relative wave function chosen in Eq. (A23), we have

$$G(r,\acute{r}) = -\frac{m}{4\hbar^2}\begin{cases}\psi_{II}^{(0)}(\acute{r})N_0(kr), & r > \acute{r}\\ \psi_{II}^{(0)}(r)N_0(k\acute{r}), & r < \acute{r}\end{cases} \tag{A33}$$

Substituting this Green's function into Eq. (31) and taking the limit $r \to \infty$, for the first-order contribution to the phase shift we have

$$\tan\delta_0 = \tan\widetilde{\delta_0} + \tan\widetilde{\widetilde{\delta_0}}, \tag{A34}$$

where

$$\tan\widetilde{\widetilde{\delta_0}} = -\frac{m}{4\hbar^2}\int_{r_0}^{\infty}\left[\psi_{II}^{(0)}(r)\right]^2 V(r)d^2r$$

$$= -\frac{\pi}{2}r_*\int_{r_0}^{\infty}\frac{\left[\psi_{II}^{(0)}(\acute{r})\right]^2}{r^2}d^2r. \tag{A35}$$

Using the formula

$$\int Z_p(x)\bar{Z}_q(x)\frac{dx}{x} = \frac{Z_{p-1}(x)\bar{Z}_q(x) - \bar{Z}_p(x)\bar{Z}_{q-1}(x)}{p^2-q^2} - \frac{Z_p(x)\bar{Z}_q(x)}{p+q}, \tag{A36}$$

where $Z_p(x)$ and $\bar{Z}_q(x)$ are arbitrary Bessel functions, and integrating by part with the use of Eq.(A27), we obtain

$$\tan\widetilde{\widetilde{\delta_0}} = 2kr_*\left(1 + \frac{\pi^2}{4Q^2}\right) - \frac{\pi}{2}\frac{r_*}{r_0}\varkappa, \tag{A37}$$

The sum $\tan\widetilde{\delta_0}$ and the first order contribution give

$$\tan\delta_0 = \frac{\pi}{2Q} + 2kr_*\left(1 + \frac{\pi}{4Q^2}\right). \tag{A38}$$

2.2.Scattering with $|l| > 1$

The presence of strong anomalous s-wave scattering, i.e., the scattering from interparticle distances$\sim 1/k$, originates from the slow $1/r^3$ decay of the potential $V(r)$ at large r. The strong anomalous scattering is also present for partial waves with higher *l*. In this section, we follow the same method as in the case of the *s*-wave scattering and calculate the amplitude of the *l*-wave scattering with$|l| > 1$. For simplicity, we consider positive *l*, having in mind that the scattering amplitude and phase shift depend only on$|l|$.

To zero order in $V(r)$, the wave function of the l wave relative motion at large distances $r > r_0$ is written

$$\psi_{l\,II}^{(0)}(r) = J_l(kr) - \tan\delta_l\, N_l(kr), \tag{A39}$$

where $\delta_l(k)$ is the l-wave scattering phase shift coming from nthe interaction at distances $r < r_0$. We then match $\psi_{l\,II}^{(0)}(r)$ at $r = r_0$, with the short-distance wave function $\psi_{l\,I}(r)$, which follows from the Schrödinger equation for the l-wave relative motion in the potential $V(r)$ at $k = 0$. This immediately gives a relation,

$$\tan\delta_l\,(k) = \frac{kJ_l'(kr_0) - \varpi_l J_l(kr_0)}{kN_l'(kr_0) - \varpi_l N_l(kr_0)}, \tag{A40}$$

where the momentum-independent quantity ϖ_l is the logarithmic derivative of $\psi_{l\,I}(r)$ at $r = r_0$. Since we have the inequality $kr_0 < 1$, the arguments of the Bessel functions in Eq. (A40) are small and they reduce to $J_l(x) \sim x^l$ and $N_l(x) \sim x^{-l}$. This leads to $\tan\delta_l\,(k) \sim (kr_0)^{2l}$.

Then, as for the s-wave scattering, we calculate the contribution to the phase shift from distances $r > r_0$ by considering the potential $V(r)$ as perturbation. To first order in $V(r)$, at $r > r_0$, we have similar expression as Eq. (A35) for the relative wave function of the l-wave motion. Following the same method as in the case of the s-wave scattering and retaining only the terms up to k, for the first-order phase shift, we have

$$\begin{aligned}\tan\delta_l &= -\frac{m}{4\hbar^2}\int_{r_0}^{\infty}\left[\psi_{II}^{(0)}(\acute{r})\right]^2 V(r)d^2r,\\ &\simeq -\frac{\pi kr_*}{2}\int_{kr_0}^{\infty}\frac{J_l^2(x)}{x^2}dx = -\frac{2kr_*}{4l^2-1},\end{aligned} \tag{A41}$$

Now for identical bosons, the full scattering amplitude $f_l = -\frac{4\hbar^2}{m}\tan\delta_l$, can be obtained by making summation over all partial amplitudes with even l.

$$f = -\frac{\hbar^2}{m}\left[\frac{4\pi}{\mathrm{Q}} + 2\pi kr_*\left(1 + \frac{1}{4\mathrm{Q}^2}\right)\right]. \tag{A42}$$

We then omit the term proportional to kr_*/Q^2 and notice that in quasi2D we have

$$r_d = l_0 e^{-\frac{l_0}{\sqrt{2\pi}a}}, \tag{A43}$$

where $l_0 = \sqrt{\hbar/m\omega_z}$ is the oscillator length.

Substituting this equation into Eq.(A42), one finds

$$f(k) = \frac{\hbar^2}{m}\left(\frac{2\sqrt{2}\pi a}{l_0} - 2\pi kr_*\right). \tag{D44}$$

In the quasi2D geometry the short range constant $g = g_{3D}/\sqrt{2}l_0$, where $g_{3D} = 4\pi\hbar^2 a/m$. Assuming that $C = 2\pi\hbar^2 r_*/mg$. We get straightforwardly the result (2.4) employed in chapter 2 of Part II

$$f(k) = g(1 - Ck), \tag{A45}$$

Strictly speaking, in order to express the coupling strength in terms of the scattering amplitude we need the off-shell scattering amplitude. However, since we employ the Bogoliubov approach, the coupling strength in front of the Hamiltonian terms $\hat{a}_{\boldsymbol{k}}^{+}\hat{a}_{\boldsymbol{k}}$, $\hat{a}_{\boldsymbol{k}}\hat{a}_{-\boldsymbol{k}}$ and $\hat{a}_{-\boldsymbol{k}}^{+}\hat{a}_{\boldsymbol{k}}^{+}$ is nothing than (A45).

It is worth noticing that the off-shell scattering amplitude can be calculated using the first-order Born approximation.

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Variational self-consistent theory for trapped Bose gases at finite temperature

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Abstract. We apply the time-dependent variational principle of Balian-Vénéroni to a system of self-interacting trapped bosons at finite temperature. The method leads to a set of coupled non-linear time dependent equations for the condensate density, the thermal cloud and the anomalous density. We solve numerically these equations in the static case for a harmonic trap. We analyze the various densities as functions of the radial distance and the temperature. We find an overall good qualitative agreement with recent experiments as well as with the results of many theoretical groups. We also discuss the behavior of the anomalous density at low temperatures owing to its importance to account for many-body effects.

1 Introduction

The Bose-Einstein condensation phenomenon was observed in dilute atomic gases for the first time in 1995 [1,2], and now becomes a very active area of research both theoretically and experimentally.

Weakly non-ideal Bose gases theory was pioneered by Bogoliubov [3–8]. The collective excitations turn out to be nicely predicted at and near zero temperature. Although there exist some generalizations to the non uniform case [9], the Bogoliubov approximation is primarily suited for homogeneous gases.

For trapped gases at zero temperature, the Gross-Pitaevskii (GP) equation [10,11] constitutes the best model for studying the properties of Bose-Einstein condensation and provides excellent predictions for relevant experimental observations (see e.g. Dodd et al. [12], Stringari [13], Proukakis et al. [14].) It is however only valid at $T = 0$. Consequently, it ignores both the thermal cloud and the anomalous average and their dynamics.

At finite temperature, the mean-field approximation is intensively used to describe the static and dynamic equilibrium properties of Bose-Einstein condensates. Depending on the regime at hand, different variants and different models do exist. Among them, we can cite in particular the Hartree-Fock-Bogoliubov theory [15–18], the generalized GP equation and the Bogoliubov-de-Gennes (BdG) equations [19]. These theories have been successfully confronted to experiments as they predict correctly, among other things, the collective and single-particle excitations, the condensate fraction and also the transition temperature.

In order to take into account the motion of the condensate coupled to a static thermal cloud, Zaremba, Nikuni and Griffin [20] used the HFB-Popov approximation and the hydrodynamic approach in a kind of generalized mean field approximation. To go beyond, Proukakis [21], using an HFB basis, developed a second order perturbation theory to include the effect of the triplets.

Another kind of extensions has been developed by Stoof [22,23] and Gardiner and Zoller [24]. It is based on the Focker-Planck equation and the quantum optics techniques to derive a kinetic equation for the condensate coupled to a time dependent thermal cloud.

Yukalov [25,26] adopted a quite different formal approach by using the notion of representative statistical ensembles.

The above theories, although being quite satisfactory, suffer from several drawbacks and inconsistencies which restrict their applicability to certain regimes and not to others. For instance, the Stoof, Gardiner-Zoller and Yukalov approaches ignore the dynamics of the anomalous density, despite its well established importance. On the other hand, the HFB approximation, which includes the anomalous average, leads to an unphysical gap in the excitation spectrum, which causes a violation of the Hugenholtz-Pines theorem [27,28] and to UV divergences which require regularization. This has been done by Morgan [29] who implemented a "generalized" HFB approximation (GHFB) by resorting to the many-body T-matrix. It is not however clear how to handle long range correlations which become more and more important as one approaches the critical regime. Moreover, going beyond the two-body contact potential is a cumbersome task in the GHFB approach. On the other hand, the perturbative approach is well suited in this respect

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but suffers from known shortcomings, especially near the critical regime.

In this paper we would like to proceed differently by using the time-dependent variational principle proposed by Balian and Vénéroni (BV) a long time ago [30]. The point is that this principle uses the notion of least biased state, which is the best ansatz compatible with the constraints imposed on the system. For our purposes, we will use a Gaussian density operator. This ansatz is reminiscent of the independent particle approximation and belongs to the class of generalized coherent states. It allows us to perform explicitly all the calculations since there exists a generalization of Wick's theorem to statistical physics. It is important to note however that despite its simple form, it by no means endows any further simplification on the interaction between particles. Indeed, the BV-machinery, together with this trial Gaussian ansatz, lead to a set of coupled time-dependent mean field equations for the condensate, the noncondensate and the anomalous average. We have to mention at this point that the equations that we derive in this paper are quite general and fully consistent as they do not require any simplifying assumption on the thermal cloud or the anomalous density. They may provide in this sense a kind of generalization to the previously discussed approximations, valid however, in the collisionless regime.

In their simplest (local) form, these equations have been derived elsewhere [31,32] and labeled TDHFB for Time Dependent Hartree-Fock-Bogoliubov. In the latter reference, these equations were solved numerically in the static case under the assumption that the spatial variations of the anomalous average were relatively small (which leads to a sort of finite temperature generalization of the Thomas-Fermi approximation). Although the results were quite satisfactory, at least on the qualitative level, there remained many unanswered questions. In particular, the thermal and anomalous density profiles seem to have no structure at the center of the trap. This is in contradistinction with what was found in the literature [18,19] (where the HFB-BdG approximation was used), and where these densities are found to have "holes". On the other hand, a recent experiment [33] seems to indicate that the Gaussian shape of the thermal cloud is maintained, therefore confirming the absence of structure near the center of the trap.

Hence, solving the full TDHFB equations, without any simplifying assumption, is of great interest in order to understand if the absence of these holes is an artifact of the finite temperature Thomas-Fermi approximation one adopted previously, or is a general prediction of the TDHFB approximation as a whole. In the latter case, one has to conclude definitely in favor of the predictions of the TDHFB approximation.

The paper is organized as follows. In Section 2, we review the main steps used to derive the TDHFB equations from the Balian-Vénéroni variational principle. In Section 3, the TDHFB equations are applied to a trapped Bose gas to derive a coupled dynamics of the condensate, the non condensate and the anomalous densities. We then restrict to the local densities and discuss the properties of the underlying equations, their relevance to the finite temperature case as well as their relations with other known approximations such as the Bogoliubov-De Gennes equations. In Section 4, we present the static equations and the physical boundary conditions relevant to the trapped Bose gas. Section 5 is devoted to the discussion of the numerical results, where we analyze the various density profiles. We confront our results with the HFB-BdG predictions and with recent experiments. Furthermore, owing to its importance to account for many-body effects, we focus on the behavior of the anomalous density for different temperatures. In Section 6, we draw our conclusions and present some perspectives.

2 The variational TDHFB equations

The time-dependent variational principle of Balian and Vénéroni requires first the choice of a trial density operator. In our case, we will consider a Gaussian time-dependent density operator. This ansatz which belongs to the class of the generalized coherent states allows us to perform the calculations since there exists a Wick's theorem, while retaining some fundamental aspects such as the pairing between atoms.

The Gaussian density operator $D(t)$ is completely characterized by the partition function $Z(t) = \mathrm{Tr}D(t)$, the one-boson field expectation values $\langle\Psi\rangle(\vec{r},t) = \mathrm{Tr}\Psi(\vec{r})D(t)/Z(t)$, $\langle\Psi^+\rangle(\vec{r},t) = \mathrm{Tr}\Psi^+(\vec{r})D(t)/Z(t)$ and the single-particle density matrix $\rho(\vec{r},\vec{r}',t)$ defined as

$$\rho((\vec{r},\vec{r}',t) = \begin{pmatrix} \langle\overline{\Psi}^+(\vec{r}')\overline{\Psi}(\vec{r})\rangle & -\langle\overline{\Psi}(\vec{r}')\overline{\Psi}(\vec{r})\rangle \\ \langle\overline{\Psi}^+(\vec{r}')\overline{\Psi}^+(\vec{r})\rangle & -\langle\overline{\Psi}(\vec{r})\overline{\Psi}^+(\vec{r}')\rangle \end{pmatrix}. \quad (2.1)$$

In the preceding definitions, $\Psi(\vec{r})$ and $\Psi^+(\vec{r})$ are the boson destruction and creation field operators (in the Schrödinger representation) satisfying the usual canonical commutation rules

$$\left[\Psi(\vec{r}),\Psi^+(\vec{r}')\right] = \delta(\vec{r}-\vec{r}'), \quad (2.2)$$

and $\overline{\Psi}(\vec{r}) = \Psi(\vec{r}) - \langle\Psi(\vec{r})\rangle$ and $\overline{\Psi}^+(\vec{r}) = \Psi^+(\vec{r}) - \langle\Psi^+(\vec{r})\rangle$ are the corresponding centered operators.

Upon introducing these variational parameters into the BV principle, one obtains

$$\begin{aligned} i\frac{\partial\langle\Psi\rangle}{\partial t}(\vec{r},t) &= \frac{\partial E}{\partial\langle\Psi^+\rangle(\vec{r},t)}, \\ i\frac{\partial\langle\Psi^+\rangle}{\partial t}(\vec{r},t) &= -\frac{\partial E}{\partial\langle\Psi\rangle(\vec{r},t)}, \\ i\frac{\partial\rho}{\partial t}(\vec{r},\vec{r}',t) &= -2\left[\rho,\frac{\partial E}{\partial\rho}\right](\vec{r},\vec{r}',t), \end{aligned} \quad (2.3)$$

where $E = \langle H\rangle$ is the mean-field energy. These equations were also derived in [34]. Let us discuss some of their general properties. We note first that the mean-field energy E is conserved when the Hamiltonian H does not

depend explicitly on time. Another property is the unitary evolution of the s.p. density matrix ρ, which means that the eigenvalues of ρ are conserved. This implies in particular the conservation of the von-Neumann entropy $S = -\mathrm{Tr} D \log D$ and the fact that an initially pure state, satisfying $\rho(\rho+1)=0$, remains pure during the TDHFB evolution. The conservation of the free energy $F = E - TS$ naturally follows. These conservation laws show that the TDHFB equations reproduce, in the single-particle space, the exact properties of the system [34].

3 Application of the TDHFB formalism to trapped Bose gases

Let us apply the previous equations (2.3) to a system of trapped bosons interacting via a two-body potential. The grand canonical Hamiltonian may be written in the form

$$H = \int_{\vec{r}} \Psi^{+}(\vec{r}) \left[-\frac{\hbar^2}{2M}\Delta + V_{ext}(\vec{r}) - \mu \right] \Psi(\vec{r}) + \frac{1}{2} \int_{\vec{r},\vec{r}'} \Psi^{+}(\vec{r}) \Psi^{+}(\vec{r}') V(\vec{r},\vec{r}') \Psi(\vec{r}') \Psi(\vec{r}'), \quad (3.1)$$

where $V\left(\vec{r},\vec{r'}\right)$ is the interaction potential, $V_{ext}(\vec{r})$ the external confining field and μ the chemical potential. For the sake of clarity, we will omit to write explicitly the time dependence whenever evident. Next, we introduce the order parameter $\Phi(\vec{r}) = \langle \Psi(\vec{r}) \rangle$ and the non-local densities

$$\tilde{n}(\vec{r},\vec{r}') \equiv \tilde{n}^{*}(\vec{r},\vec{r}') = \langle \Psi^{+}(\vec{r}) \Psi(\vec{r}') \rangle - \Phi^{*}(\vec{r}) \Phi(\vec{r}'),$$
$$\tilde{m}(\vec{r},\vec{r}') \equiv \tilde{m}(\vec{r}',\vec{r}) = \langle \Psi(\vec{r}) \Psi(\vec{r}') \rangle - \Phi(\vec{r}) \Phi(\vec{r}'). \quad (3.2)$$

where we note that $\tilde{n}(\vec{r},\vec{r}) \equiv \tilde{n}(\vec{r})$ and $\tilde{m}(\vec{r},\vec{r}) \equiv \tilde{m}(\vec{r})$ are respectively the non condensate and the anomalous densities. The energy may be readily computed to yield

$$\begin{aligned} E = & \int_{\vec{r}} h^{sp}(\vec{r}) \left[\tilde{n}(\vec{r},\vec{r}) + \Phi(\vec{r}) \Phi^{*}(\vec{r}) \right] \\ & + \int_{\vec{r},\vec{r}'} V(\vec{r},\vec{r}') |\Phi(\vec{r})|^2 |\Phi(\vec{r}')|^2 \\ & + \frac{1}{2} \int_{\vec{r},\vec{r}'} V(\vec{r},\vec{r}') \left[\tilde{m}^{*}(\vec{r},\vec{r}') \tilde{m}(\vec{r},\vec{r}') \right. \\ & \left. + \tilde{n}(\vec{r},\vec{r}') \tilde{n}(\vec{r}',\vec{r}) + \tilde{n}(\vec{r},\vec{r}) \tilde{n}(\vec{r}',\vec{r}') \right] \\ & + \frac{1}{2} \int_{\vec{r}\vec{r}'} V(\vec{r},\vec{r}') \left[\tilde{n}(\vec{r},\vec{r}') \Phi(\vec{r}) \Phi^{*}(\vec{r}') \right. \\ & + \tilde{n}(\vec{r}',\vec{r}) \Phi^{*}(\vec{r}) \Phi(\vec{r}') + \tilde{n}(\vec{r},\vec{r}) \Phi(\vec{r}') \Phi(\vec{r}') \\ & \left. + \tilde{n}(\vec{r}',\vec{r}') \Phi(\vec{r}) \Phi(\vec{r}) \right] + \frac{1}{2} \int_{\vec{r},\vec{r}'} V(\vec{r},\vec{r}') \\ & \times \left[\tilde{m}^{*}(\vec{r},\vec{r}') \Phi(\vec{r}) \Phi(\vec{r}') + \tilde{m}(\vec{r},\vec{r}') \Phi^{*}(\vec{r}) \Phi^{*}(\vec{r}') \right]. \end{aligned} \quad (3.3)$$

In equation (3.3), $h^{sp} = -\frac{\hbar^2}{2M}\Delta + V_{ext}(\vec{r}) - \mu$ is the single particle Hamiltonian.

Now, one inserts the expression (3.3) in the general equations of motion (2.3) to get the explicit form of the TDHFB equations for a trapped Bose gas:

$$\begin{aligned} i\hbar\dot{\Phi}(\vec{r}) = & h^{sp}(\vec{r}) \Phi(\vec{r}) + \int_{\vec{r}'} V(\vec{r},\vec{r}') \left[|\Phi(\vec{r}')|^2 \Phi(\vec{r}) \right. \\ & + \Phi^{*}(\vec{r}') \tilde{m}(\vec{r},\vec{r}') + \Phi(\vec{r}') \tilde{n}(\vec{r},\vec{r}') \\ & \left. + \Phi(\vec{r}) \tilde{n}(\vec{r}',\vec{r}') \right], \end{aligned} \quad (3.4a)$$

$$\begin{aligned} i\hbar\dot{\tilde{n}}(\vec{r},\vec{r}') = & \left[h^{sp}(\vec{r}) - h^{sp}(\vec{r}') \right] \tilde{n}(\vec{r},\vec{r}') + \int_{\vec{r}''} V(\vec{r}',\vec{r}'') \\ & \times \left[a(\vec{r}'',\vec{r}') \tilde{n}(\vec{r},\vec{r}'') + a(\vec{r}'',\vec{r}'') \tilde{n}(\vec{r},\vec{r}') \right. \\ & \left. + b(\vec{r}',\vec{r}'') \tilde{m}(\vec{r}'',\vec{r}) \right] - \int_{\vec{r}''} V(\vec{r}',\vec{r}'') \\ & \times \left[a(\vec{r},\vec{r}'') \tilde{n}(\vec{r}'',\vec{r}) + a(\vec{r}'',\vec{r}'') \tilde{n}(\vec{r},\vec{r}') \right. \\ & \left. + b(\vec{r},\vec{r}'') \tilde{m}(\vec{r}'',\vec{r}') \right], \end{aligned} \quad (3.4b)$$

$$\begin{aligned} i\hbar\dot{\tilde{m}}(\vec{r},\vec{r}') = & \left[h^{sp}(\vec{r}) + h^{sp}(\vec{r}') \right] \tilde{m}(\vec{r},\vec{r}') + \int_{\vec{r}''} V(\vec{r}',\vec{r}'') \\ & \times \left[a(\vec{r}'',\vec{r}') \tilde{m}(\vec{r},\vec{r}'') + a(\vec{r}'',\vec{r}'') \tilde{m}(\vec{r},\vec{r}') \right. \\ & \left. + b(\vec{r}',\vec{r}'') \left(\tilde{n}^{*}(\vec{r},\vec{r}'') + \delta(\vec{r}-\vec{r}'') \right) \right] \\ & + \int_{\vec{r}''} V(\vec{r}',\vec{r}'') \left[a(\vec{r}'',\vec{r}) \tilde{m}(\vec{r}',\vec{r}'') \right. \\ & \left. + a(\vec{r}'',\vec{r}'') \tilde{m}(\vec{r},\vec{r}') + b(\vec{r},\vec{r}'') \tilde{n}(\vec{r}'',\vec{r}') \right]. \end{aligned} \quad (3.4c)$$

In equations (3.4), the dots denote time derivatives and we have introduced the quantities

$$a(\vec{r},\vec{r}') = \tilde{n}(\vec{r},\vec{r}') + \Phi^{*}(\vec{r}) \Phi(\vec{r}'),$$
$$b(\vec{r},\vec{r}') = \tilde{m}(\vec{r},\vec{r}') + \Phi(\vec{r}) \Phi(\vec{r}'). \quad (3.5)$$

It is worth noticing that similar equations have been derived elsewhere using quite different approaches. For instance, Stoof [35] used a variational plus perturbative effective action, Proukakis [21] a truncation of the Heisenberg equations and Chernyak et al. [36] the generalized coherent state representation. The latter approach yields equations very close to ours, but the authors did not pursue further their analysis. In particular, an important diverging term in their equations was completely ignored. In our case, this term appears in equation (3.4c) and becomes highly non trivial when considers the contact potential. This is precisely the term which leads to UV- divergences in the anomalous density [19] and which requires a regularization. We do this by a very natural recipe which consists in defining the renormalized anomalous average by

$$\tilde{m}(\vec{r},\vec{r}') = \tilde{m}_R(\vec{r},\vec{r}') + \frac{1}{i\hbar} \int_{t} b(\vec{r},\vec{r}',t) \delta(\vec{r}-\vec{r}'), \quad (3.6)$$

and replacing $\tilde{m}(\vec{r},\vec{r}')$ by $\tilde{m}_R(\vec{r},\vec{r}')$ wherever it appears. This time-dependent renormalization turns out to be quite similar to the static regularization scheme introduced by Morgan [29] and also to the rigorous derivation of Olshanii and Pricoupenko [28,37] based on the pseudo-potential method. In what follows, we will omit the index "R" and simply write $\tilde{m}$ instead of $\tilde{m}_R$.

Equations (3.4) remain complicated even for a contact potential. To proceed further, and by the same way, to investigate the behavior of the various density profiles, we will change to a local representation by taking the limit $\vec{r}' \to \vec{r}$. We further consider the contact potential $V(\vec{r},\vec{r}') = g\delta(\vec{r}-\vec{r}')$, where g is related to the s-wave scattering length a by $g = 4\pi\hbar^2 a/M$. For an isotropic trap, and due to the spherical symmetry, equations (3.4) become

$$\begin{aligned}
i\hbar\dot{\Phi}(r) &= \left(-\frac{\hbar^2}{2M}\Delta + V_{ext}(r) - \mu + gn_c(r) + 2g\tilde{n}(r)\right) \\
&\quad \times \Phi(r) + g\tilde{m}(r)\Phi^*(r), \\
i\hbar\dot{\tilde{m}}(r) &= g\left(2\tilde{n}(r)+1\right)\Phi^2(r) + 4\Bigg(-\frac{\hbar^2}{2M}\Delta + V_{ext}(r) \\
&\quad - \mu + 2gn(r) + \frac{g}{4}\left(2\tilde{n}(r)+1\right)\Bigg)\tilde{m}(r), \\
i\hbar\dot{\tilde{n}}(r) &= g\left(\tilde{m}^*(r)\Phi^2(r) - \tilde{m}(r)\Phi^{*2}(r)\right), \qquad (3.7)
\end{aligned}$$

where $n_c(r) = |\Phi(r)|^2$ is the condensate density and $n(r)$ the total density $n(r) = n_c(r) + \tilde{n}(r)$.

It is important to note that equations (3.7) are not totally independent. Indeed, $\tilde{n}$ and $\tilde{m}$ are related by the equality

$$(1+2\tilde{n})^2 - |2\tilde{m}|^2 = I, \qquad (3.8)$$

where I is the Heisenberg parameter. At thermal equilibrium, it is related to the temperature by $\sqrt{I} = 1+2f_B(E)$, where f_B is the Bose-Einstein distribution for a system of energy E. Hence, at $T=0$, $I=1$. As it stands, I describes the degree of mixing of the system. It indeed satisfies the continuity equation

$$\frac{\partial I}{\partial t} + \vec{\nabla}\cdot\vec{J}_I = 0, \qquad (3.9)$$

where the current density is $\vec{J}_I = -\frac{2i\hbar}{M}(\tilde{m}^*\vec{\nabla}\,\tilde{m} - \tilde{m}\vec{\nabla}\tilde{m}^*)$. The deviation from the pure state situation ($I=1$) is therefore mainly controlled by the anomalous density. This result shows that neglecting $\tilde{m}$ while maintaining $\tilde{n}$ will necessarily lead to inconsistencies when talking about the mixing of the condensed and non-condensed phases. Furthermore, the total density also obeys a continuity equation of the form

$$\frac{\partial n}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0, \qquad (3.10)$$

where $\vec{J} = -\frac{i\hbar}{2M}\left(\Phi^*\vec{\nabla}\Phi - \Phi\vec{\nabla}\Phi^*\right)$, which leads to the conservation of the total number of atoms $N = \int_{\vec{r}} n(r)$. It is also interesting to observe here that even at finite temperature, there is no current associated with the thermal cloud.

Let us now turn to discuss the relationship between our TDHFB equations (3.7) and the HFB-De Gennes equations [18,19]. In fact, we may easily show that upon linearizing the first equation in (3.7) around a static solution, we obtain

$$i\hbar\delta\dot{\Phi} = \left(h^{sp} + 2gn\right)\delta\Phi + g\left(\tilde{m} + \Phi^2\right)\delta\Phi^*. \qquad (3.11)$$

Using the parameterization $\delta\Phi = \sum_p (u_p e^{-i\hbar\omega_p t} - v_p e^{i\hbar\omega_p t})$ in which ω_p are the quasi-particle frequencies and u_p and v_p the quasi-particle amplitudes, we get from (3.11) the HFB-BdG equations:

$$\begin{aligned}
\varepsilon_p u_p &= \left(h^{sp} + 2gn\right)u_p - g\left(n_c + \tilde{m}\right)v_p, \\
-\varepsilon_p v_p &= \left(h^{sp} + 2gn\right)v_p - g\left(n_c + \tilde{m}\right)u_p. \qquad (3.12)
\end{aligned}$$

Hence, the HFB-BdG equations found in the literature are just the random phase approximation to the first of our equations (3.7), which are therefore more general since the two last equations in (3.7) have no analogues in the HFB formalism.

4 The static TDHFB equations

The static TDHFB equations are obtained by setting to zero the right hand sides of (3.7). For numerical purposes, it is convenient to start our treatment with the dimensionless form of the set (3.7). Let us consider a spherical trap with frequency ω, $V_{ext}(r) = \frac{1}{2}m\omega^2 r^2$ and use the harmonic oscillator length $a_{\rm HO} = \sqrt{\hbar/m\omega}$, as well as $a_{\rm HO}^{-3}$ and $\hbar\omega$ as units of length, density and energy respectively. The dimensionless radial distance is $q = r/a_{\rm HO}$. The dimensionless condensed, non-condensed and anomalous densities are respectively $\hat{n}_c = a_{\rm HO}^3 n_c$, $\hat{\tilde{n}} = a_{\rm HO}^3\tilde{n}$ and $\hat{\tilde{m}} = a_{\rm HO}^3\tilde{m}$. Therefore, $\hat{n} = \hat{n}_c + \hat{\tilde{n}}$ is the dimensionless total density. However, in order to avoid the appearance of first order spatial derivatives in the final equations (which are always cumbersome in a numerical treatment), it is preferable to introduce a dimensionless "order parameter" $\hat{\Psi} = q\hat{n}_c$ and a dimensionless "anomalous density" $\hat{\chi} = q\hat{\tilde{m}}$. With these definitions, the static equations corresponding to (3.7) write as:

$$\begin{aligned}
&\left(-\frac{d^2}{dq^2} + q^2 - \nu + 8\pi\frac{a}{a_{\rm HO}}\left(\frac{\hat{\Psi}^2}{q^2} + 2\hat{\tilde{n}} + \frac{\hat{\chi}}{q}\right)\right)\hat{\Psi} = 0, \\
&\left(-\frac{d^2}{dq^2} + q^2 - \nu + 8\pi\frac{a}{a_{\rm HO}}\left(2\hat{n} + \frac{2\hat{\tilde{n}} + \hat{V}^{-1}}{4}\right)\right)\hat{\chi} \\
&\qquad + 8\pi\frac{a}{a_{\rm HO}}\left(\frac{2\hat{\tilde{n}} + \hat{V}^{-1}}{4}\right)\frac{\hat{\Psi}^2}{q} = 0, \qquad (4.1)
\end{aligned}$$

where $\hat{V} = V/a_{\rm HO}^3$ is the normalized volume and we have introduced the dimensionless chemical potential

$\nu = \mu/\frac{1}{2}\hbar\omega$. We have deliberately omitted the third equation in (3.7) since it is of no interest for our purposes. Indeed, the quantity $\hat{\tilde{n}}$ is determined via the relation (3.8) which becomes in our units

$$\hat{\tilde{n}} = \frac{1}{2}\left[\left(I + 4\frac{\hat{\chi}^2}{q^2}\right)^{1/2} - 1\right]. \tag{4.2}$$

The atom-atom interaction is now completely specified by the parameter $a/a_{\rm HO}$. The normalization condition writes in these new units as $\int d^3q\hat{n}\,(q) = N$, where N is the total number of atoms.

As one notes from (4.1), the problem becomes formally one-dimensional. Its solution requires a set of boundary conditions as $r \to \infty$. We have therefore to determine the asymptotic behavior of Φ and $\tilde{m}$ or equivalently $\hat{\Psi}$ and $\hat{\chi}$. To this end, we note first that for a confined gas, Φ and $\tilde{m}$ must vanish at infinity. However, these boundary conditions are numerically useless since they always lead to the trivial solution. Hence, it is preferable to solve the equations (4.1) in the asymptotic region (where the non linear terms can be neglected) and then to consider these asymptotic solutions as boundary conditions for the problem (4.1). In the region $q \to \infty$, the two equations in (4.1) become identical and lead to the same generic solution: $\hat{\Psi} \approx \hat{\chi} \approx q\exp(-q^2)$.

Next we discretize the set of equations (4.1) by using a finite difference scheme with step h. The chemical potential must be computed self-consistently in order to ensure the normalization condition. One may associate with the algorithm a gradient method, which searches for the best value of ν that satisfies the previous condition. However, this procedure is rather slowly converging and we prefer instead to use a more intuitive and less expensive technique. The idea is to start our calculations for $a/a_{\rm H0} \ll 1$, in which case we know that the value of ν is very close to that of the ideal gas, namely $\nu = 3$ (or $\mu = \frac{3}{2}\hbar\omega$). By gradually increasing the ratio $a/a_{\rm H0}$, we may correspondingly determine ν.

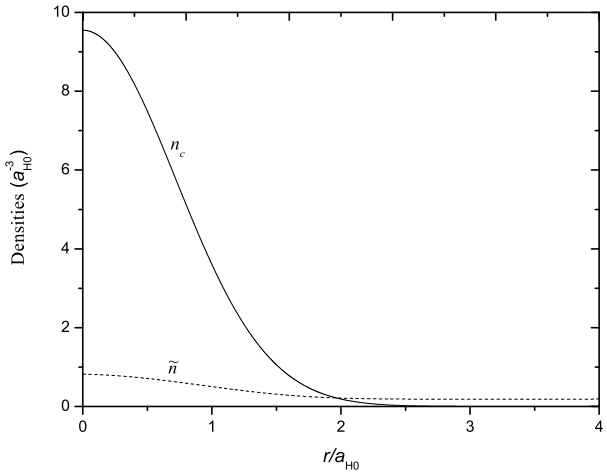

Fig. 1. The condensate (solid) and non-condensate (dashed) densities versus the radial distance (in units of $a_{\rm H0}$) for: $a/a_{\rm H0} = 7.64 \times 10^{-3}$, $N = 2000$ atoms and $N_c/N = 85\%$.

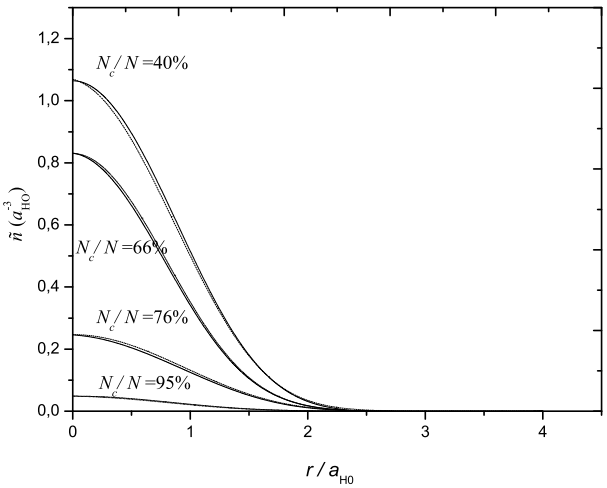

Fig. 2. The non-condensate density versus the radial distance for various condensate fractions, $a/a_{\rm H0} = 7.64\times10^{-3}$ and $N =$ 2000 atoms. Solid: our result; dashed: the ideal gas result.

5 Numerical results

To illustrate our formalism at finite temperature, we consider the ^{87}Rb gas with $a/a_{\rm H0} = 7.64 \times 10^{-3}$ and $N =$ 2000 atoms.

We begin by plotting the condensate, the non condensate and the anomalous densities as functions of the radial distance for several values of the condensate fraction N_c/N and hence of the temperature. Densities and lengths are measured in units of $a_{\rm HO}^{-3}$ and $a_{\rm HO}$ respectively.

In Figure 1, we show the two components of the gas at low temperature. We notice that the non condensate density is rather small compared to the condensate density, since in this range of temperature, almost all the atoms are condensed in the center of the trap. We also observe that the thermal cloud has a larger tail compared to the condensate. This image illustrates clearly the fact that the condensate is surrounded by the thermal cloud. The previous results have also been obtained by several authors, see e.g. [18,19,38].

In Figure 2, we see that the non-condensate density is increasing significantly with decreasing condensate fraction. Furthermore, it is quite interesting to observe that the ideal gas model (dashed line) is still a good approximation.

In Figure 3, we compare our non condensate density with the one predicted by the HFB-BdG equations. What is important to note here is that we clearly disagree with the HFB-BdG calculations [19]. The discrepancies are more pronounced near the center of the trap, where the HFB-BdG approximation predicts a hole. On the other hand, our result is in accordance with the experiments of references [33,39], where no special structure is observed near the center and where the Gaussian shape of the thermal cloud seems to be maintained. These observations

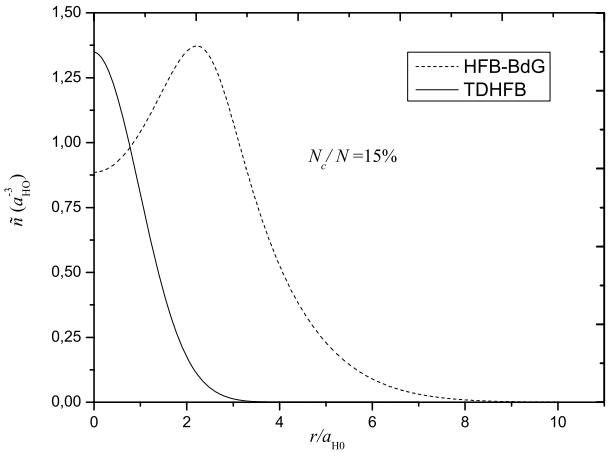

Fig. 3. The non-condensate density versus the radial distance for $N_c/N = 15\%$, $a/a_{H0} = 7.64 \times 10^{-3}$ and $N = 2000$ atoms. Solid: our result; dashed: HFB-BdG.

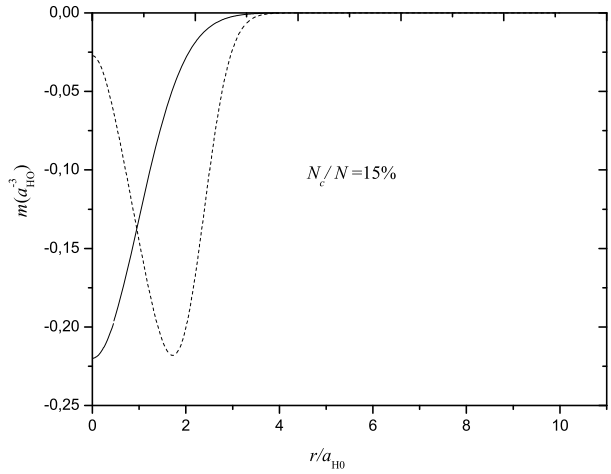

Fig. 4. The anomalous density versus the radial distance for $N_c/N = 15\%$, $a/a_{H0} = 7.64 \times 10^{-3}$ and $N = 2000$ atoms. Solid: our result; dashed: HFB-BdG.

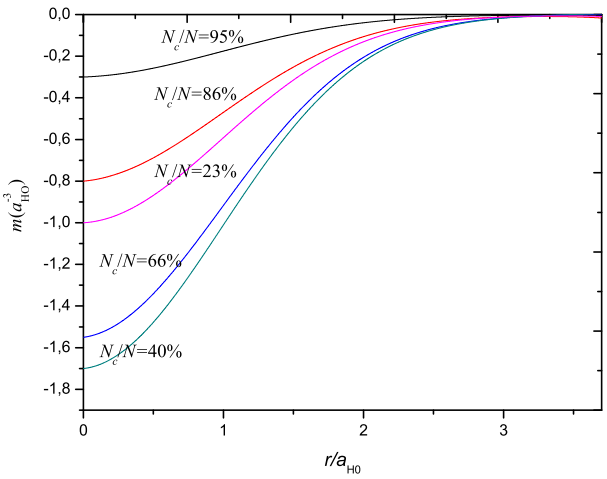

Fig. 5. (Color online) The anomalous density versus the radial distance for various condensate fractions, $a/a_{H0} = 7.64 \times 10^{-3}$ and $N = 2000$ atoms.

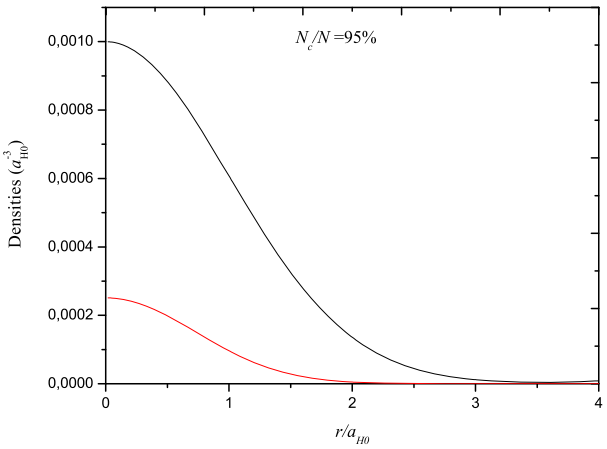

Fig. 6. (Color online) The absolute value of the anomalous density (black) and the non condensate density (red) vs. the radial distance for $N_c/N = 95\%$.

may be extended to the anomalous average. Indeed, we see in Figure 4 that our results are again in clear disagreement with the HFB-BdG approximation which also predicts a hole in the center while we predict a Gaussian shape.

Figure 5 depicts the anomalous density for varying condensation fraction. We notice that by decreasing N_c/N, $\tilde{m}$ begins to increase in absolute value then decreases when N_c/N approaches 50%. This overall behavior has also been obtained in [18,19]. Therefore, our calculations predict no special structure of $\tilde{n}$ and $\tilde{m}$ near the center and a monotonic behavior from the center to the edges of the trap. In fact, $\tilde{m}$ is still ill known and an experiment (although highly non trivial) focusing on this quantity would be welcome in the future.

Figures 6–8 compare the absolute value of the anomalous density $|\tilde{m}|$ (in black) and the non condensate density $\tilde{n}$ (in red). We observe that at high condensate fraction (that is at very low temperatures), for instance at $N_c/N = 95\%$, $|\tilde{m}|$ is greater than $\tilde{n}$, although both are very small. For $N_c/N \approx 50\%$ (Fig. 7), the anomalous density is comparable to the thermal cloud and at low enough condensate fraction (Fig. 8), the anomalous density becomes much smaller than the non condensate density. Hence, we may infer from that that the anomalous density plays a central role at low temperatures. It is therefore highly unlikely to neglect it for $T \ll T_c$. These observations are consistent with the results of Yukalov [25,26,40–42].

6 Conclusions and perspectives

By using a Gaussian density operator, we derive from the time-dependent variational principle of Balian-Vénéroni a set of coupled equations of motion for a self-interacting trapped Bose gas. These equations govern in a self-consistent way the dynamics of the condensate, the

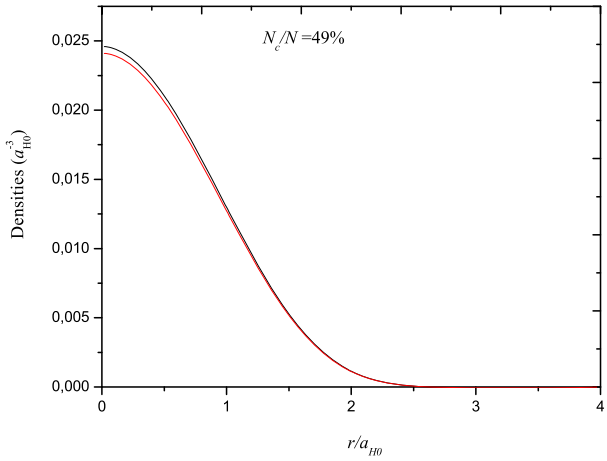

Fig. 7. (Color online) Same as Figure 6 for $N_c/N = 49\%$.

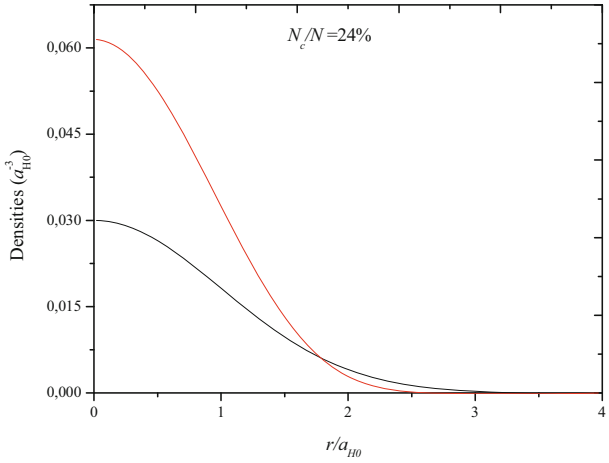

Fig. 8. (Color online) Same as Figure 6 for $N_c/N = 24\%$.

thermal cloud and the anomalous average. Our time dependent Hartree-Fock-Bogoliubov (TDHFB) equations generalize in a natural way many of the famous approximations found in the literature such as the Bogoliubov, the Gross-Pitaevskii, the Popov, the Beliaev and the Bogoliubov-de Gennes equations.

In order to apprehend better the advantages of our approach, we solve numerically the static TDHFB equations in the local limit for a contact potential and a harmonic trap. The outcomes of our numerical explorations are the following. First of all, the numerical resolution of our equations is relatively easy and is not as time-consuming as the HFB-BdG calculations especially for large atom numbers. For instance, the latter cannot be handled correctly as soon as $N \sim 10^4 - 10^5$. By contrast, there are no such limitations in our case. Secondly, although we obtain for the condensate density a quite good agreement with the literature and with the experiments, our predicted thermal cloud and anomalous average differ substantially from the HFB-BdG results especially near the center of the trap. Indeed, we obtain Gaussian shapes for both densities while the HFB-BdG calculations predict "holes" (that is local minima) near the center. These holes are absent (at least concerning $\tilde{n}$) in the experiments of Gerbier et al. and Caracanhas et al. We recall that the HFB-BdG numerical calculations have been performed for a reduced atom number ($N \sim 2000$). The question that naturally arises is whether these holes may disappear for large atom numbers. In fact, a preliminary HFB-BdG calculation seems to confirm this conclusion. We plan to publish more details in the near future [43].

On the other hand, owing to its importance to account for many-body effects, we have analyzed the behavior of the anomalous density. We recover a well-known prediction of HFB-BdG since $\tilde{m}$ increases with the temperature and then decreases as one approaches the transition. Moreover, we show that at low temperatures, the anomalous density is greater than the non condensate density, although both are very small. The former necessarily plays a major role in the condensation phenomenon. Any approach neglecting the anomalous average at low temperatures will inevitably lead to inconsistencies [40–42].

Finally, as for any variational approach, one has to discuss the relevance of the trial space for the problem at hand and how to extend it in order to take into account many important effects which we did not deal with in this paper. Among the most important phenomena, we can cite in particular the effect of the inclusion of the triplets, the damping of the excitations (Landau and Beliaev) and the particle exchange. While the former may be easily handled by the "post-Gaussian" approximation, the two latter require dissipative effects which are totally absent in the present formalism since the von-Neumann entropy is conserved.

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Thermodynamics of a trapped Bose gas at low temperature: Departure from the Thomas-Fermi regime

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Abstract

We apply the finite temperature Thomas-Fermi (TF) approximation by using the Time dependent Hartree-Fock-Bogoliubov equations. The exploration of these equations at finite temperature leads to the fact that all the thermodynamics quantities deviate from the standard values in the TF regime

Keywords: Bose-Einstein condensation; variational equations; TDHFB; Thomas-Fermi .

1. Introduction

Our starting point is the Time Dependent Hartree-Fock-Bogoliubov (TDHFB) equations, which were derived in [1] using the Ballian-Vénéroni (BV) variational principle [2]. For a Hamiltonian *H* of the type:

$$H = \int_{\vec{r}} \psi^{+}(\vec{r}) \left[-\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(r) - \mu \right] \psi(\vec{r}) + \frac{g}{2}\int_{\vec{r}} \psi^{+}(\vec{r})\psi^{+}(\vec{r})\psi(\vec{r})\psi(\vec{r}) \quad , (1.1)$$

and a Gaussian Ansatz for the density operator, they write:

$$\begin{aligned} i\hbar\dot{\Phi} &= \left(H^{sp} + gn_C + 2g\tilde{n} \right)\Phi + g\tilde{m}\Phi^{*}, \\ i\hbar\dot{\tilde{m}} &= 4\left(H^{sp} + 2gn + \frac{g}{4V}\left(2V\tilde{n}+1\right) \right)\tilde{m} + \frac{g}{V}\left(2V\tilde{n}+1\right)\Phi^{2}, \\ i\hbar\dot{\tilde{n}} &= g\left(\tilde{m}^{*}\Phi^{2} - \tilde{m}\Phi^{*2} \right). \end{aligned} \quad (1.2)$$

where $H^{sp} = -\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(r) - \mu$ is the single particle Hamiltonian.

In equation (1.1), *m* is the atom mass, $\psi^{+}(\vec{r})$, $\psi(\vec{r})$ are the boson creation and annihilation operators respectively , $V_{\text{ext}}(r)$ is the external confining potential, μ the chemical potential and *g* is the coupling constant. Furthermore, in the Eqs. (1.2), Φ is the order parameter, $n_c = |\Phi|^2$ is the condensate density, $\tilde{n}$ the thermal cloud and $\tilde{m}$ is the anomalous density, $n = n_c + \tilde{n}$ is the total density. The volume *V* of the gas is introduced for dimensional reasons.

One may understand in few words how (1.2) have been derived simply by recalling that the BV variational principle provides dynamical equations for the variational parameters of the density operator. These parameters are directly related to the expectation values (with respect to the density operator) of the operators $\psi(\vec{r})$, $\psi^{+}(\vec{r})\psi(\vec{r})$ and $\psi(\vec{r})\psi(\vec{r})$, which determine the various densities. For

instance, $\Phi(\vec{r}) = \langle \psi(\vec{r}) \rangle$,

$\tilde{n}(\vec{r}) = \langle \psi^+(\vec{r})\psi(\vec{r}) \rangle - \langle \psi^+(\vec{r}) \rangle \langle \psi(\vec{r}) \rangle$ and

$\tilde{m}(\vec{r}) = \langle \psi(\vec{r})\psi(\vec{r}) \rangle - |\psi(\vec{r})|^2$. For further computational details, see Ref. [1].

The quantities $\tilde{n}$ and $\tilde{m}$ are related by the unitarity relation

$$I = (1 + 2V\tilde{n})^2 - (2V|\tilde{m}|)^2, \qquad (1.3)$$

where the Heisenberg parameter *I* is directly related to the temperature by $\sqrt{I} = Coth(\hbar\omega / 2kT)$. For instance, *I*=1 at zero temperature.

The TDHFB equations possess a number of interesting properties such as the conservation of the energy and of the total number of particles. They are also characterized by a gapless excitation spectrum, which is compatible with the Hugenholtz-Pines theorem [3]. Furthermore, they provide a self-consistent dynamics of the order parameter, the thermal cloud and the anomalous density. They constitute in this sense a natural generalization of well known approximations such as the Gross-Pitaevskii, the Bogoliubov, the Popov, the Beliaev and the Hartree-Fock-Bogoliubov-De Gennes equations (HFB-BdG). See e.g. [4, 5, 6 and 7].

The HFB-de Gennes equations seem to derive from the linearization of the first equation in (1.2) around a static solution. Indeed, we easily get the equation

$$i\hbar\delta\dot{\Phi} = (H^{sp} + 2gn)\delta\Phi + g(\tilde{m} + \Phi^2)\delta\Phi^*, \qquad (1.4)$$

which, upon setting $\delta\Phi = \sum_p \left(u_p e^{-i\varepsilon_p t} - v_p e^{i\varepsilon_p t} \right)$ where u_p and v_p are real space function, turns out to be the HFB-De Gennes equations

$$\begin{aligned} \varepsilon_p u_p &= (H^{sp} + 2gn)u_p - g(n_c + \tilde{m})v_p \\ -\varepsilon_p v_p &= (H^{sp} + 2gn)v_p - g(n_c + \tilde{m})u_p \end{aligned}. \qquad (1.5)$$

The properties of the Bose-Einstein condensation in the TF regime at finite temperature were explored by many experimental and theoretical groups. A recent experimental result shows a deviation of the condensate radius from the standard TF approximation [8]. Moreover, in Ref.[9], it was clearly demonstrated that the thermal cloud compresses the condensate. From these experiments and from the Ref. [10], one notes that the validity of the TF approximation depends not only on the number of atoms but also on the trap properties.

2. The Thomas-Fermi approximation at finite temperature

In this section, we would like to generalize the TF method worked out in Ref [11] to the finite temperature. To this end, the kinetic energy operator is replaced by its classical counterpart $p^2/2m$ in the equations (1.2). We simplify our model by neglecting the anomalous density. The equations (1.2)-(1.3) take the form:

$$\left(\frac{p^2}{2m} + V_{ext}(r) + g(n_c + 2\tilde{n}) \right) \Phi = \mu\Phi, \qquad (2.1)$$

$$\tilde{n} = \frac{\sqrt{I} - 1}{2V}. \qquad (2.2)$$

The equation (2.1) can also be written:

$$(\bar{\mu} - H_{cl})\Phi = 0, \qquad (2.3)$$

where $H_{cl} = \frac{p^2}{2m} + V_{ext}(r) + gn_c$ is the ''classical'' Hamiltonian of the system and $\bar{\mu} = \mu - \frac{g}{V}(\sqrt{I} - 1)$. The solution of equation (2.1) for a repulsive case is given by

$$n_c(r) = Ag\left(\sqrt{1 + \frac{2}{Ag}\xi(r)} - 1 \right), \qquad (2.4)$$

where

$A = \left(\frac{m\alpha}{2\pi^2\hbar^3} \right)^2 mN_c^2$, $\xi(r) = (\bar{\mu} - V_{est}(r))/g$ and $\frac{1}{\alpha} = \int \frac{d\vec{r}d\vec{p}}{(2\pi\hbar)^3} \delta(\mu - H_{cl})$. In turn, the number of condensed atoms N_c is computed via $N_c = \int d\vec{r}\, n_c(r)$. Further details are given in [11].

It is worth noticing that in the case of a repulsive interaction and for large values of N_c (that is very low temperatures), we can expand $n_c(r)$ around $\xi(r)$. The equation (2.4) becomes

$$n_c \approx \xi(r) + \frac{1}{KgN_c^2}\xi^2(r) + \ldots \qquad (2.5)$$

We see that the first order result

$$n_c = \frac{\mu - V_{ext}}{g} - \frac{\sqrt{I} - 1}{V}, \qquad (2.6)$$

which is the finite temperature correction to the TF condensate density is just a temperature dependent term.

3. Thermodynamic quantities

For later convenience let us write the temperature dependence of the chemical potential. Integrating equation (2.6) over the available space and substituting the number conservation $N = N_c + \tilde{N}$, where $\tilde{N}$ is the number of non-condensed atoms, we find

$$\frac{\mu}{kT_c^0} = \left[\left(1-t^3\right)^{2/5} + \frac{0.8t^3}{\left(1-t^3\right)^{3/5}}\right]\eta . \qquad (3.1)$$

Here, we have used the ideal gas result $N_c = N\left(1-t^3\right)$, where $t = T/T_c^0$ is the reduced temperature (T_c^0 is the ideal gas transition temperature). The scaling parameter $\eta = 1.57\left(N^{1/6}\frac{a}{a_{H0}}\right)^{2/5}$, where N is the total number of atoms, a the s-wave scattering length and a_{H0} the oscillator length, describes the balance between interaction and thermal effects. Due to its relatively weak N dependence, η assumes values from 0.3 to 0.49 [10]. Equation (3.1) provides a useful correction of μ at finite temperature, which is expected to be valid in the range $T \le T_c$.

Let us first discuss the problem of the condensate fraction. Using the semi-classical picture for the thermal cloud[12], one may write

$$\tilde{N} = c\int_0^\infty d\varepsilon \frac{\varepsilon^2}{e^{(\varepsilon-\mu)/kT}}, \qquad (3.2)$$

were c is an integration constant. It is clear that at temperatures at and above T_c, the condensed and the anomalous densities can be neglected. The single particle energies are directly deducted from equation (1.5)

$$\varepsilon_p = \frac{p^2}{2M} + V_{ext}(r) + 2gn(r). \qquad (3.3)$$

Explicit integration of (3.2) provides a corrected expression for the condensate fraction

$$\frac{N_c}{N} = 1-t^3 - 1.37t^2\left[\left(1-t^3\right)^{2/5} + \frac{0.8t^3}{\left(1-t^3\right)^{3/5}}\right]\eta . \qquad (3.4)$$

A similar calculation yields an approximate expression for the total energy of the system

$$\frac{E}{NkT_c^0} = 2.70t^4 + \frac{5+16t^3}{7}\left[\left(1-t^3\right)^{2/5} + \frac{0.80t^3}{\left(1-t^3\right)^{3/5}}\right]\eta \qquad (3.5)$$

Notice that this expression can be obtained directly starting from the result (3.1), through the use of general thermodynamic properties.

The equations (3.4)-(3.5) show that the effects of the interaction depend linearly on η and are consequently expected to deviate from the predictions Ref. [10] and [12].

4. Results and discussions

Let us consider a system of ^{87}Rb atoms trapped by an isotropic harmonic potential. We use the following parameters $a/a_{H0} = 7.64\,10^{-3}$ and a total number of atoms $N = 2000$. Distances are measured in units of $a_{HO} = \sqrt{\hbar/m\omega_0}$ and densities in units of a_{HO}^{-3}. We begin by studying the chemical potential as a function of the scaling parameter for various temperatures.

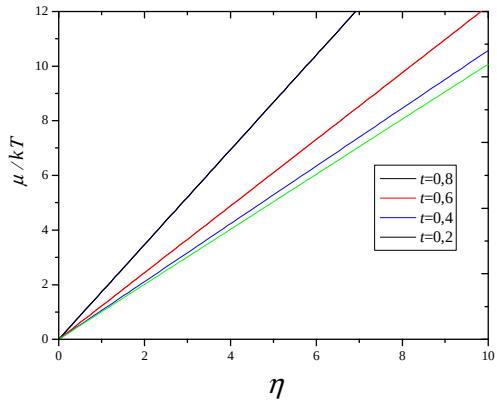

Fig 1: Chemical potential as function of the scaling parameter

The figure 1 shows that the chemical potential depends linearly on the scaling parameter and increases with temperature.

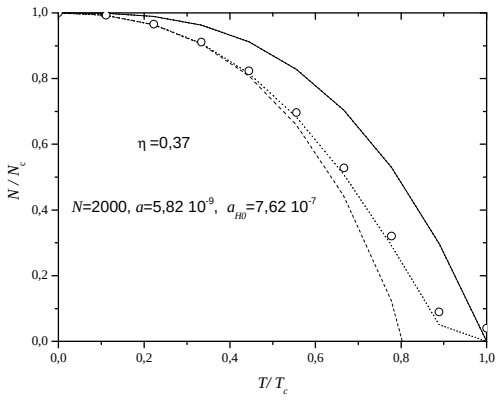

Fig 2: Condensate fraction as a function of the reduced temperature. The circles are the results of Ref.[13] for η = 0.37, obtained without using the semi classical approximation. The dotted line is the result of ref [12] for the same configuration. The dashed line is our calculation for the same configuration. The solid line is the ideal gas result in the large N limit.

Figure 2 shows that our prediction for the condensate fraction is much likely close to HFB-De Gennes calculation

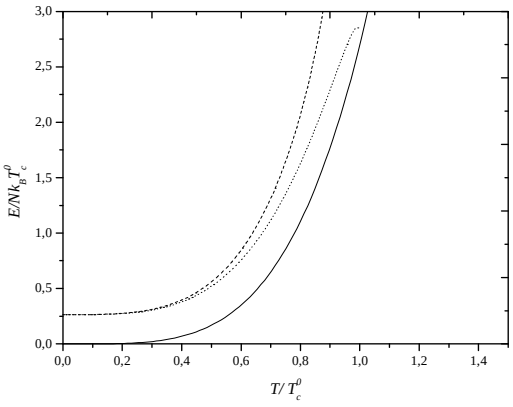

Fig 3: Total energy of the system as function of the reduced temperature for η =0.37. The dotted line is from Ref.[12]. The dashed line is our calculation for the same configuration. The solid line is the ideal gas result in the large *N* limit.

Figure 3 represents the total energy of the system and it is predicted to be larger than the one predicted by the non interacting gas. It coincides with the result of [12] for $T/T_c^0 \leq 0.5$.

5. Conclusion

In this work, we have studied the Thomas-Fermi approximation for trapped Bose gases at finite temperature. We have extended a semi classical method developed for the *T*=0 case.

Our calculations allow us first to establish original analytical expressions for the condensate density and some other thermodynamic quantities such as the chemical potential, the condensate fraction and the total energy of the system. These expressions are natural extensions of those obtained in Refs [11, 12].

Moreover, our numerical results show a linear dependence of the chemical potential with the scaling parameter and with the temperature. The total energy of the system is also shown to be larger than what has been predicted by semi classical methods.

Finally, we may conclude that the finite temperature extension of the Thomas-Fermi approximation, together with the full TDHFB equations can offer a powerful tool for the study of trapped self-interacting Bose quantum gases.

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Anomalous density for Bose gases at finite temperature

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We analyze the behavior of the anomalous density as function of the radial distance at different temperatures in a variational framework. We show that the temperature dependence of the anomalous density agrees with the Hartree-Fock-Bogoliubov (HFB) calculations. Comparisons between the normal and anomalous fractions at low temperature show that the latter remains higher and, consequently, the neglect of the anomalous density may destabilize the condensate. These results are compatible with those of Yukalov. Surprisingly, the study of the anomalous density in terms of the interaction parameter shows that the dip in the central density is destroyed for sufficiently weak interactions. We explain this effect.

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I. INTRODUCTION

The investigation of the Bose-Einstein condensation (BEC) phenomenon at finite temperature has attracted a great number of physicists in the recent years. The traditional theories to describe Bose-Einstein condensation at finite temperature are based on the Bogoliubov quasiparticle approach, developed originally for a spatially homogeneous Bose-condensed gas at $T \to 0$ [1] and employed by Lee and Yang [2] at finite temperatures. The generalization of the Bogoliubov method for spatially inhomogeneous systems has been described by De Gennes [3]. The main idea of Bogoliubov is to separate out the condensate part in the field operator $\Psi(\vec{r}) = \Phi(\vec{r}) + \tilde{\Psi}(\vec{r})$. The system may be split into two subcomponents; namely, the condensate described by its density, $n_c(r) = |\Phi(r)|^2$ and the thermal cloud $\tilde{n}(\vec{r},\vec{r}') = \langle\tilde{\Psi}^\dagger(\vec{r})\tilde{\Psi}(\vec{r}')\rangle$. These two components have been intensively studied both theoretically and experimentally [4–34]. Similarly, this approximation motivates the definition of an additional mean-field contribution $\tilde{m}(\vec{r},\vec{r}') = \langle\tilde{\Psi}(\vec{r})\tilde{\Psi}(\vec{r}')\rangle$. This is often referred to as the pair anomalous average and bears its name from the fact that there is an unequal number of creation and annihilation operators being averaged over. An analogous correlation plays a dominant role in the BCS theory of superconductivity [3], where fermionic atoms pair up to form the so-called Cooper pairs. In the case of Bose-Einstein condensation of neutral bosonic atoms, where the condensate mean field $\Phi(r)$ is the dominant parameter, the anomalous average plays a minor role for sufficiently repulsive interaction atoms in the condensate. However, this contribution becomes crucial in the presence of attractive interactions and molecular BECs [35].

Among the theoretical investigations of the anomalous density, we can cite in particular those of Hutchinson *et al.* [36] and Giorgini [37] based on the mean-field HFB-Bogoliubov–de Gennes (BdG) approximation. To go beyond the mean field, Fedichev *et al.* [38] and Proukakis *et al.* [39,40] developed a finite-temperature perturbation theory using an HFB basis. Another kind of approach has been developed by Griffin [41] based on the Green's function method to derive an equation for the condensate and its fluctuations. Yukalov [42] adopted a quite different approach by using the notion of representative statistical ensembles. Recently, Wright *et al.* [43,44] have used the classical-field trajectories of the projected Gross-Pitaevskii equation.

An interesting alternative nonperturbative and nonclassical-field approach to the finite-temperature Bose gas is provided by the so-called time-dependent variational principle. This principle was proposed by Balian and Vénéroni (BV) a long time ago [45]. The BV variational principle has been applied to various quantum problems including heavy-ion reactions [46], quantum fields out of equilibrium [47], and attempts to go beyond the Gaussian approximation for fermion systems [48]. Therefore, the BV principle has been used to provide the best approximation to the generating functional for two- and multi-time correlation functions of a set of bosonic and fermionic observables [49–52]. More recently, it was used to derive a set of equations governing the dynamics of trapped Bose gases [53,54]. The point is that this principle uses the notion of least-biased state, which is the best ansatz compatible with the constraints imposed on the system. For our purposes, we use a Gaussian density operator. The main difference between our approach and the earlier variational treatments is that, in our variational theory, we do not minimize only the expectation values of a single operator such as the free energy in the variational HF and HFB approximation or the thermodynamics potential as is done in the variational approach of Bijlsma and Stoof [24]. Conversely, our variational theory is based on the minimization of an action in addition to a Gaussian variational ansatz. The action to minimize involves two types of variational objects: one related to the observables of interest and the other that is akin to a density matrix [45,52,53]. This leads to a set of coupled time-dependent mean-field equations for the condensate, the noncondensate, and the anomalous average. We call this approach "time-dependent Hartree-Fock-Bogoliubov" (TDHFB). The TDHFB equations that we derive in this paper are quite general and fully consistent because they do not require any simplifying assumption for the thermal cloud or the anomalous density. They may provide in this sense a kind of generalization to the previously discussed approximations. Moreover, what is important in the TDHFB approach for Bose systems is that there have been no assumptions on weak interactions. Therefore, the theory is valid even for strong interactions.

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In fact, in many approximations, the anomalous density is always neglected. This is based in the general claim that its contributions are negligibly small. However, Yukalov [42] pointed out that, even if it is the case, it is an essential ingredient for the consistency of the formalism. We will go further by using our TDHFB formalism to show that the contribution of the anomalous density is not as small as claimed. On the other hand, the anomalous density profiles seem to have no structure at the center of the trap for weak interactions. This is in contradiction with what was found in the literature [36,43], where the HFB-BdG approximation and the classical-field trajectories of the projected Gross-Pitaevskii equation were used, and where these densities are found to have a "dip."

The paper is organized as follows: In Sec. II, we review the main steps used to derive the TDHFB equations from the Balian-Vénéroni variational principle. In Sec. III, the TDHFB equations are applied to a trapped Bose gas to derive a coupled dynamics of the condensate, the noncondensate, and the anomalous densities. We then restrict ourselves to the local densities and discuss the properties of the underlying equations, their relevance to the finite-temperature case, as well as their relations with other known approximations such as the mean-field Bogoliubov-de Gennes equations. In Sec. IV, we study the behavior of the TDFHB equations in homogeneous Bose gases; in particular, we discuss some properties of the normal and anomalous densities as functions of the temperature. Section V is devoted to presenting the static equations and the physical boundary conditions relevant to the trapped Bose gas. We analyze the profiles of the anomalous density for different temperatures both for large and small values of the interaction parameter. We confront our results with the HFB-BdG predictions. Furthermore, we focus on the comparison between the normal and anomalous fractions at low, intermediate, and high temperatures. Our conclusions are drawn in Sec. 6.

II. THE VARIATIONAL TDHFB EQUATIONS

The time-dependent variational principle of Balian and Vénéroni requires first the choice of a trial density operator. In our case, we will consider a Gaussian time-dependent density operator. This ansatz, which belongs to the class of the generalized coherent states, allows us to perform the calculations since there exists Wick's theorem, while retaining some fundamental aspects such as the pairing between atoms.

The Gaussian density operator $D(t)$ is completely characterized by the partition function $Z(t) = \mathrm{Tr}D(t)$, the one-boson field expectation value $\langle\Psi\rangle(\vec{r},t) \equiv \Phi(\vec{r},t) = \mathrm{Tr}\Psi(\vec{r})D(t)/Z(t)$ and the single-particle density matrix $\rho(\vec{r},\vec{r}',t)$ defined as

$$\rho(\vec{r},\vec{r}',t) = \begin{pmatrix} \langle\bar{\Psi}^\dagger(\vec{r}')\bar{\Psi}(\vec{r})\rangle & -\langle\bar{\Psi}(\vec{r}')\bar{\Psi}(\vec{r})\rangle \\ \langle\bar{\Psi}^\dagger(\vec{r}')\bar{\Psi}^\dagger(\vec{r})\rangle & -\langle\bar{\Psi}(\vec{r})\bar{\Psi}^\dagger(\vec{r}')\rangle \end{pmatrix}. \quad (2.1)$$

In the preceding definitions, $\Psi(\vec{r})$ and $\Psi^\dagger(\vec{r})$ are the boson destruction and creation field operators (in the Schrödinger representation), respectively, satisfying the usual canonical commutation rules

$$[\Psi(\vec{r}),\Psi^\dagger(\vec{r}')] = \delta(\vec{r}-\vec{r}'), \quad (2.2)$$

and

$$\bar{\Psi}(\vec{r}) = \Psi(\vec{r}) - \langle\Psi(\vec{r})\rangle.$$

Upon introducing these variational parameters into the BV principle, one obtains dynamical equations for the expectation values of the one- and two-boson field operators:

$$i\frac{\partial\langle\Psi\rangle}{\partial t}(\vec{r},t) = \frac{\partial E}{\partial\langle\Psi^\dagger\rangle(\vec{r},t)}, \quad i\frac{\partial\langle\Psi^\dagger\rangle}{\partial t}(\vec{r},t) = -\frac{\partial E}{\partial\langle\Psi\rangle(\vec{r},t)},$$
$$i\frac{\partial\rho}{\partial t}(\vec{r},\vec{r}',t) = -2\left[\rho,\frac{\partial E}{\partial\rho}\right](\vec{r},\vec{r}',t), \quad (2.3)$$

where $E = \langle H\rangle$ is the mean-field energy. We may notice at this point that the system (2.3) is closed and does not require any further ingredients. The truncation of the full hierarchy is no longer brutally performed but rather obtained by softly restricting the full Hilbert space to the single-particle one.

One of the most noticeable properties of the TDHFB equations (2.3) is the unitary evolution of the single-particle density matrix ρ, which means that the eigenvalues of ρ are conserved. This implies, in particular, the conservation of the von Neumann entropy $S = -\mathrm{Tr}(D)\ln D$ and the fact that an initially pure state, satisfying$\rho(\rho\ln+1) = 0$, remains pure during the evolution. This property also leads to conservation of the Heisenberg parameter [52]

$$I(\vec{r},\vec{r}') = \int d\vec{r}''[\langle\bar{\Psi}^\dagger(\vec{r})\bar{\Psi}(\vec{r}'')\rangle\langle\bar{\Psi}(\vec{r}'')\bar{\Psi}^\dagger(\vec{r}')\rangle$$
$$-\langle\bar{\Psi}^\dagger(\vec{r})\bar{\Psi}^\dagger(\vec{r}'')\rangle\langle\bar{\Psi}(\vec{r}'')\bar{\Psi}(\vec{r}')\rangle]. \quad (2.4)$$

III. APPLICATION OF THE TDHFB FORMALISM TO TRAPPED BOSE GASES

Let us apply the previous equations (2.3) to a system of trapped bosons interacting via a two-body potential. The grand canonical Hamiltonian may be written in the form

$$H = \int d\vec{r}\Psi^\dagger(\vec{r})\left[-\frac{\hbar^2}{2M}\Delta + V_{\mathrm{ext}}(\vec{r}) - \mu\right]\Psi(\vec{r})$$
$$+\frac{1}{2}\int d\vec{r}d\vec{r}'\Psi^\dagger(\vec{r})\Psi^\dagger(\vec{r}')V(\vec{r},\vec{r}')\Psi(\vec{r}')\Psi(\vec{r}), \quad (3.1)$$

where $V(\vec{r},\vec{r}')$ is the interaction potential, $V_{\mathrm{ext}}(\vec{r})$ is the external confining field, and μ is the chemical potential. For the sake of clarity, we will omit the time dependence whenever they are obvious. Next, we introduce the order parameter $\Phi(\vec{r}) = \langle\Psi(\vec{r})\rangle$ and the nonlocal densities

$$\tilde{n}(\vec{r},\vec{r}') \equiv \tilde{n}^*(\vec{r},\vec{r}') = \langle\Psi^\dagger(\vec{r})\Psi(\vec{r}')\rangle - \Phi^*(\vec{r})\Phi(\vec{r}'),$$
$$\tilde{m}(\vec{r},\vec{r}') \equiv \tilde{m}(\vec{r}',\vec{r}) = \langle\Psi(\vec{r})\Psi(\vec{r}')\rangle - \Phi(\vec{r})\Phi(\vec{r}'). \quad (3.2)$$

where we note that $\tilde{n}(\vec{r},\vec{r}) \equiv \tilde{n}(\vec{r})$ and $\tilde{m}(\vec{r},\vec{r}) \equiv \tilde{m}(\vec{r})$ are respectively the noncondensate and the anomalous densities.

The energy may be readily computed to yield

$$E = \int d\vec{r} h^{\rm sp}(\vec{r})[\tilde{n}(\vec{r},\vec{r}) + \Phi(\vec{r})\Phi^*(\vec{r})] + \int d\vec{r}d\vec{r}' V(\vec{r},\vec{r}')|\Phi(\vec{r})|^2|\Phi(\vec{r}')|^2$$
$$+ \frac{1}{2}\int d\vec{r}d\vec{r}' V(\vec{r},\vec{r}')[\tilde{m}^*(\vec{r},\vec{r}')\tilde{m}(\vec{r},\vec{r}') + \tilde{n}(\vec{r},\vec{r}')\tilde{n}(\vec{r}',\vec{r}) + \tilde{n}(\vec{r},\vec{r})\tilde{n}(\vec{r}',\vec{r}')]$$
$$+ \frac{1}{2}\int d\vec{r}d\vec{r}' V(\vec{r},\vec{r}')[\tilde{n}(\vec{r},\vec{r}')\Phi(\vec{r})\Phi^*(\vec{r}') + \tilde{n}(\vec{r}',\vec{r})\Phi^*(\vec{r})\Phi(\vec{r}') + \tilde{n}(\vec{r},\vec{r})\Phi(\vec{r}')\Phi(\vec{r}') + \tilde{n}(\vec{r}',\vec{r}')\Phi(\vec{r})\Phi(\vec{r})]$$
$$+ \frac{1}{2}\int d\vec{r}d\vec{r}' V(\vec{r},\vec{r}')[\tilde{m}^*(\vec{r},\vec{r}')\Phi(\vec{r})\Phi(\vec{r}') + \tilde{m}(\vec{r},\vec{r}')\Phi^*(\vec{r})\Phi^*(\vec{r}')]. \tag{3.3}$$

In Eq. (3.3), $h^{\rm sp} = -\frac{\hbar^2}{2M}\Delta + V_{\rm ext}(\vec{r}) - \mu$ is the single particle Hamiltonian.

Now one inserts the expression (3.3) in the general equations of motion (2.3) to get the explicit form of the TDHFB equations for a trapped Bose gas:

$$i\hbar\dot{\Phi}(\vec{r}) = h^{\rm sp}(\vec{r})\Phi(\vec{r}) + \int d\vec{r}' V(\vec{r},\vec{r}')[|\Phi(\vec{r}')|^2\Phi(\vec{r}) + \Phi^*(\vec{r}')\tilde{m}(\vec{r},\vec{r}') + \Phi(\vec{r}')\tilde{n}(\vec{r},\vec{r}') + \Phi(\vec{r})\tilde{n}(\vec{r}',\vec{r}')], \tag{3.4a}$$

$$i\hbar\dot{\tilde{n}}(\vec{r},\vec{r}') = [h^{\rm sp}(\vec{r}) - h^{\rm sp}(\vec{r}')]\tilde{n}(\vec{r},\vec{r}') + \int d\vec{r}'' V(\vec{r}',\vec{r}'')[a(\vec{r}'',\vec{r}')\tilde{n}(\vec{r},\vec{r}'') + a(\vec{r}'',\vec{r}'')\tilde{n}(\vec{r},\vec{r}') + b(\vec{r}',\vec{r}'')\tilde{m}(\vec{r}'',\vec{r})]$$
$$- \int d\vec{r}'' V(\vec{r}',\vec{r}'')[a(\vec{r},\vec{r}'')\tilde{n}(\vec{r}'',\vec{r}) + a(\vec{r}'',\vec{r}'')\tilde{n}(\vec{r},\vec{r}') + b(\vec{r},\vec{r}')\tilde{m}(\vec{r}'',\vec{r}')], \tag{3.4b}$$

$$i\hbar\dot{\tilde{m}}(\vec{r},\vec{r}') = [h^{\rm sp}(\vec{r}) + h^{\rm sp}(\vec{r}')]\tilde{m}(\vec{r},\vec{r}') + \int d\vec{r}'' V(\vec{r}',\vec{r}'')\{a(\vec{r}'',\vec{r}')\tilde{m}(\vec{r},\vec{r}'') + a(\vec{r}'',\vec{r}'')\tilde{m}(\vec{r},\vec{r}') + b(\vec{r}',\vec{r}')[\tilde{n}^*(\vec{r},\vec{r}'') + \delta(\vec{r}-\vec{r}'')]\}$$
$$+ \int d\vec{r}'' V(\vec{r}',\vec{r}'')[a(\vec{r}'',\vec{r})\tilde{m}(\vec{r}',\vec{r}'') + a(\vec{r}'',\vec{r}'')\tilde{m}(\vec{r},\vec{r}') + b(\vec{r},\vec{r}'')\tilde{n}(\vec{r}'',\vec{r}')]. \tag{3.4c}$$

In the Eqs. (3.4), the dots denote time derivatives and we have introduced the quantities

$$a(\vec{r},\vec{r}') = \tilde{n}(\vec{r},\vec{r}') + \Phi^*(\vec{r})\Phi(\vec{r}'),$$
$$b(\vec{r},\vec{r}') = \tilde{m}(\vec{r},\vec{r}') + \Phi(\vec{r})\Phi(\vec{r}'). \tag{3.5}$$

It is worth noticing that similar equations have been derived elsewhere using quite different approaches. For instance, Stoof [24] used a variational plus perturbative effective action, Proukakis [35,39] used truncation of the Heisenberg equations, and Chernyak *et al.* [55] used the generalized coherent state representation. The latter approach yields equations very close to ours, but the authors did not pursue further their analysis.

For contact potential $V(\vec{r},\vec{r}') = g\delta(\vec{r}-\vec{r}')$, where g is related to the s-wave scattering length a by $g = 4\pi\hbar^2 a/M$. This implies that the integrations in Eqs (3.4) are removed:

$$i\hbar\dot{\Phi}(r) = [h^{\rm sp} + gn_c(r) + 2g\tilde{n}(r)]\Phi(r) + g\tilde{m}(r)\Phi^*(r), \tag{3.6a}$$

The equations of motion for $\tilde{n}(r,r')$and $\tilde{m}(r,r')$ may be written in the compact form

$$i\hbar\frac{d\rho}{dt} = \Im\rho - \rho\Im^+, \tag{3.6b}$$

where we have defined the 2×2 matrices

$$\Im(r,r') = \begin{pmatrix} h(r,r') & \Delta(r',r') \\ -\Delta^*(r,r) & -h^*(r,r') \end{pmatrix},$$
$$\rho(r,r') = \begin{pmatrix} \tilde{n}(r,r') & \tilde{m}(r,r') \\ \tilde{m}^*(r,r') & \tilde{n}^*(r,r')+1 \end{pmatrix}$$

and

$$h(r,r') = h^{\rm sp}(r) + 2ga(r',r'), \quad \Delta(r,r) = gb(r,r).$$

Equations (3.6) constitute the TDHFB equations for the contact interaction potential approximation in real space.

It is well known that, in the HFB theory, the issues of the ultraviolet (uv) divergence of the anomalous density arise from the zero-point occupation of quasiparticle modes [36]. In our case, the diverging term appears in Eq. (3.4c) and becomes highly nontrivial when one considers the contact potential. This is precisely the term which leads to uv divergences in the anomalous density in HFB theory [36]. Having identified the origin of this divergence, we can habitually eliminate it from the problem, by regularizing the anomalous average. This is achieved by following the method of Refs. [56,57].

Equations (3.6) remain complicated even for the contact potential where the noncondensate and anomalous densities are nonlocal functions of two spatial points $\tilde{n}\left(r,r'\right)$ and $\tilde{m}\left(r,r'\right)$. To proceed further and to investigate the behavior of

the various density profiles both for homogeneous and trapped gases, we consider in this article only the quantities for $r = r'$ since these are the most physically accessible.

IV. ANOMALOUS DENSITY FOR HOMOGENEOUS BOSE GAS

In the uniform case $[V_{\rm ext}(r) = 0]$ and for a thermal distribution at equilibrium, the relation (2.4) may rewritten as

$$I_p = (2\tilde{n}_p + 1)^2 - 4|\tilde{m}_p|^2 = \coth^2[\varepsilon_p/(2kT)], \tag{4.1}$$

where $\varepsilon_p$is the Bogoliubov energy spectrum defined by the expression

$$\varepsilon_p = [(E_p + 2gn - \mu)^2 - g^2(n_c + \tilde{m})^2]^{1/2}, \tag{4.2}$$

with $E_p = p^2/(2m)$ being the energy of a free particle.

Note that the expression (4.2) can be derived by computing the random-phase approximation (RPA) modes from (3.6a). It is well known that, to satisfy the Goldstone or the Hugenholtz-Pines [58] theorem, the spectrum (4.2) should be gapless in the long-wavelength limit. This is indeed satisfied provided

$$\mu = g(n + \tilde{n} - \tilde{m}), \tag{4.3}$$

where $n = n_c + \tilde{n}$ is the total density.

Moreover, at zero temperature, the relation (4.1) becomes

$$|\tilde{m}_p|^2 = \tilde{n}_p(\tilde{n}_p + 1). \tag{4.4}$$

Equation (4.4) constitutes an explicit relationship between the normal and the anomalous densities at zero temperature and indicates that the anomalous density and the thermal cloud density are of the same order of magnitude at low temperatures, which leads to the fact that neglecting $\tilde{m}$ while maintaining $\tilde{n}$ is a quite hazardous approximation. Finally, as a technical remark, note that the dependence of $\tilde{n}$ and $\tilde{m}$ at zero temperature allows us to eliminate the noncondensate density from the TDHFB equations, thereby reducing the dimensionality of the problem and simplifying the numerical solution.

A straightforward calculation using Eq. (4.1) leads to a novel form of the normal and anomalous densities as a function of $\sqrt{I_p}$:

$$\begin{aligned} \tilde{n}_p &= \frac{1}{2}\left[\frac{E_p + g\,(n_c + \tilde{m})}{\varepsilon_p}\sqrt{I_p} - 1\right], \\ \tilde{m}_p &= -\frac{g\,(n_c + \tilde{m})}{2\varepsilon_p}\sqrt{I_p}, \end{aligned} \tag{4.5}$$

where $\sqrt{I_p} = \coth[\varepsilon_p/(2kT)]$.

It is worth noticing that Eqs. (4.5) together with (3.6a) constitute the generalized HFB equations at finite temperature. This shows that our formalism can be reproduced easily by the full HFB equations both at finite and zero temperatures [see Eqs. (4.6)].

It is convenient now to analyze the asymptotic behavior of Eqs. (4.5) with respect to temperature.

At low temperature $\tilde{n}_p$ and $\tilde{m}_p$ behave as

$$\begin{aligned} \tilde{n}_p &= \frac{1}{2}\left[\frac{E_p + g\,(n_c + \tilde{m})}{\varepsilon_p} - 1\right] \quad (T \to 0)\,, \\ \tilde{m}_p &= -\frac{g\,(n_c + \tilde{m})}{2\varepsilon_p} \quad (T \to 0)\,. \end{aligned} \tag{4.6}$$

At high temperature we can use the asymptotic form $\sqrt{I_p} \cong 2kT/\varepsilon_p$. Then, $\tilde{n}_p$ and $\tilde{m}_p$ take the form

$$\begin{aligned} \tilde{n}_p &= \frac{E_p + g\,(n_c + \tilde{m})}{\varepsilon_p}\left(\frac{kT}{\varepsilon_p}\right) - \frac{1}{2} \quad (T \to T_c)\,, \\ \tilde{m}_p &= -\frac{g\,(n_c + \tilde{m})}{\varepsilon_p}\left(\frac{kT}{\varepsilon_p}\right) \quad (T \to T_c)\,. \end{aligned} \tag{4.7}$$

To illustrate comparatively the behavior of the normal and anomalous densities as functions of temperature for a uniform Bose gas, it is useful to introduce the

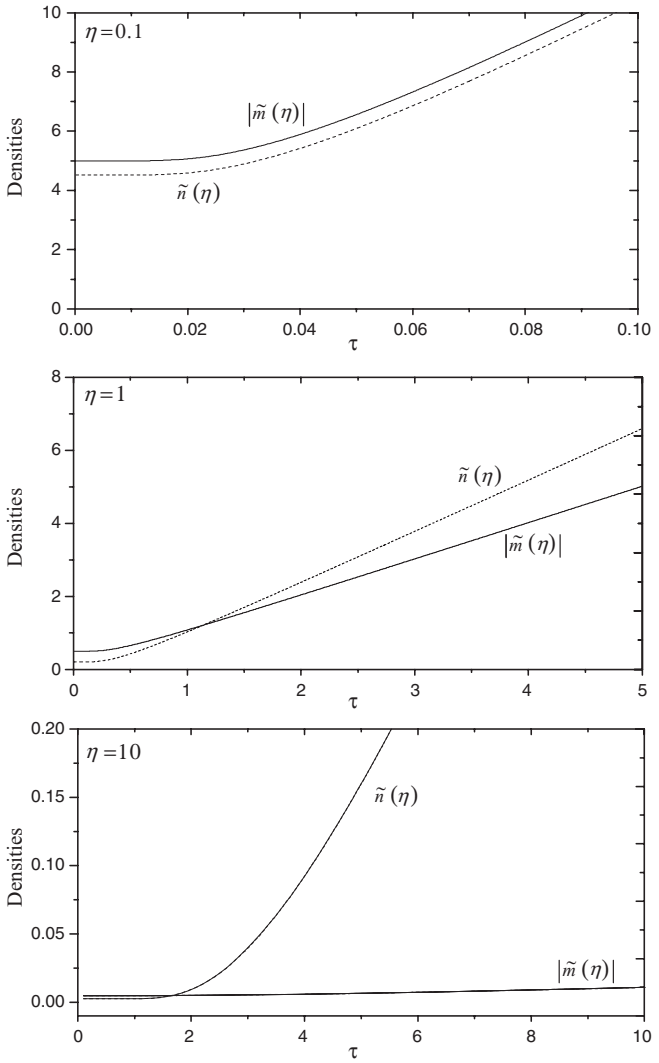

FIG. 1. Absolute value of the anomalous density $\tilde{m}(\eta)$ (solid line) and the noncondensate density $\tilde{n}(\eta)$ (dashed line) vs the temperature τ for different values of η.

dimensionless variables $\eta = \varepsilon_p/[g(n_c + \tilde{m})]$ and $\tau = kT/[g(n_c + \tilde{m})]$. Equations (4.5) become

$$\tilde{n}(\eta) = \frac{\sqrt{1+\eta^2}}{2\eta}\sqrt{I(\eta)} - \frac{1}{2},$$
$$\tilde{m}(\eta) = -\frac{1}{2\eta}\sqrt{I(\eta)}, \tag{4.8}$$

where $\sqrt{I(\eta)} = \coth[\eta/(2\tau)]$.

In Fig. 1 we show that the absolute value of the anomalous density is always larger than the noncondensed value for small values of $\eta = 0.1$ at low temperature. Moreover, the absolute value of the anomalous density is comparable with the noncondensed density for $\eta = 1$ ($|\tilde{m}| \approx \tilde{n}$ for $\tau \approx 1.2$). However, at high temperatures, the anomalous density becomes much smaller than the noncondensed density. As can be seen from these figures, the behavior of the normal and anomalous densities found here is in good agreement with the recent theoretical results of Refs. [59–61].

Finally, we can check that omitting the anomalous density, while keeping the normal one, is mathematically inappropriate; this is clearly shown in (4.4). From these facts, it is understandable now that neglecting the anomalous density at low temperature for a homogeneous Bose gas as one habitually does in the literature is principally an unjustified approximation. Let us turn now to analyze the situation for a trapped Bose gas.

V. ANOMALOUS DENSITY FOR TRAPPED BOSE GAS

The static TDHFB equations are obtained by setting to zero the right-hand sides of Eqs. (3.6) in their local form. For numerical purposes, it is convenient to start our treatment with the dimensionless form of the set (3.6). Let us consider a spherical trap with frequency ω, $V_{\rm ext}(r) = \frac{1}{2}m\omega^2 r^2$and use the harmonic oscillator length $a_{\rm HO} = \sqrt{\hbar/(m\omega)}$, as well as $a_{\rm HO}^{-3}$ and $\hbar\omega$ as units of length, density, and energy respectively. The dimensionless radial distance is $q = r/a_{\rm HO}$. The dimensionless condensed, noncondensed, and anomalous densities are, respectively, $\hat{n}_c = a_{\rm HO}^3 n_c$, $\hat{\tilde{n}} = a_{\rm HO}^3\tilde{n}$, and $\hat{\tilde{m}} = a_{\rm HO}^3\tilde{m}$. Therefore, $\hat{n} = \hat{n}_c + \hat{\tilde{n}}$ is the dimensionless total density. The static TDHFB equations can be solved numerically. The numerical method divides into two parts: The first part consists of finding the solutions of the static TDHFB equations that satisfies the boundary conditions summarized as follows: since the full wave function and the normal and anomalous averages must vanish as $q \to \infty$, the nonlinear term inside Eq. (3.6a) becomes negligible compared to the other terms. Therefore, the two equations of $\hat{\Phi}$ and $\hat{\tilde{m}}$ have the same approximate form $\hat{\Phi} \approx \hat{\tilde{m}} \approx q^{-3/2}\exp(-q^2/4)$ for $q \to \infty$. The second part is used to propagate the solutions of the static TDHFB equations with an adaptable numerical method.

To illustrate our finite temperature formalism, we consider the ^{87}Rb gas with the following parameters [30,62]: $a = 5.82 \times 10^{-9}$ m, $a_{\rm H0} = 7.62 \times 10^{-7}$ m and $\hbar\omega = 1.32 \times 10^{-31}$ J. A convenient dimensionless parameter describing the effective strength of the interactions is $\gamma = Na/a_{\rm H0}$ [20,63]. We begin by plotting the anomalous density as functions of the radial distance for several values of temperatures for $N = 20\,000$ atoms, i.e., $\gamma = 153$.

Figure 2(a) depicts the anomalous density for varying condensation fraction and for $\gamma = 153$. We notice that, by decreasing N_c/N, $\tilde{m}$ begins to increase in absolute value then decreases when N_c/N approaches 50%. This overall behavior has also been obtained in [36,43]. The anomalous density remains real and negative whatever the temperature and position. The presence of effective repulsive atomic interactions between the atoms, and thus also between the condensate and the thermal cloud, leads to the appearance of a local dip in the anomalous density at the center of the trap.

In Fig. 2(b) we show that, for a small value of the interaction parameter ($\gamma = 1.53$), the shape of the anomalous density is surprisingly modified. In particular, we observe that the dip in the neighborhood of the center of the trap disappears and the curve takes a Gaussian form. The central anomalous density is lowered for weak interactions. Such a result can be justified by the effect of interactions (i.e., for a small number of particles or a small value of γ). The interactions between the atoms

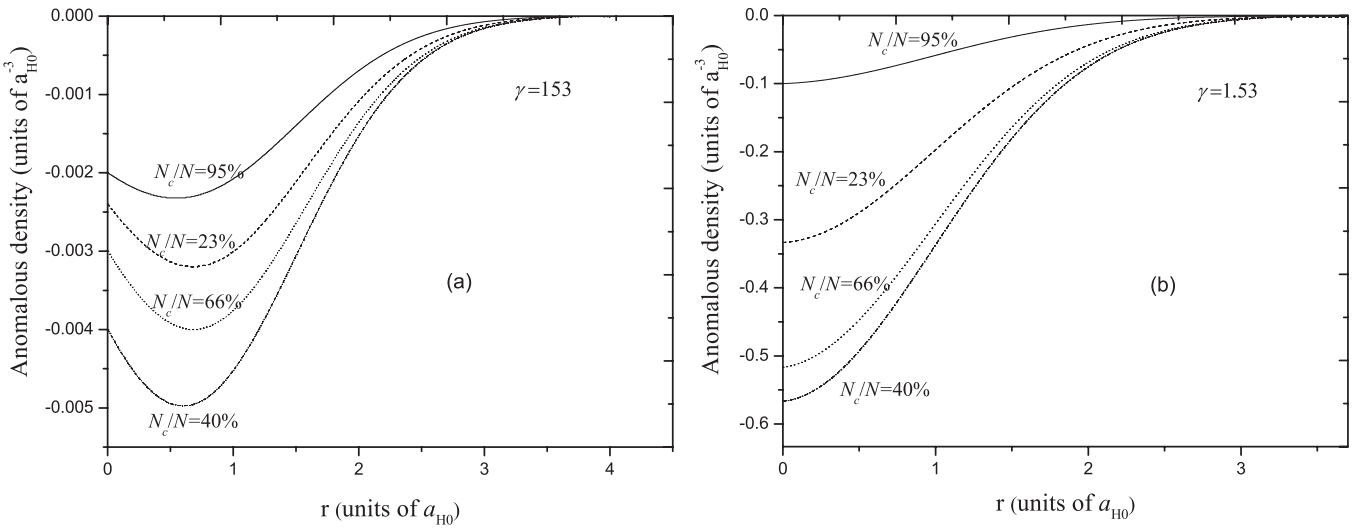

FIG. 2. Anomalous density profiles for various condensate fractions.

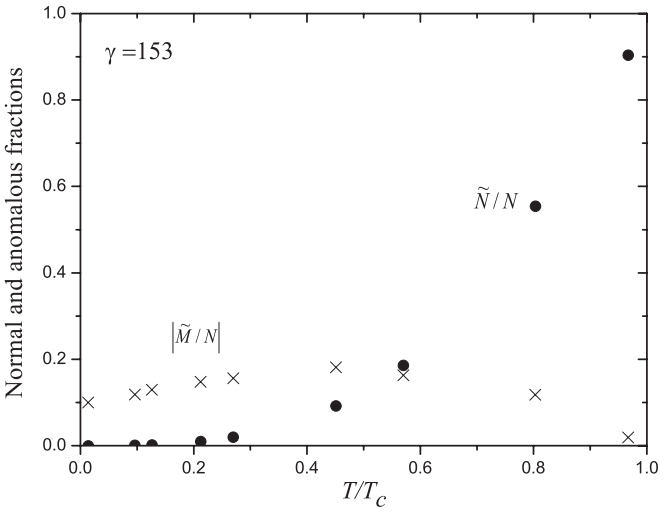

FIG. 3. Normal and anomalous fractions vs reduced temperature for $\gamma = 153$.

of the condensate and the thermal cloud are lowered, which leads automatically to the correlations becoming weak which is why the anomalous density remains small and takes a Gaussian shape together with the thermal and the condensate density. We note that the effect of interactions on the anomalous density was studied theoretically earlier by many authors, but no one looked at how the shape of this quantity varies as a function of the interactions.

We now turn our attention to analyze more obviously the temperature-dependent behavior of the noncondensate and the anomalous fractions defined, respectively, as $\tilde{n}/N$ and $|\tilde{M}/N|$ where $\tilde{N} = \int d\vec{r}\tilde{n}(r)$ and $\tilde{M} = \int d\vec{r}\tilde{m}(r)$ are the integrated values of the noncondensate and the anomalous densities.

In Fig. 3, we plot the noncondensate and the absolute value of anomalous fractions as function of the reduce temperature T/T_c for $\gamma = 153$ (where we follow the method outlined in [36]). It can be seen that $\tilde{N}/N$ is increasing significantly with increasing temperature, which is why $\tilde{N}$ reaches a maximum value close to the BEC transition temperature. Furthermore, it is quite interesting to observe that the absolute value of the anomalous fraction $|\tilde{M}/N|$ becomes small as the temperature approaches zero or T_c. It reaches a maximum at intermediate temperatures ($T \approx 0.5T_c$).

On the other hand, a careful observation of Fig. 3 shows that $|\tilde{M}/N|$ is larger than $\tilde{N}/N$ at low temperature ($T \leqslant 0.5T_c$), which is justified mathematically by our relation (4.4). This result is in disagreement with what is given in the literature [36]. In fact, the authors of this Ref. [36] were still based on the idea that the anomalous fraction is always smaller than the normal fraction for any range of temperature, even at low temperatures, without any physical or mathematical justifications. Second, when the temperature approaches its critical value, the fraction of noncondensed particles approaches unity. That's why at $T \cong T_c$ the anomalous fraction simultaneously with the condensate fraction become much smaller than the normal fraction. Such a feature is well understood and explained in the literature [36,42,43,61], although the absolute value of the anomalous and normal fractions are of the same order at intermediate temperatures. It is worth noticing that this behavior persists even for $\gamma = 1.53$ with a small change in the amplitudes of these fractions. Hence, we may infer from these results that the anomalous fraction plays a central role at low temperatures. It is therefore highly unlikely to neglect it for $T < T_c$.

It is well known that the anomalous density is proportional to the *s*-wave scattering length (i.e., the interactions between atoms). In fact, $\tilde{m}(\vec{r},\vec{r}') = \langle\bar{\Psi}(\vec{r})\bar{\Psi}(\vec{r}')\rangle = 0$ for the ideal Bose gas. Indeed, the anomalous average appears in all calculations for a Bose system with broken gauge symmetry. Its importance will be highlighted if we compare the expressions, derived with and without taking into account the anomalous averages, with measured quantities, thus measuring the contributions from the anomalous averages. In some cases, the difference is drastic. For instance, the BEC transition is of first order when the anomalous average is not taken into account, while it is second order when we take it into account. Another example is the fact that the compressibility becomes infinite, implying that the system is unstable if the anomalous averages are absent. Moreover, the superfluid transition does not occur if the anomalous averages are omitted [61].

Since the presence of anomalous average means that particles in the system are correlated, it is important for the current experiments with ultracold atoms to find new methods of characterizing the correlated many-body states, such as systems near the Feshbach resonance, rotating condensates, atoms in optical lattices, and low-dimensional systems [64]. An interesting question to ask is whether the anomalous averages can be measured experimentally. In their recent papers, Polkovnikov *et al.* [65,66] argued that this can be done by using interference experiments with two independent condensates for any geometry. Nevertheless this technique is not applicable for a single condensate as in our case where there are correlations between the atoms of the condensate and the thermal cloud. To this point, as far as we know, there is no experimental technique to directly measure the anomalous density itself. Experimental data about the anomalous density remain a great challenge for experimentalists.

VI. CONCLUSIONS

By using a Gaussian density operator, we derive from the time-dependent Balian-Vénéroni variational principle a set of coupled equations of motion for a self-interacting trapped Bose gas. These equations govern in a self-consistent way the dynamics of the condensate, the thermal cloud, and the anomalous average. Our time-dependent Hartree-Fock-Bogoliubov (TDHFB) equations generalize in a natural way many of the famous approximations found in the literature such as the Bogoliubov, the Gross-Pitaevskii [67,68], the Popov [69], the Beliaev [70], the Bogoliubov-de Gennes [36], Zaremba-Nikuni-Griffin (ZNG) equations [22], and others.

The comparison between the normal and anomalous densities at different temperatures is analyzed for a homogeneous Bose gas. This analysis shows the significance of the anomalous density compared to the normal density at low temperature [42].

To better understand the advantages of our approach and owing to the importance of accounting for many-body effects, we analyzed the behavior of the anomalous density for trapped Bose gases. We solve numerically the static TDHFB equations in the local limit and for a contact potential. The outcomes of our numerical explorations are numerous. First of all, the numerical resolution of our equations is relatively easy and is not as time-consuming as the HFB-BdG calculations, especially for large atom numbers. For instance, the latter cannot be handled correctly as soon as $N \sim 10^4$ to 10^5. By contrast, there are no such limitations in our case. We recover a well-known theoretical prediction of HFB-BdG [36] since $\tilde{m}$ increases with the temperature and then decreases as one approaches the transition. Furthermore, we found that the dip of the anomalous density is destroyed for sufficiently weak interactions. Moreover, we show that, at low temperatures, the anomalous fraction is larger than the noncondensate fraction. The former necessarily plays a major role in the Bose-Einstein condensation phenomenon. Any approach neglecting the anomalous fraction at low temperatures will inevitably lead to inconsistencies.

The dynamics of the anomalous density will be the goal of our next work with the aim of understanding how this quantity evolves in time. Furthermore, to examine more carefully our TDHFB formalism we will focus in the future on the behavior of the anomalous density in dipolar Bose-Einstein condensates at finite temperature both in the static and the dynamic cases.

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Low Dimensional Behavior of Normal and Anomalous Densities for Homogeneous Bose Gases

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Abstract: We analyze the behavior of the normal and anomalous densities at two dimensions for homogenous Bose gas in a Hartree-Fock-Bogoluibov (HFB) framework. A comparison between the normal and the anomalous densities at zero shows that the latter remains larger and consequently the neglect of the anomalous density may destabilize the condensate.

Key words: Bose-Einstein condensation, HFB equations, low dimension, anomalous density.
PACS: 05.30.Jp; 11. 15. Tk; 32. 80. Pj

INTRODUCTION

During the last decade, the physics of ultracold gases in low dimensions has attracted considerable attention both experimentally and theoretically. The properties of these fluids are radically different from those in three dimensions. The famous Mermin-Wagner-Hohenberg theorem states that long wavelength thermal fluctuations destroy long range order in a homogeneous one-dimensional Bose gas at all temperatures and in a homogeneous two-dimensional Bose gas at any nonzero temperature, preventing formation of both condensate and anomalous density.

In this communication we analyze the behavior of the normal and anomalous densities in low dimensional homogenous Bose gas in the Hartree-Fock-Bogoliubov (HFB) framework. A comparison between the normal and the anomalous densities at zero temperature shows that the latter remains higher. In the limit of weak interactions, the expressions of the above quantities allow us to calculate the chemical potential. The superfluid fraction is also obtained at low temperature.

THE HFB-EQUATIONS

Starting with the equation of motion for the Bose field operator $\hat{\psi}(\vec{r})$, and its decomposition $\hat{\psi}(\vec{r}) = \overline{\psi}(\vec{r}) + \Phi(\vec{r})$ in term of condensate and noncondensate parts, the condensate wavefunction $\Phi(\vec{r})$ is defined in 2D Bose gas within the generalized Gross-Pitaevskii equation [1-3]

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$$\mu\Phi = \left[\frac{\hbar^2}{2m}\Delta + V_{ext}(\vec{r}) + g_2\left(n_c + 2\tilde{n}\right) \right]\Phi + g_2\, \tilde{m}\, \Phi^*, \tag{1}$$

here $n_c = |\Phi(\vec{r})|^2$, $\tilde{n}(\vec{r}) = <\overline{\Psi}^+(\vec{r})\overline{\Psi}(\vec{r})>$ and $\tilde{m}(\vec{r}) = <\overline{\Psi}(\vec{r})\overline{\Psi}(\vec{r})>$ are the condensate, noncondensate and the anomalous densities respectively. g_2 is the two body *T*-matrix given as

$$g_2 = \frac{4\pi\hbar^2}{m}\frac{1}{\log\left(2\hbar^2/m\mu\, a^2\right)}, \tag{2}$$

where a is the two dimensional scattering length (See e.g.[4,5]). The usual Bogoliubov transformation $\overline{\psi}(\vec{r}) = \sum_k \left[u_k(\vec{r}) b_k - v_k(\vec{r}) b_k^+ \right]$ leads to the coupled Bogoliubov-de Gennes equations

$$\begin{pmatrix} \hat{\mathcal{L}} & \hat{\mathcal{M}} \\ -\hat{\mathcal{M}}^* & -\hat{\mathcal{L}}^* \end{pmatrix} \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} = \varepsilon_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix}, \tag{3}$$

where $\hat{\mathcal{L}} = \frac{\hbar^2}{2m}\Delta + V_{ext}(r) + 2g_2 n - \mu$, $\hat{\mathcal{M}} = g_2\left(\Phi^2 + \tilde{m}\right)$ and $n = n_c + \tilde{n}$ is the total density. These equations define the Bogoliubov energy spectrum ε_k and the quasiparticle amplitudes u_k and v_k. Once these quantities have been determined, the noncondensate and the anomalous densities for a homogeneous Bose gas are obtained from the following expressions

$$\tilde{n} = \frac{1}{2}\int \frac{d^2k}{(2\pi)^2}\left[\frac{E_k + g_2\left(n_c + \tilde{m}\right)}{\varepsilon_k} \coth\left(\varepsilon_k / 2T\right) - 1 \right], \tag{4}$$

$$\tilde{m} = -\frac{1}{2}\int \frac{d^2k}{(2\pi)^2}\left[\frac{g_2\left(n_c + \tilde{m}\right)}{\varepsilon_k} \coth\left(\varepsilon_k / 2T\right) \right], \tag{5}$$

where

$$\varepsilon_k = \sqrt{E_k^2 + 2E_k g_2\left(n_c + \tilde{m}\right)}, \tag{6}$$

and $E_k = \frac{\hbar^2 k^2}{2m}$ is the energy of a free particle.

It is well known that in order to satisfy the Hugenholtz–Pines theorem, the spectrum (6) should be gapless in the long wavelength limit. This is indeed satisfied provided

$$\mu = g_2\left(n + \tilde{n} - \tilde{m}\right) \tag{7}$$

Eqs.(4) and (5) are not totally independent since $\tilde{n}$ and $\tilde{m}$ are related by

$$\left(2\tilde{n}_k + 1\right)^2 - 4\left|\tilde{m}_k\right|^2 = \coth^2\left(\varepsilon_k / 2T\right), \tag{8}$$

The most important feature of Eq.(8) is that it allows us to calculate in very useful way the dissipated heat (see Eq.14). Moreover, at zero temperature, this relation becomes

$$\left|\tilde{m}_k\right|^2 = \tilde{n}_k(\tilde{n}_k + 1). \tag{9}$$

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Eq.(9) constitutes an explicit relationship between the normal and the anomalous densities at zero temperature and it indicates that these two quantities are of the same order of magnitude at low temperatures which leads to the fact that neglecting $\tilde{m}$ while maintaining $\tilde{n}$ is a quite hazardous approximation.

NORMAL AND ANOMALOUS DENSITIES IN A WEAKLY INTERACTING 2D BOSE GAS

In this section we discuss the behavior of the normal and anomalous densities in uniform 2D Bose gas at zero temperature. From now on, we will consider the regime in weakly repulsive interactions at zero temperature.

In the very dilute limit, when $g_2 \to 0$ and $\tilde{m}/n_c << 1$, the integrals (4) and (5) may be computed by means of dimensional regularization [6]. We finally obtain for the normal and anomalous densities

$$\tilde{n} = \frac{n_c}{\log\left(2\hbar^2 / m\mu a^2\right)}, \tag{10}$$

$$\tilde{m} = \frac{4n_c}{\log\left(2\hbar^2 / m\mu a^2\right)}, \tag{11}$$

It is worth noticing that in the case of $n_c \approx n$, we recover easily the well-known result of Schick, Al-Kawaja et al [7] and Petrov et al [8]. Furthermore, Eqs. (10) and (11) show clearly that the anomalous density is always greater than the normal one at zero temperature in 2D Bose gas ($\tilde{m}/\tilde{n} = 4$). From these results we can infer that omitting the anomalous density, while keeping the normal one is physically and mathematically inappropriate which is clearly shown in Eq.(9). Moreover, Eq.(12) has no analogue in the literature.

CONCLUSION

The two-dimensional behavior of the normal and anomalous densities at zero temperature is analyzed for homogeneous Bose gases by using the standard HFB formalism. By using the dimensional regularization we find that the anomalous density has a finite value in the limit of weak interactions. Furthermore, we show the significance of the anomalous density when it compared to the normal one in 2D uniform Bose gas.

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Behavior of the anomalous correlation function in a uniform two-dimensional Bose gas

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We investigate the behavior of the anomalous correlation function in two-dimensional Bose gas. In the local case, we find that this quantity has a finite value in the limit of weak interactions at zero temperature. The effects of the anomalous density on some thermodynamic quantities are also considered. These effects can modify, in particular, the chemical potential, the ground-state energy, the depletion, and the superfluid fraction. Our predictions are in good agreement with recent analytical and numerical calculations. We show also that the anomalous density presents a significant importance compared to the noncondensed one at zero temperature. The single-particle anomalous correlation function is expressed in two-dimensional homogenous Bose gases by using the density-phase fluctuation. We then confirm that the anomalous average accompanies in analogous manner the true condensate at zero temperature, while it does not exist at finite temperature.

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I. INTRODUCTION

The experimental progress of the ultracold gases in two dimensions (2D) [1–8] has recently attracted great attention. The properties of these fluids are radically different from those in 3D. The famous Mermin-Wagner-Hohenberg theorem [9,10] states that long-wavelength thermal fluctuations destroy long-range order in a homogeneous 1D Bose gas at all temperatures and in a homogeneous 2D Bose gas at any nonzero temperature, preventing formation of condensate.

Since the earlier works of Schick [11] and Popov [12], several theoretical studies of fluctuations, scattering properties, and the appropriate thermodynamics have been performed in [13–16]. In fact, in most of the previous references, the anomalous density is neglected under the claim that it is a divergent and unmeasured quantity, as well as its contribution being very small compared to the other terms. Otherwise, the importance of the anomalous density in 3D Bose gas has been shown in our recent theoretical results [17,18] and also by several authors [19–24] using different approaches. Theoretically, the anomalous average arises of the symmetry-breaking assumption [17,19,24]. It quantifies the correlations of pairs of noncondensate atoms with pairs of condensate atoms due to the Bogoliubov pair promotion process in which two condensate atoms scatter each other out of the condensate which is responsible for the well-known Bogoliubov particle-hole structure of excitations in the system [24]. The anomalous density can also be interpreted as a measure of the squeezing of the noncondensate field fluctuations [25]. Certainly, the presence of this quantity adds new features to the well-known problems and attracts our attention to the 2D systems. A number of questions arise naturally in this paper. Does the anomalous density exist even at finite temperature in 2D Bose gas? How does its behavior compare with the normal density at zero temperature? What are the effects of this quantity on the thermodynamics of the system?

Due to the complexity and the particularity of dilute 2D Bose gases, many analytical investigations have been performed recently to find corrections beyond mean field at zero temperature. One should cite at this stage that Pricoupenko [26] employs the pseudopotential with a Gaussian variational approach. Mora and Castin [27], on the other hand, used their lattice model, which is a sort of regularization scheme to treat ultraviolet divergences. Cherny *et al.* [28] used a reduced-density matrix of second order and a variational procedure to derive results identical to those of Refs. [26,27] for equation of state (EoS) and ground-state energy. The above analytical results have been checked using Monte Carlo calculations to find numerical agreement with beyond-mean-field terms in 2D [29,30]. Recently, Mora and Castin [31] have been also extended their approach [27] one step beyond Bogoliubov theory, which gives good accuracy with the simulations of [30]. Another kind of extension has been developed recently by Sinner *et al.* [32] which is based on using the functional renormalization group to study dynamical properties of the 2D Bose gas at $T = 0$. The approach is free from infrared divergences and satisfies both the Hungeholtz-Pines (HP) [33] relation and the Nepomnyashchy identity [34], which states that the anomalous self-energy vanishes at zero frequency and momentum. The spectrum energy thus satisfies a Bogoliubov-type expression with a renormalized sound velocity. Although the above approaches provide good predictions for the thermodynamic of 2D Bose gas in the universal regime, they are limited only at zero temperature.

The present paper deals with extending our variational time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory to the case of 2D Bose systems. The theory was previously presented for 3D systems in [17,18]. In fact, the main difference between our approach and the earlier variational HFB treatments is that in our variational theory we do not minimize only the expectation values of a single operator like the free energy in the standard HFB approximation. Conversely, our variational theory is based on the minimization of an action also with a Gaussian variational ansatz. The action to minimize involves two types of variational objects: one related to the observables of interest and the other akin to a density matrix [35,36].

The paper is organized as follows. In Sec. II, we briefly review the derivation of the TDHFB formalism and give the different quantities which we study in 2D homogeneous system. In Sec. III, we restrict ourselves to the behavior of the anomalous density and its effects on the depletion, the

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chemical potential, and the ground-state energy. We therefore compare our results with recent Monte Carlo simulations and analytic predictions. The validity of the HP theorem and Nepomnyashchy identity are also discussed within the present formalism. In Sec. IV, we extend our results at finite temperature where we calculate, in particular, the one-body anomalous correlation function. In Sec. V, we apply our formalism to analyze the behavior of the superfluid fraction. We then emphasize the importance of the anomalous density for the occurrence of superfluid transition and sound velocity. Our conclusion and perspectives are drawn in Sec. VI.

II. FORMALISM

Our starting point is the TDHFB equations which describe the dynamics of d-dimensional interacting trapped Bose systems. For a short-range interaction potential and sufficiently dilute gas, the TDHFB equations read

$$i\hbar\dot{\Phi}(r) = [h^{sp} + gn_c(r) + 2g_d\tilde{n}(r)]\Phi(r) + g_d\tilde{m}(r)\Phi^*(r), \tag{1a}$$

$$i\hbar\frac{d\rho}{dt} = \Im\rho - \rho\Im^+, \tag{1b}$$

where $h^{sp} = -\frac{\hbar^2}{2m}\Delta + V_{\rm ext}(\vec{r}) - \mu$ is the single-particle Hamiltonian, $V_{\rm ext}(\vec{r})$ is the external trapping potential, μ is the chemical potential, and g_d is the interaction parameter in d dimensions.

Here we have defined the 2×2 matrices

$$\Im(r,r') = \begin{pmatrix} h(r,r') & \Delta(r',r') \\ -\Delta^*(r,r) & -h^*(r,r') \end{pmatrix}$$

and

$$\rho(r,r') = \begin{pmatrix} \tilde{n}(r,r') & \tilde{m}(r,r') \\ \tilde{m}^*(r,r') & \tilde{n}^*(r,r') + \delta(r,r') \end{pmatrix},$$

where $h(r,r') = h^{sp}(r) + 2g_d[\tilde{n}(\vec{r}',\vec{r}') + \Phi^*(\vec{r}')\Phi(\vec{r}')]$, $\Delta(r,r) = g_d[\tilde{m}(\vec{r},\vec{r}) + \Phi(\vec{r})\Phi(\vec{r})]$, and

$$\begin{aligned} \tilde{n}(\vec{r},\vec{r}') &\equiv \tilde{n}^*(\vec{r},\vec{r}') = \langle\Psi^+(\vec{r})\Psi(\vec{r}')\rangle - \Phi^*(\vec{r})\Phi(\vec{r}'), \\ \tilde{m}(\vec{r},\vec{r}') &\equiv \tilde{m}(\vec{r}',\vec{r}) = \langle\Psi(\vec{r})\Psi(\vec{r}')\rangle - \Phi(\vec{r})\Phi(\vec{r}'), \end{aligned} \tag{2}$$

are, respectively, the normal and anomalous single-particle correlation functions. In the local case they play the role of the noncondensed and anomalous densities. Moreover, our formalism provides a direct link between these two later quantities as

$$I(\vec{r},\vec{r}') = \int d\vec{r}''[\rho_{11}(\vec{r},\vec{r}'')\rho_{22}(\vec{r}'',\vec{r}') - \rho_{12}(\vec{r},\vec{r}'')\rho_{21}(\vec{r}'',\vec{r}')]. \tag{3}$$

Notice that Eq. (3) is often known as the Heisenberg invariant; it is a direct consequence of the conservation of the von Neumann entropy $S = -{\rm Tr}\mathcal{D}\ln\mathcal{D}$. For the pure state Eq. (3) takes the form $I(\vec{r},\vec{r}') = \delta^d(\vec{r} - \vec{r}')$ [37].

Among the advantages of the TDHFB equations is that the three densities are coupled in a consistent and closed way. Second, they should in principle yield the general time, space, and temperature dependence of the various densities. Furthermore, they satisfy the energy and number conserving laws. In addition, the most important feature of the TDHFB equations is that they are valid for any Hamiltonian H and for any density matrix operator. Interestingly, our TDHFB equations can be extended to provide self-consistent equations of motion for the triplet correlation function by using the post-Gaussian ansatz.

In the uniform case [$V_{\rm ext}(r) = 0$] and for a thermal distribution at equilibrium, by working in the momentum space,

$$\rho_{ij}(\vec{r},\vec{r}\prime) = \int \frac{d^dk}{(2\pi)^d} e^{i\vec{k}\cdot(\vec{r}-\vec{r}\prime)}\rho_{ij}(k), \tag{4}$$

where $\rho_{ij}(k)$ is the Fourier transform of $\rho_{ij}(\vec{r},\vec{r}')$. We can then easily rewrite Eq. (3) as

$$I_k = \tilde{n}_k(\tilde{n}_k + 1) - |\tilde{m}_k|^2 = \frac{1}{4\sinh^2(\varepsilon_k/2T)}, \tag{5}$$

where ε_k is the Bogoliubov energy spectrum given below.

The physical meaning of Eq. (5) is that it allows us to calculate in a very useful way the dissipated heat for d-dimensional Bose gas as

$$Q_d = \frac{1}{n}\int E_k I_k \frac{d^dk}{(2\pi)^d}, \tag{6}$$

where $E_k = \hbar^2k^2/2m$ is the energy of a free particle.

Furthermore, at zero temperature, Eq. (5) reduces to $|\tilde{m}_k|^2 = \tilde{n}_k(\tilde{n}_k + 1)$, which constitutes an explicit relationship between the normal and the anomalous densities at zero temperature and indicates that these two quantities are of the same order of magnitude at low temperatures which leads to the fact that neglecting $\tilde{m}$ while maintaining $\tilde{n}$ is a quite unsafe approximation.

The excitation energy ε_k is determined in our formalism via the random-phase approximation (RPA) [36], which can be found by expanding all quantities around their equilibrium solution. The RPA appears as a direct application of the general Balian-Vénéroni formalism to the Lie algebra of single boson operators [36,37].

Thus, we write

$$\begin{aligned} \Phi(k,t) = \Phi(k) + \delta\Phi(k,t), \quad \tilde{n}(k,t) = \tilde{n}(k) + \delta\tilde{n}(k,t), \\ \tilde{m}(k,t) = \tilde{m}(k) + \delta\tilde{m}(k,t). \end{aligned} \tag{7}$$

Then, we have written these quantities on a diagonal basis (RPA matrix), which derived from the set (1), and kept only the first-order terms. After a long, but straightforward, calculation, we arrive at the gapless expression of the Bogoliubov spectrum [18,38]

$$\varepsilon_k = \sqrt{(E_k - \mu + \Sigma_{11})^2 - \Sigma_{12}^2}, \tag{8}$$

where $\Sigma_{11} = 2g_dn$ and $\Sigma_{12} = g_d(n_c + \tilde{m})$ are, respectively, the first-order normal and anomalous self-energies, where $n = n_c + \tilde{n}$ is the total density.

A detailed derivation of the Bogoliubov spectrum with the RPA method will be given elsewhere.

Note that Eq. (8) can be also obtained using the Green's functions (see, e.g., [38]). It provides a useful finite-temperature version of the healing length and the sound

velocity c_s as

$$\xi = \hbar/\sqrt{m\Sigma_{12}} = \hbar \Big/ \sqrt{m n_c g_d \left(1 + \frac{\tilde{m}}{n_c}\right)} = \hbar/mc_s. \quad (9)$$

In order to get explicit formulas for the noncondensed and the anomalous averages in d-dimensions we may use Eq. (5). A simple calculation yields

$$\tilde{n} = \frac{1}{2}\int \frac{d^d k}{(2\pi L^{-1})^d}\left[\frac{E_k + g_d(n_c + \tilde{m})}{\varepsilon_k}\sqrt{I_k} - 1\right], \quad (10a)$$

$$\tilde{m} = -\frac{1}{2}\int \frac{d^d k}{(2\pi L^{-1})^d}\left[\frac{g_d(n_c + \tilde{m})}{\varepsilon_k}\sqrt{I_k}\right]. \quad (10b)$$

It is worth noting that Eqs. (1a) and (10) together form the generalized HFB equations. This shows that, in the static case, our formalism recovers easily the full HFB equations at both finite and zero temperatures.

III. ANOMALOUS DENSITY AT ZERO TEMPERATURE

Let us now discuss the behavior of the normal and anomalous densities in homogeneous 2D Bose gas at both zero and finite temperatures. From this point we consider the regime in weakly repulsive interaction at zero temperature, where $\sqrt{I_k} = 1$. In 2D Bose gas, the interaction parameter ($g_d = g_2$) depends logarithmically on the chemical potential as

$$g_2 = \left[\frac{4\pi\hbar^2}{m}\frac{1}{\ln(2\hbar^2/m\mu a^2)}\right], \quad (11)$$

where a is the 2D scattering length among the particles and g_2 is the two-body T matrix (see, e.g., [15,26,27]).

The calculation of the integral in Eq. (10a) leads us to the following expression of the depletion:

$$\frac{\tilde{n}}{n} = \frac{1}{4\pi n\xi^2}. \quad (12)$$

This equation is in good agreement with that obtained in [26].

The integral in Eq. (10b) has an ultraviolet divergence in both two and three dimensions. This divergence is well known and arises due to the use of the contact potential. To regulate the ultraviolet divergences, we may use the dimensional regularization [39,40]. In such a technique one calculates the loop integrals in $d = 2 - 2\eta$ dimensions for values of η where the integrals converge. One then analytically continues back to $d = 2$ dimensions. With dimensional regularization, an arbitrary renormalization scale M is introduced. This scale can be identified with the simple momentum cutoff. An advantage of dimensional regularization is that in 2D systems it automatically sets power divergences to zero, while logarithmic divergences show up as poles in η [40]. Using this technique one gets for the anomalous density

$$\tilde{m}^{\Lambda}_{T=0} = -\frac{\Lambda^2}{4}J_{0,1}, \quad (13)$$

where Λ is the regularized part, which is related to the size of particles and interactions as $\Lambda = 2/\xi$. This parameter is similar to that used in [26,32,40].

And $J_{0,1} = \frac{1}{4\pi}\left[\frac{1}{\eta} - L + O(\eta)\right]$ with $L = \ln(\Lambda^2/4M^2)$.

Thus, the convergent part of the anomalous density provides

$$\tilde{m}^{\Lambda}_{T=0} = \frac{\Lambda^2}{16\pi}\ln(\Lambda^2/4M^2). \quad (14)$$

A useful remark at this level, the noncondensed density of Eq. (12), can be rewritten also in terms of Λ as $\tilde{n} = \Lambda^2/16\pi$.

At $T = 0$, the condensed density has a significant value and hence constitutes the dominant quantity in the system, while both the noncondensed and the anomalous densities vanish for $\Lambda \to 0$, which ensures that $\Sigma_{11}^{\Lambda=0} = 2\mu$ and $\Sigma_{12}^{\Lambda=0} = \mu$, in good accordance with the Hugenholtz-Pines theorem $\Sigma_{11}^{\Lambda=0} - \Sigma_{12}^{\Lambda=0} = \mu$ [33]. On the other hand, once we find $\Sigma_{12}^{\Lambda=0} \neq 0$, this means that the actual version of our extended variational TDHFB including a dimensional regularization does not satisfy the Nepomnyashchy identity [32] as it should for any limited approximation order (see, for example, Griffin and Shi [38], Yukalov and Graham [19], Pricoupenko [26], and Andersen and Haugerud [40]). Indeed, in a Bose-condensed system, the anomalous self-energy must be nonzero in order to define a meaningful nonzero sound velocity and healing length. In addition, a zero sound velocity leads evidently to an unstable system [see Eq. (9)].

Indeed, our approach can be an effective way to verify the Nepomnyashchy identity, but on the condition that we sum over all terms of perturbation theory for the self-energy with renormalization of the sound velocity to ensure the stabilization of the system as it has been demonstrated in [32].

Conversely, at finite-temperature 3D Bose gas, the chemical potential satisfies the generalized version of HP theorem given by Hohenberg and Martin [41] $\Sigma_{11}^{\Lambda} - \Sigma_{12}^{\Lambda} = \mu$. In such a situation, when $T \geqslant T_c$, both the condensate and the anomalous densities vanish [17–19,24,25] whatever the value of Λ, which implies directly that $\Sigma_{12}^{\Lambda} = 0$ and $\Sigma_{11}^{\Lambda} = 2g\tilde{n} \approx 2\mu$. Consequently, a vanishing anomalous self-energy is further guaranteed at high temperature and momentum in 3D systems. Physically, this result is reasonable because the gas becomes completely thermalized and therefore there is neither superfluid nor acoustic waves when the temperature reaches its critical value.

On the other side, the dimensional regularization gives an asymptotically exact result at weak interactions ($g_2 \to 0$). The extrapolation to finite interactions requires that the limiting condition $\tilde{m}/n_c \ll 1$ be verified. In real systems, however, the interactions have a finite range a and so $1/a$ provides a natural ultraviolet cutoff M [40]. Hence, using this technique presupposes that value of the healing length in Eqs. (12) and (13) takes the form $\xi = \hbar/\sqrt{mn_c g_2}$. In the case where $n_c \approx n$, we recover easily the well-known result of Schick [11] for the depletion, while Eq. (14) has no analog in the literature. Under these conditions, the anomalous average turns out to be given as

$$\tilde{m}_{T=0} = \frac{m\mu_0}{4\pi\hbar^2}\ln\left(\frac{m\mu_0 a^2}{\hbar^2}\right), \quad (15)$$

where $\mu_0 = g_{2d}n$.

Figure 1 shows that the noncondensed and the anomalous densities, as function of the dimensionless parameter $x = m\mu_0 a^2/\hbar^2$, are competitive contributions at zero temperature. For small values of x, we observe that the noncondensed

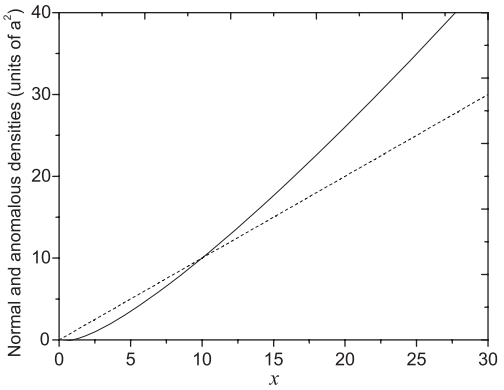

FIG. 1. Noncondensed (dashed line) and anomalous (solid line) densities as function of $x = m\mu_0 a^2/\hbar^2$.

density is greater than the anomalous one while this later becomes the dominant quantity for the whole range of $x(x > 10)$. $\tilde{n}$ and $\tilde{m}$ are comparable only for $x \approx 10$. Therefore, we deduce that omitting the anomalous density, while keeping the normal one, is physically and mathematically inappropriate. It is noticed that this behavior holds also in 3D Bose gas [17–25].

It is important now to discuss how the anomalous density can modify the chemical potential and hence the other thermodynamic quantities of dilute Bose gas. The first-order quantum corrections to the chemical potential are given by $\delta\mu = g_d\,(\tilde{n} + \tilde{m})$ [42]. Therefore, using the results obtained in Eqs. (12) and (15) with the assumption $n \approx n_c$ at $T = 0$. One obtains for the chemical potential

$$\mu = \mu_0 \left[1 + \frac{m\mu_0}{4\pi\hbar^2 n} \ln\left(\frac{m\mu_0 a^2 e}{\hbar^2}\right)\right]. \tag{16}$$

The ground-state energy is obtained through

$$E/N = \int_0^n \mu dn = \frac{\mu_0}{2}\left[1 + \frac{mg_2}{8\pi\hbar^2} \ln\left(\frac{m\mu_0 a^2\sqrt{e}}{\hbar^2}\right)\right]. \tag{17}$$

The leading term in Eq. (16) was first obtained by Schick [11], while the second represents our correction to the chemical potential. Clearly, this correction is *universal*, depending only on the interactions and scattering length. It is worth mentioning that the additional logarithm term in Eq. (16) is analogous to

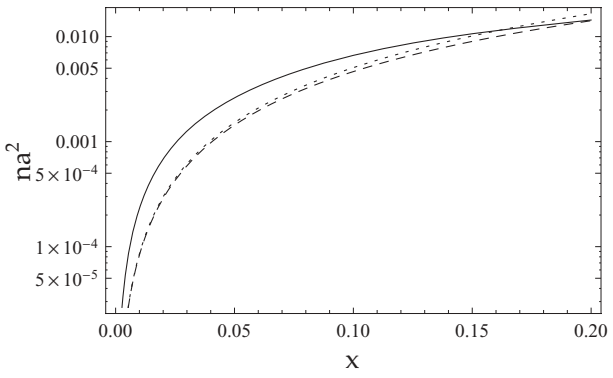

FIG. 2. Equation of state of a 2D homogeneous Bose gas. Solid line, our extended variational approach; dashed line, EoS predicted in [26,27]; dotted line, first correction beyond Bogoliubov theory [31].

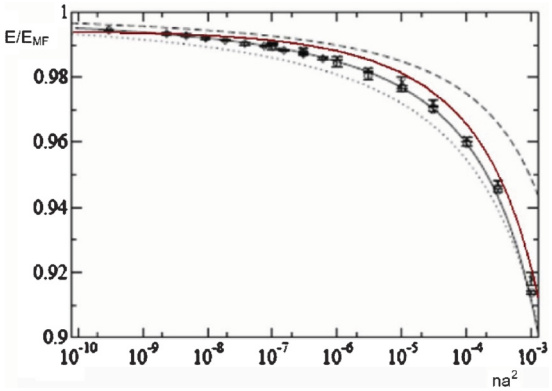

FIG. 3. (Color online) Ground-state energy of a 2D Bose gas, as a function of the gas density, in units of the mean-field prediction $E_{\rm MF}$. Brown solid line, our calculations; dark solid line, energy obtained from the beyond Bogoliubov [31]; dashed line, analytical prediction of [28]; dotted line, analytical calculations of [26]. Plotting symbols with error bars, numerical results of [29], for interactions given by hard disks (crosses) and by soft disks (circles); numerical results of [30], for dipolar interactions (diamonds).

that found recently in [31]. Moreover, what is interesting in Eq. (16) is that if we invert it and take the limit of vanishing density, we thereby recover the well-known Popov's EoS [12].

Before plotting Figs. 2 and 3, we use the dimensionless relation $na^2 = x^2[\frac{1}{2} - \ln(\frac{xe^\gamma}{2})]$, where γ is the Euler's constant [26,31].

One can see from Fig. 2 that for the value of the gas parameter around 5×10^{-5} there is a difference of 10% between diverse EoS, while for na^2 larger than 5×10^{-3} all EoS are practically identical.

Figure 3 shows that our expression of the ground-sate energy [Eq. (17)] gives also an estimate compatibility within error bars of Monte Carlo simulations [29,30] and analytic results of [26–28,31]. Furthermore, it is clearly seen from Figs. 2 and 3 that there is an upward shift of our curve relative to that of Ref. [31], which is indeed due to a prefactor which appears in the expansion of the later reference.

Another important feature revealed in Fig. 3 is that there is no difference between dipolar and short-range interaction for densities lower than 10^{-10} [30].

IV. ANOMALOUS DENSITY AT FINITE TEMPERATURE

Now we turn to analyze the finite-temperature case. As we mentioned in the Introduction, the finite-temperature uniform 2D Bose gas is characterized by the absence of a true Bose-Einstein condensate and long-range order [9,10]. So the physics of 2D Bose gas at finite T can be understood in the context of the density-phase representation. Accordingly, the single-particle anomalous correlation function is found by using the field operator in the form $\Psi = \sqrt{n}e^{i\phi}$. Following the hydrodynamic approach described in [14,15,43] with the assumptions $\tilde{m}/n_c \ll 1$ and $n_c \approx n$ for $T \to 0$. Then on the basis of Eq. (2), we obtain for the single-particle anomalous

correlation function

$$\tilde{m}(\vec{r},0) = n \exp\left[-\frac{1}{2n}\int d\vec{k}\,\frac{\varepsilon_k}{E_k}\coth(\varepsilon_k/2T)\cos^2\left(\frac{\vec{k}\cdot\vec{r}}{2}\right)\right]. \tag{18}$$

At low temperatures ($T \ll \mu$) the main contribution to the integral of Eq. (18) comes from the region of small momentum; then the single-particle anomalous correlation function undergoes a slow law decay at large distances:

$$\tilde{m}(r) = n\left(\frac{\xi}{r}\right)^{T/2T_d}, \tag{19}$$

where $T_d = \frac{2\pi\hbar^2 n}{m}$ is the temperature of quantum degeneracy.

We can infer from these results that the anomalous average does not exist at finite temperature. This is strictly confirmed by Eq. (19), where one finds that $\tilde{m}(r)$ vanishes for $r \to \infty$. Similarly to the 2D situation at finite temperature regarding the normal correlator $\tilde{n}(\vec{r},\vec{r}') = \langle\Psi^+(\vec{r})\Psi(\vec{r}')\rangle - \Phi^*(\vec{r})\Phi(\vec{r}')$, which tends to zero as$r \to \infty$, confirming that there is no true condensate, but one identifies instead the existence of a quasicondensate. However, this result also implies that there is no symmetry breaking, and consequently the anomalous average should not exist at any nonzero temperature. The butter of this result is that the anomalous density accompanies in a manner analogous the true condensate in a system of 2D homogeneous Bose gas.

V. SUPERFLUID FRACTION

Usually, Bose-Einstein condensation (BEC) is accompanied by superfluidity. However, in a 2D system at finite temperature, there is no BEC, but there still exists superfluidity. The relation between them depends on the Bogoliubov-type nature of the spectrum Eq. (7) [13]. Also, what is important is that our formalism provides a useful relation between the superfluid fraction and the dissipated heat, which is equivalent to that obtained in Refs. [13,19],

$$f_s = \frac{n_s}{n} = 1 - \frac{\hbar^2}{2mnT}\int \frac{d^2k}{(2\pi)^2}k^2\frac{e^{\varepsilon_k/T}}{(e^{\varepsilon_k/T}-1)^2} = 1 - \frac{Q_{d=2}}{T}, \tag{20}$$

where $n_s$is the superfluid density.

It is very important to mention that the superfluid fraction f_s will be a divergent quantity and thus the superfluid transition does not occur when the anomalous average is omitted in Eq. (20).

At low temperature and weak interaction, we get

$$f_s = 1 - \frac{3\varsigma(3)}{2\pi\hbar^2 mnc_s^4}T^3, \tag{21}$$

where $\varsigma(3)$ is a Riemann ζ function and the sound velocity turns out to be given

$$c_s = c_s^{(0)}\sqrt{\left(1 - \frac{\tilde{n}}{n} + \frac{\tilde{m}}{n}\right)}, \tag{22}$$

where $c_s^{(0)} = \sqrt{\mu_0/m}$ is the zero-order sound velocity.

Upon neglecting the normal and the anomalous fractions we recover straightforwardly the superfluid fraction obtained earlier by Popov [12] and by Fisher and Hohenberg [13].

VI. CONCLUSION

We have studied in this paper the behavior of the anomalous density in 2D homogeneous Bose gases. We find that this quantity has a finite value in the limit of weak interactions. We have discussed also the effects of the anomalous average on some thermodynamic quantities. As an example, we have given formulas for the chemical potential, ground-state energy, the depletion, and superfluid fraction. The later does not occur if the anomalous density is neglected. In the ultradilute limit, the known results are reproduced. This feature makes our predictions in accordance with Monte Carlo simulations and analytical calculations. Also, we have shown that our approach well satisfies the HP theorem at zero temperature, while it does not verify the Nepomnyashchy identity as it should be for any limited approximation. Moreover, the importance of the anomalous density compared to the normal one at low temperature has been also highlighted. In addition, by using the density phase fluctuation we found that the single-particle anomalous correlation function undergoes a slow law decay at large distances. Such a result implies that the anomalous average does not exist at finite temperature.

Finally, an interesting question to ask is whether some quantity can exist in this system which accompanies the quasicondensate density in a manner analogous to that in which the anomalous density accompanies a true condensate?

The goal of our next work is to use our approach to answer this important question. On the other hand, we will try to extract something useful about superfluidity in 2D Bose system. The idea is to relate our predictions with appropriate numerical simulations for some realistic experiments in traps to study, for example, the vortex stability without rotating fluid.

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Two-dimensional dipolar Bose gas with the roton-maxon excitation spectrum

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We discuss fluctuations in a dilute two-dimensional Bose-condensed dipolar gas, which has a roton-maxon character of the excitation spectrum. We calculate the density-density correlation function, fluctuation corrections to the chemical potential, compressibility, and normal (superfluid) fraction. It is shown that the presence of the roton strongly enhances fluctuations of the density, and we establish the validity criterion of the Bogoliubov approach. At $T = 0$ the condensate depletion becomes significant if the roton minimum is sufficiently close to 0. At finite temperatures exceeding the roton energy, the effect of thermal fluctuations is stronger and it may lead to a large normal fraction of the gas and compressibility.

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In the last decade, ultracold gases of dipolar particles, which include atoms with a large magnetic moment and polar molecules, have attracted a great deal of interest [1–4]. Being electrically or magnetically polarized, such particles interact with each other via long-range anisotropic dipole-dipole forces, which drastically changes the nature of quantum degenerate regimes. Experiments with chromium atoms (magnetic moment $6\mu_B$) [2], together with theoretical studies [5,6], have revealed the dependence of the shape and stability diagram of trapped dipolar Bose-Einstein condensates on the trapping geometry and interaction strength. They initiated spinor physics with quantum dipoles [7,8], and now dysprosium [9] and erbium [10] atoms (magnetic moments $10\mu_B$ and $7\mu_B$, respectively) have also entered the game. Recently, fascinating prospects for the observation of novel quantum phases have been opened by the creation of ultracold clouds of polar molecules and their cooling almost to quantum degeneracy [3,11]. In this case, the dipole-dipole forces can be orders of magnitude larger, and one has the possibility of manipulating the molecules by making use of their rotational degrees of freedom.

For dipolar Bose-condensed gases, one of the key issues was related to the presence of the roton-maxon character of the excitation spectrum and to the possibility of obtaining supersolid states in which the condensate wave function is the superposition of a uniform background and a lattice structure. The roton-maxon structure of the spectrum was first predicted for strongly pancaked Bose-Einstein condensates [12]. However, the idea of obtaining a supersolid state when the roton reaches 0 and the uniform BEC becomes unstable did not succeed because of the collapse of the system [13,14]. Since that time, several proposals have been made for the creation of supersolid states with bosons [15]. They rely on the potential of interatomic interaction which is flat at short distances and decays at large separations, and the results then indicate the presence of dense supersolid clusters [16].

This activity brought in analogies with liquid helium, where studies of the roton-maxon spectrum and attempts to observe the supersolid state experimentally have spanned decades [17,18] since the early theoretical prediction [19]. However, the most credible claim to observation of the supersolid [20] has now been withdrawn [21]. It is worth mentioning that the old idea of obtaining a stable density-modulated state (supersolid) in superfluid helium moving at a supercritical velocity [22] is now being discussed in the general context of superfluidity in Bose gases flowing with velocities higher than the Landau critical velocity [23].

The roton-maxon character of the excitation spectrum has also attracted great attention by itself. In relation to liquid helium, it has been discussed how the position of the roton minimum influences the phenomenon of superfluidity [18]. In the context of dipolar bosons in two dimensions, numerical calculations of the zero-temperature phase diagram [24–26] found that the reduction of the condensed fraction with an increase in density can be attributed to the appearance of the roton minimum. Finite-temperature Monte Carlo calculations [27] have revealed that the rotonization of the spectrum can decrease the Kosterlitz-Thouless superfluid transition temperature. Although the calculations [24–27] were focused on fairly high densities, they raised the question of the applicability of the Bogoliubov approach for dipolar bosons [26]. At the same time, there was extended activity on the static and dynamical properties of dilute trapped dipolar BECs on the basis of the Bogoliubov approach [28–31].

It is therefore instructive to identify the validity criterion of the Bogoliubov approach for Bose-condensed dipolar gases with the roton-maxon excitation spectrum, and this is the subject of the present paper. We show that at zero temperature the density fluctuations originating from the presence of the roton minimum lead to a significant depletion of the condensate and modify thermodynamic quantities if the roton minimum is sufficiently close to 0. At finite temperatures exceeding the roton energy, thermal density fluctuations may have a much stronger influence, leading to a large increase in the normal fraction and compressibility.

We consider a dilute Bose-condensed gas of dipolar bosons (tightly) confined in one direction (z) to zero-point oscillations and assume that in the x, y plane the translational motion is free (see Fig. 1). The dipole moments are oriented perpendicularly to the x, y plane, which, for electric dipoles (polar molecules), can be done by applying an electric field and, for magnetic atoms, by using a magnetic field. In this quasi-two-dimensional (2D) geometry, at large interparticle

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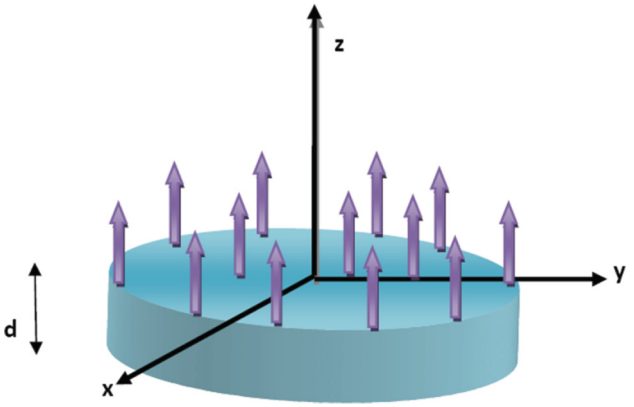

FIG. 1. (Color online) Dipolar Bose-Einstein condensate tightly confined in one direction.

separations r the interaction potential is

$$V(r) = \frac{d^2}{r^3} = \frac{\hbar^2 r_*}{m r^3}, \tag{1}$$

with d being the dipole moment, m the particle mass, and $r_* = md^2/\hbar^2$ the characteristic dipole-dipole distance. The short-range part of the potential is assumed to be such that there is a roton-maxon excitation spectrum. In the ultracold limit where the particle momenta satisfy the inequality $kr_* \ll 1$, the off-shell scattering amplitude, defined as $f(\vec{k},\vec{k}') = \int \exp(-i\vec{k}' \cdot \vec{r}')V(r)\psi_{\vec{k}}(\vec{r})d^2r$ ($\psi_{\vec{k}}(\vec{r})$ is the wave function of the relative motion with momentum $\vec{k}$), is given by (see [32] and references therein):

$$f(\vec{k},\vec{k}') = \frac{\hbar^2}{m}\left[\frac{2\pi}{\ln(\kappa/k) + i\pi/2} - 2\pi r_*|\vec{k} - \vec{k}'|\right], \tag{2}$$

where we omit higher order terms in k. The second term on the right-hand side represents the so-called anomalous contribution coming from distances of the order of the de Broglie wavelength of particles [33]. It takes into account all partial waves and is obtained using a perturbative approach in $V(r)$. The first term on the right-hand side of Eq. (2) describes the short-range contribution. It is obtained by putting $k' = 0$ and proceeding along the lines of the 2D scattering theory [33]. The parameter κ depends on the behavior of $V(r)$ at short distances. In the quasi-2D geometry it also depends on the confinement length in the z direction, $l_0 = \sqrt{\hbar/m\omega_0}$, where ω_0 is the confinement frequency. One then can express κ through the 3D coupling constant g_{3D}. If the 3D s-wave scattering length, $a_{3D} = mg_{3D}/4\pi\hbar^2 \ll l_0$, then κ is exponentially small [34,35] and we may omit the k dependence under logarithm in Eq. (2), as well as $i\pi/2$ in the denominator of the first term. This gives $f(\vec{k},\vec{k}') = g(1 - C|\vec{k} - \vec{k}'|)$, where the 2D short-range coupling constant is $g = g_{3D}/\sqrt{2}l_0$ and $C = 2\pi\hbar^2 r_*/mg = 2\pi d^2/g$. Employing this result in the secondly quantized Hamiltonian [13,14], we obtain

$$\hat{H} = \sum_{\vec{k}} E_k \hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}} + \frac{g}{2S}\sum_{\vec{k},\vec{q},\vec{p}}(1 - C|\vec{q} - \vec{p}|)\hat{a}^\dagger_{\vec{k}+\vec{q}}\hat{a}^\dagger_{\vec{k}-\vec{q}}\hat{a}_{\vec{k}+\vec{p}}\hat{a}_{\vec{k}-\vec{p}}, \tag{3}$$

where S is the surface area, $E_k = \hbar^2k^2/2m$, and $\hat{a}^\dagger_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}$ are the creation and annihilation operators of particles. At zero temperature there is a true BEC in two dimensions, and we may use the standard Bogoliubov approach. Assuming the weakly interacting regime where $mg/2\pi\hbar^2 \ll 1$ and $r_* \ll \xi$, with $\xi = \hbar/\sqrt{mng}$ being the healing length, we reduce Hamiltonian (3) to a bilinear form, use the Bogoliubov transformation $\hat{a}^\dagger_{\vec{k}} = u_k\hat{b}^\dagger_{\vec{k}} - v_k\hat{b}_{-\vec{k}}$, and obtain the diagonal form $\hat{H} = E_0 + \sum_{\vec{k}}\varepsilon_k\hat{b}^\dagger_{\vec{k}}\hat{b}_{\vec{k}}$ in terms of operators $\hat{b}^\dagger_{\vec{k}}$ and $\hat{b}_{\vec{k}}$ of elementary excitations. The Bogoliubov functions u_k and v_k are expressed in a standard way, $u_k, v_k = (\sqrt{\varepsilon_k/E_k} \pm \sqrt{E_k/\varepsilon_k})/2$, and the Bogoluibov excitation energy is given by $\varepsilon_k = \sqrt{E_k^2 + 2ngE_k(1 - Ck)}$.

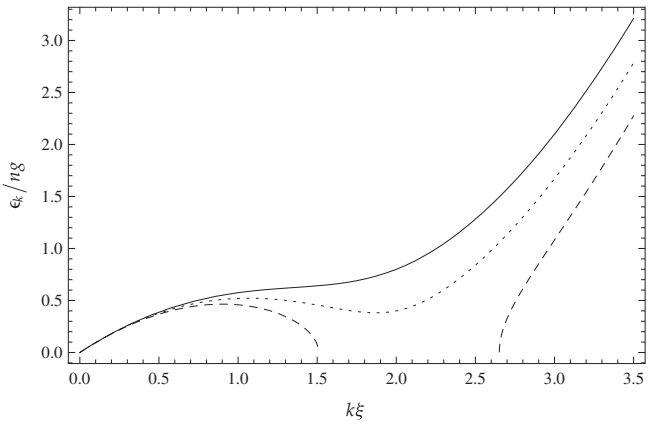

FIG. 2. Excitation energy ε_k of a quasi-2D dipolar BEC as a function of momentum k for several values of k_r. The solid curve ($k_r\xi = 1.84$) shows a monotonic dependence ε_k, the dotted curve ($k_r\xi = 1.96$) is ε_k with the roton-maxon structure, and the dashed curve ($k_r\xi = 2.08$) corresponds to a dynamically unstable BEC.

To zero order the chemical potential is $\mu = ng$. For small momenta the excitations are sound waves, $\varepsilon_k = \sqrt{ng/m}k$. The dependence of ε_k on k remains monotonic with increasing k if $C \leqslant \sqrt{8}\xi/3$ (see Fig. 2). For the constant C in the interval

$$\frac{\sqrt{8}}{3}\xi \leqslant C \leqslant \xi, \tag{4}$$

the excitation spectrum has a roton-maxon structure. It is then convenient to represent ε_k in the form

$$\varepsilon_k = \frac{\hbar^2 k}{2m}\sqrt{(k - k_r)^2 + k_\Delta^2}, \tag{5}$$

where $k_r = 2C/\xi^2$ and $k_\Delta = \sqrt{4/\xi^2 - k_r^2}$. If the roton is close to 0, then k_r is the position of the roton, and

$$\Delta = \hbar^2 k_r k_\Delta/2m = 2ngC\sqrt{mng/\hbar^2 - C^2(mng/\hbar^2)^2} \tag{6}$$

is the height of the roton minimum (see Fig. 2). For $C = \xi$ the roton minimum touches 0, and at larger C the uniform Bose condensate becomes dynamically unstable.

It should be noted that the coupling constant g can be tuned by using Feshbach resonances or by modifying the frequency of the tight confinement ω_0. Therefore, although the range of C given by Eq. (4) is rather narrow, it can be reached without serious difficulties. The condition $C = 2\pi d^2/g = \xi$ is reduced to $(mg/2\pi\hbar^2) = a_{3D}/\sqrt{2}l_0 \simeq 2\pi n r_*^2$. For dysprosium atoms we have the dipole-dipole distance $r_* \simeq 200$ Å, and at 2D densities $\sim 10^9$ cm^{-2} the roton-maxon spectrum is realized for

the 3D scattering length a_{3D} of several tens of angstroms at the frequency of the tight confinement of 10 kHz, leading to a confinement length l_0 of about 1000 Å.

The Bogoliubov approach assumes that the density and phase fluctuations are small. In the 2D case at $T = 0$, the presence of the roton does not significantly change the phase fluctuations and they remain small. However, the situation with density fluctuations is different. Writing the operator of the density fluctuations as (see [36]) $\delta\hat{n} = \sqrt{n}\sum_{\vec{k}}(u_k - v_k)\exp(i\vec{k}\cdot\vec{r})\hat{b}_{\vec{k}} + \text{H.c.}$, we obtain for the density-density correlation function:

$$\frac{\langle\delta\hat{n}(\vec{r})\delta\hat{(0)}\rangle}{n^2} = \frac{1}{n}\int\frac{d^2k}{(2\pi)^2}\frac{E_k}{\varepsilon_k}(1+2N_k)\exp(i\vec{k}\cdot\vec{r}), \quad (7)$$

where $N_k = [\exp(\varepsilon_k/T) - 1]^{-1}$ are occupation numbers for the excitations. It is instructive to single out the roton contribution to the correlation function, (7). Asuming that the roton is close to 0 and the roton energy is $\Delta \ll ng$, we have the coefficient C close to ξ, and $k_r \simeq 2/\xi$. Then, using Eqs. (5) and (7), for the contribution of momenta near the roton minimum at, $T = 0$ we obtain

$$\frac{\langle\delta\hat{n}(\mathbf{r})\delta\hat{n}(0)\rangle_r}{n^2} = \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right)J_0(2r/\xi); \quad \Delta \ll ng, \quad (8)$$

where J_0 is the Bessel function.

We thus see that the density fluctuations grow logarithmically when the roton minimum is approaching 0 and they can become strong for very small Δ. In this case they lead to a significant depletion of the condensate. The noncondensed density of particles is $n' = \int v_k^2 d^2k/(2\pi)^2$ and the integral over dk is logarithmically divergent at large momenta because of the dipolar contribution to the interaction strength, $-gCk$. However, this form of the dipole-dipole contribution is valid only for $k \ll 1/r_*$. We thus may set a high momentum cut-off, $1/r_*$, which leads to (see Fig. 3)

$$\frac{n'}{n} = \frac{mg}{4\pi\hbar^2}\left[1 - k_r\xi - \frac{3(k_r\xi)^2}{4} + \frac{(k_r\xi)^2}{2}\ln\left(\frac{\xi}{r_*(2-k_r\xi)}\right)\right]. \quad (9)$$

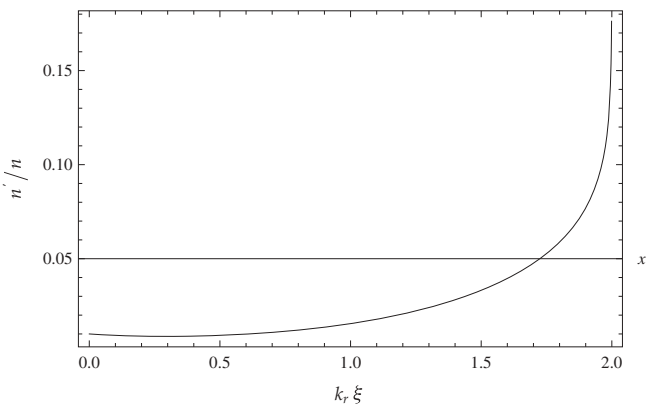

FIG. 3. Noncondensed fraction as a function of $k_r\xi$ for $mg/4\pi\hbar^2 = 0.01$ ($\xi/r_* = 100/k_r\xi$). A similar increase in the noncondensed fraction with decreasing roton energy Δ was found in numerical calculations in Ref. [28].

In the absence of the dipole-dipole interaction ($r_* = 0$ and $k_r = 0$) we recover the usual result for the 2D BEC with short-range interparticle repulsion, $n' = n(mg/4\pi\hbar^2)$. For $\Delta \ll ng$ we have $(2 - k_r\xi) \simeq (k_\Delta\xi)^2/4$ and Eq. (9) transforms to

$$\frac{n'}{n} \simeq \frac{mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\zeta\right), \quad \Delta \ll ng, \quad (10)$$

where $\zeta = \sqrt{2\pi\hbar^2/e^2mg}$.

As we see from Eqs. (8) and (10), for a roton minimum close to 0 a small condensate depletion and small fluctuations of the density require the inequality $(mg/\pi\hbar^2)\ln(2ng/\Delta) \ll 1$. It differs only by a logarithmic factor $\ln(2ng/\Delta)$ from the small parameter of the theory, $(mg/2\pi\hbar^2) \ll 1$, in the absence of a roton. The same logarithmic factor appears in the fluctuation correction to the chemical potential and in the one-body density matrix $g_1(r) = \langle\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(0)\rangle$, where $\hat{\Psi}(\vec{r})$ is the field operator. Assuming that the roton minimum is close to 0 and taking into account only the contribution of momenta near this minimum, for $\Delta \ll ng$ we have

$$g_1(r) = n_0\left[1 + \frac{mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right)J_0(2r/\xi)\right]. \quad (11)$$

The correction to the chemical potential due to quantum fluctuations is given by

$$\frac{\delta\mu}{\mu} \simeq \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right), \quad \Delta \ll ng. \quad (12)$$

However, the situation changes in the calculation of the compressibility. At $T = 0$ the inverse compressibility is equal to $n^2\partial\mu/\partial n$. Then, using Eqs. (12) and (6), for a roton minimum close to 0, at $\Delta \ll ng$ we obtain

$$\frac{\partial\mu}{\partial n} = g\left[1 + \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right) + \frac{mg}{\pi\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\right], \quad (13)$$

where g is the mean-field contribution, and the second and third terms originate from quantum fluctuations. Small deviations of the compressibility from the mean-field result require the inequality

$$\frac{mg}{\pi\hbar^2}\left(\frac{2ng}{\Delta}\right)^2 \ll 1. \quad (14)$$

We thus conclude that at $T = 0$ the validity of the Bogoliubov approach is guaranteed by the presence of the small parameter, (14). For the dysprosium example given after Eq. (6) we have $ng \sim 5$ nK, and criterion (14) is satisfied for a roton energy above 2 nK.

In two dimensions at finite temperatures, long-wave fluctuations of the phase destroy the condensate [37–39]. There is the so-called quasicondensate, or condensate with fluctuating phase. In this state fluctuations of the density are suppressed but the phase still fluctuates. The transition from a noncondensed state to a quasi-BEC is of the Kosterlitz-Thouless type and it occurs through the formation of bound vortex-antivortex pairs [40]. Somewhat below the Kosterlitz-Thouless transition temperature the vortices are no longer important, and in the weakly interacting regime that we consider the phase

coherence the length l_ϕ is exponentially large. Thermodynamic properties, excitations, and correlation properties on a distance scale smaller than l_ϕ are the same as in the case of a true BEC. Moreover, for realistic parameters of quantum gases, l_ϕ exceeds the size of the system [41], so that one can employ the ordinary BEC theory.

Irrespective of the relation between l_ϕ and the size of the system, one may act in terms of the density and phase variables (hydrodynamic approach). We now show that the rotonization of the spectrum can strongly increase thermal fluctuations of the density and destroy the Bose-condensed state even at very low T. Using Eq. (7) we calculate the density-density correlation function. Assuming that the roton energy Δ is very low (at least $\Delta \ll T$), the main contribution to the integral in Eq. (7) comes from momenta near k_r, and we obtain

$$\frac{\langle \delta\hat{n}(\mathbf{r})\delta\hat{(}0)\rangle}{n^2} = \frac{4mg}{\hbar^2}\frac{T}{\Delta}J_0(2r/\xi), \tag{15}$$

where it is also assumed that $k_\Delta r \ll 1$. Comparing this result with Eq. (8) we see that instead of the logarithmic factor we have $2\pi T/\Delta \gg 1$.

The same factor appears in the correction to the chemical potential due to thermal fluctuations:

$$\frac{\delta\mu}{\mu} = \sum_{\mathbf{k}}(u_k - v_k)^2 N_k \simeq \frac{2mg}{\hbar^2}\frac{T}{\Delta}, \quad \Delta \ll T. \tag{16}$$

We now calculate the density of the normal component in the presence of the roton. In two dimensions the expression for this quantity reads (cf. [36])

$$n_T = -\int \frac{\hbar^2 k^2}{2m}\frac{\partial N_k}{\partial \varepsilon_k}\frac{d^2k}{(2\pi)^2}.$$

If the roton minimum is close to 0 and $\Delta \ll T$, then the momenta near the roton minimum are the most important, and the integration over dk yields

$$\frac{n_T}{n} = \frac{2mg}{\hbar^2}\frac{T}{\Delta}. \tag{17}$$

The employed approach requires the condition $n_T \ll n$ because we used the spectrum of excitations obtained by the Bogoliubov method. Again, at temperatures $T \gtrsim \Delta$ we should have the inequality $(2mg/\hbar^2)T/\Delta \ll 1$.

A different small parameter appears in the calculation of the compressibility. The inverse isothermal compressibility is proportional to $(\partial P/\partial n)_T$, where the pressure is $P = -(\partial F/\partial S)_T$, with the free energy given by $F = E_0 + T\sum_{\mathbf{k}} \ln[1 - \exp(-\varepsilon_k/T)]$. For a roton minimum close to 0 and $\{T, ng\} \gg \Delta$, we obtain

$$\left(\frac{\partial P}{\partial n}\right)_T = ng\left[1 - \frac{mg}{\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\frac{T}{\Delta} + \cdots\right], \tag{18}$$

where we omitted less important finite-temperature contributions and the zero-temperature contribution proportional to the small parameter, (14). Equation (18) shows that at $T \gg \Delta$ the Bogoliubov approach requires the inequality

$$\frac{mg}{\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\frac{T}{\Delta} \ll 1, \tag{19}$$

whereas for $T \lesssim \Delta$ it is sufficient to have criterion (14).

For certain quantities the Bogoliubov approach may give good results at $T \gg \Delta$ if $(mg/\hbar^2)T/\Delta \ll 1$ and at $T \lesssim \Delta$ in the presence of the ordinary small parameter $mg/2\pi\hbar^2$ amplified by a logarithmic factor $\ln(2ng/\Delta)$ for $ng \gg \Delta$. However, the validity of this approach is guaranteed only if inequalities (19) and (14) are satisfied. For $T \gg \Delta$ the compressibility following from Eq. (18) and the normal fraction given by Eq. (17) can become significant, by far exceeding similar quantities in an ordinary 2D Bose gas with short-range interactions at the same temperature, coupling constant g, and density.

In conclusion, we have shown that the roton-maxon structure of the excitation spectrum, which can be achieved in dipolar Bose-condensed gases in 2D geometry, strongly enhances the density fluctuations. We obtained the validity criterion of the Bogoliubov approach and found that at finite temperatures in the dilute regime where $nr_*^2 \ll 1$, thermal fluctuations may significantly increase the compressibility and reduce the superfluid fraction even at temperatures well below the Kosterlitz-Thouless transition temperature.

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