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# Overview and introduction

Since the dramatic discovery of Bose–Einstein condensation (BEC) in trapped atomic gases in 1995 (Anderson *et al.*, 1995), there has been an explosion of theoretical and experimental research on the properties of Bose-condensed dilute gases. The first phase of this research was discussed in the influential review article by Dalfovo *et al.* (1999) and in the proceedings of the 1998 Varenna Summer School on BEC (Inguscio *et al.*, 1999). More recently, this research has been well documented in two monographs, by Pethick and Smith (2008, second edition)[1] and by Pitaevskii and Stringari (2003). Most of this research, both experimental and theoretical, has concentrated on the case of low temperatures (well below the BEC transition temperature, $T_{\rm BEC}$), where one is effectively dealing with a *pure* Bose condensate. The total fraction of noncondensate atoms in such experiments can be as small as 10% of the total number of atoms and, equally importantly, this low-density cloud of thermally excited atoms is spread over a much larger spatial region compared with the high-density condensate, which is localized at the centre of the trapping potential. Thus most studies of Bose-condensed gases at low temperatures have concentrated entirely on the condensate degree of freedom and its response to various perturbations. This region is well described by the famous Gross–Pitaevskii (GP) equation of motion for the condensate order parameter $\Phi(\mathbf{r}, t)$. As shown by research since 1995, this pure condensate domain is very rich in physics.

The main goal of the present book, in contrast, is to describe the dynamics of dilute trapped atomic gases at finite temperatures such that the noncondensate atoms also play an important role. This means that we shall be concerned with a trapped Bose gas composed of two distinct components,

[1] The first edition of the Pethick and Smith book was published in 2002. We give page references to the expanded second edition, published in 2008. The first 13 chapters in both editions cover similar material.

the condensate and the noncondensate. These two components satisfy quite different equations of motion but can be strongly coupled to each other and hence can modify each other significantly. The coupled dynamics of a two-component superfluid Bose gas brings in a whole new class of phenomena. At a theoretical level, one clearly has to deal with a "generalized" GP equation for $\Phi(\mathbf{r}, t)$ which now includes the effect of the mean fields and collisions associated with the noncondensate atoms. Broadly speaking, the thermal cloud atoms will be described by a kinetic equation for a normal gas of atoms, such as the well-known Boltzmann equation for a classical gas. The major difference is that in a trapped Bose-condensed gas the thermal atoms are coupled to the condensate component via mean fields and collisions.

The theory of Bose-condensed gases has been an active research topic since the ground-breaking work of Bogoliubov in 1947. The present book is built on the rich body of research carried out in the period 1957–67 by Lee and Yang, Beliaev, Pitaevskii, Hugenholtz and Pines, Hohenberg and Martin, Gavoret and Nozières, Kane and Kadanoff and many others. More specifically, what we shall call the Zaremba–Nikuni–Griffin (ZNG) approximation (see the preface and Chapter 3) is very much an extension for trapped gases of the pioneering studies by Kirkpatrick and Dorfman (1983, 1985a,b). These authors derived a kinetic equation for the thermal atoms in a uniform Bose-condensed gas and used it to give an explicit derivation of the Landau two-fluid equations that account for transport coefficients. However, when their papers were published in 1985, research interest in BEC in gases was very low and their work had little impact.

Looking back, it is perhaps surprising that in the early work on Bose-condensed gases there was almost no explicit discussion of a time-dependent equation of motion for the condensate. It was only after the discovery of BEC in trapped ultracold atomic gases in 1995 that the time-dependent Gross–Pitaevskii equation and its extensions became central in theoretical discussions, even though this equation had been developed in 1961. The ZNG theory "stitches" together a generalized GP equation for the Bose condensate (which includes the coupling to the thermal cloud atoms) and a kinetic equation for the thermal cloud atoms. The ZNG approximation is thus the offspring of a "civil union" between Gross–Pitaevskii and Bogoliubov on the one hand and Boltzmann on the other.

So far, the study of the dynamics of a trapped Bose-condensed gas at finite temperatures has not been a topic of systematic experimental studies. Part of the reason for this, we believe, has been the implicit belief that the presence of a thermal cloud of noncondensate atoms just complicates the behaviour of a pure $T = 0$ condensate and is not the source of any interesting "new physics". A theme of this book is that this attitude is not justified. The coupling of the condensate and noncondensate degrees of freedom at finite temperatures leads to a two-component system in which *both* components can exhibit coherent collective behaviour, resulting in many new phenomena. Indeed, under certain conditions, a trapped Bose gas at finite temperatures can exhibit two-fluid phenomena that are precisely analogous to the well-known macroscopic quantum behaviour in superfluid $^4$He (For details, see Chapters 15 and 17).

The present book is devoted first (Chapters 3–7) to deriving coupled equations for a two-component superfluid Bose gas within a simple but realistic microscopic approximation for each component. The second major goal (Chapters 8–19) is to solve these approximate equations for the dynamics of a trapped Bose gas at finite temperatures in two different regions, the collisionless (or mean-field dominated) domain and the hydrodynamic (or collision-dominated) domain. In the collisionless region, for which there are considerable experimental data, our coupled equations give results that are in quantitative agreement with the observed temperature-dependent frequency and damping of the many kinds of collective modes that can be excited in ultracold Bose gases.

In the quite different hydrodynamic region, collisions bring the system into a state of local thermodynamic equilibrium. We prove that our approximate model equations lead to the well-known two-fluid hydrodynamical description first derived (Landau, 1941; Khalatnikov, 1965) for superfluid $^4$He. This connection allows one to make a very detailed comparison between the hydrodynamics of a trapped Bose-condensed gas and that of liquid $^4$He and emphasizes the key role of the Bose broken symmetry (Hohenberg and Martin, 1965; Anderson, 1966, 1994; Bogoliubov, 1970). Strangely enough, the hydrodynamics of a dilute Bose-condensed gas can be even more complex than that of superfluid $^4$He. The reason, as we discuss in Chapter 15, is that in a trapped gas the condensate and noncondensate can be out of *diffusive* local equilibrium with each other.

Discussions that start with the dynamics of a pure condensate at $T = 0$ can give the impression that a trapped Bose-condensed gas is some completely new phase of matter, unconnected with other interacting many body systems. The point of view of the present book is quite different, in that we start with the normal phase. That is, a Bose superfluid (gas or liquid) is viewed as a normal fluid in which, as a result of a second-order phase transition, an extra new degree of freedom emerges, namely, a condensate described by the macroscopic wavefunction $\Phi(\mathbf{r},t)$. A crucial question is how this new "superfluid" degree of freedom couples into and modifies the "normal fluid" degrees of freedom. Answering this question leads, in our opinion, to a deeper insight into the dynamics of a two-component Bose superfluid. This approach allows one to put the two extreme limits, a pure condensate ($T \ll T_{\rm BEC}$) and a pure thermal cloud ($T > T_{\rm BEC}$) into a broader context. It also sets the stage for developing a two-fluid description in trapped gases similar to that used to describe the low-frequency hydrodynamics of superfluid $^4$He.

The theory of interacting Bose-condensed fluids is most usefully discussed using quantum field operators. This approach was initiated by Bogoliubov (1947) in a simple model calculation, formalized in a systematic way by Beliaev (1958a), and then developed by Gavoret and Nozières (1964), Hohenberg and Martin (1965), Bogoliubov (1970) and many others in the early 1960s. This many body formalism is discussed in detail in the well-known texts Abrikosov *et al.* (1963) and Fetter and Walecka (1971). We recall that

$$\begin{array}{c}\text{the operator } \hat{\psi}^\dagger(\mathbf{r}) \text{ creates an atom at } \mathbf{r};\\ \text{the operator } \hat{\psi}(\mathbf{r}) \text{ destroys an atom at } \mathbf{r}.\end{array} \tag{1.1}$$

These quantum field operators satisfy the usual Bose commutation relation

$$\left[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\right] = \delta(\mathbf{r} - \mathbf{r}'). \tag{1.2}$$

All observables can be written in terms of these operators; for example, the density $\hat{n}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$ and the interaction energy is given by

$$\hat{V} = \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}'\, \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r})v(\mathbf{r} - \mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}), \tag{1.3}$$

where $v(\mathbf{r})$ is the interatomic potential.

The crucial idea, due to Bogoliubov (1947) and later generalized by Beliaev (1958a,b), is to separate out the condensate component of the quantum field operators, setting

$$\hat{\psi}(\mathbf{r}) = \langle\hat{\psi}(\mathbf{r})\rangle + \tilde{\psi}(\mathbf{r}), \tag{1.4}$$

where

$$\langle\hat{\psi}(\mathbf{r})\rangle \equiv \Phi(\mathbf{r}) \tag{1.5}$$

is the Bose macroscopic wavefunction. This quantity plays the role of the "order parameter" for the Bose superfluid phase transition:

$$\Phi(\mathbf{r}) = \begin{cases} 0, & \text{if } T > T_{\rm BEC},\\ \neq 0, & \text{if } T < T_{\rm BEC}.\end{cases} \tag{1.6}$$

We note that $\Phi(\mathbf{r}) = \sqrt{n_{\rm c}}e^{i\theta}$ is a two-component order parameter in that it has both amplitude and phase. Clearly, $\Phi(\mathbf{r})$ is not simply related to many-particle wavefunctions $\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$. The thermal average in $\langle\hat{\psi}(\mathbf{r})\rangle$ involves introducing a small *symmetry-breaking* perturbation that allows $\Phi(\mathbf{r})$ to be finite,

$$\hat{H}_{\rm SB} = \lim_{\eta\to 0}\int d\mathbf{r}\left[\eta(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}) + \eta^*(\mathbf{r})\hat{\psi}(\mathbf{r})\right]. \tag{1.7}$$

The philosophy behind the concept of symmetry-breaking and its use in a variety of condensed matter systems was extensively discussed by Bogoliubov (1970) in a beautiful and convincing article which is highly recommended to all readers. Since the early 1960s, the concept of a broken-symmetry order parameter has increasingly become the basis of all modern treatments of different phases of matter in all branches of physics. A lucid systematic account of this approach as a basis for statistical mechanics is developed in recent monographs by Mazenko (2000, 2003).

The Beliaev (1958a) decomposition (1.4) of the quantum field operator implies that the single-particle density matrix has the property

$$\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty} \rho_1(\mathbf{r},\mathbf{r}') \equiv \langle\hat{\psi}(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\rangle = \Phi(\mathbf{r})\Phi^*(\mathbf{r}'). \tag{1.8}$$

Penrose (1951) and Penrose and Onsager (1956) first gave a formal definition of what BEC is in an interacting Bose gas in terms of the asymptotic property given in (1.8). Specifically, they defined the wavefunction of the Bose condensate as the eigenstate of $\rho_1(\mathbf{r},\mathbf{r}')$ which is macroscopically occupied. The Penrose–Onsager approach is nicely summarized in Section 2.1 of Pitaevskii and Stringari (2003) and Section 2.1 of Leggett (2006).

The later, independent, formulation of Beliaev (1958a), based on separating the condensate part of the quantum field operator $\hat{\psi}(\mathbf{r})$ as in (1.4), extended the powerful field theoretic techniques for dealing with the dynamics of many body systems to include Bose condensation. The Beliaev Green's function approach allows one to avoid working directly with many body wavefunctions (as in the original approach of Penrose and Onsager, 1956) and instead work with equations of motion for Green's functions. The Beliaev formulation involves defining the Bose condensate as a broken-symmetry order parameter (1.5), which can be time dependent. This extends the original Penrose–Onsager formulation, which was based on number conserving eigenstates. The usefulness of working with number nonconserving states and anomalous Green's functions was clarified by Anderson in a classic article written in 1965 (reprinted in Anderson, 1994, p. 229). See also Section 2.2 of Pitaevskii and Stringari (2003).

To avoid any misunderstanding about the use of number nonconserving states, we emphasize that all conservation laws (including the continuity equation for density fluctuations) can be satisfied in theories based on a broken-symmetry order parameter. As is well understood (see for example Griffin, 1993), conservation laws play a crucial role in Bose superfluids.

We note that Beliaev's name is attached to two papers on interacting Bose systems which have quite different goals. In the first paper, Beliaev (1958a) set up a *general* formalism to deal with an interacting Bose-condensed system using diagrammatic methods incorporating the presence of a Bose order parameter $\Phi(\mathbf{r})$. In a companion paper, Beliaev (1958b) used this formalism to calculate the excitation spectrum of the single-particle Green's functions $\tilde{G}_{\alpha\beta}(\mathbf{q},\omega)$ to second order in the interaction. This is the famous Beliaev second-order approximation, generalizing the first-order Bogoliubov approximation.

The condensate wavefunction $\Phi(\mathbf{r},t)$ is a *coherent* state, with a "clamped" value of the phase, rather than a Fock state of fixed $N$ with no well-defined phase. The order parameter $\Phi(\mathbf{r},t)$ acts like a *classical* field, since quantum fluctuations are negligible when the number of atoms $N_{\rm c}$ in the single-particle condensate wavefunction is large. As noted above, Anderson (1966, 1994) deserves great credit for understanding (in the period 1958–1963) the new physics involved in working with a broken-symmetry state $\Phi(\mathbf{r},t)$ with a well-defined phase, both in BCS superconductors and in superfluid $^4$He. This broken-symmetry state nicely captures the physics of the Josephson effect and superfluidity. The external symmetry-breaking perturbation (1.7) allows the system to set up off-diagonal symmetry-breaking fields internally, which persist even when the external perturbation is set to zero at the end of the calculation ($\eta \to 0$).

The same sort of physics is the basis of the well-known Bardeen–Cooper–Schrieffer (BCS) theory of superconductors, based on the formation of bound pairs of fermions called Cooper pairs, which are bosons and hence can Bose-condense. Indeed, it is interesting to recall that before the BCS theory appeared in 1957, Bogoliubov's pioneering paper, published in 1947, was largely unknown or ignored. After the physics of the BCS theory was reformulated in a simple fashion involving symmetry-breaking mean fields related to a Cooper-pair condensate (Gor'kov, 1958), theorists quickly realized that the Bogoliubov theory of Bose-condensed gases involved a similar kind of "off-diagonal" mean field. Since the 1960s, in condensed matter physics our understanding of superconductors has gone hand-in-hand with our understanding of superfluid $^4$He. In particular, the BCS theory has played an important role as an example of how a broken-symmetry theory captures the physics of superfluid motion, and it has the advantage of *not* working with a number-conserving approximation.

One of the stunning developments in ultracold gases is the experimental realization of the BCS–BEC crossover in a two-component Fermi gas (for an introduction, see Chapter 17 of Pethick and Smith, 2008). Using a Feshbach resonance to tune the magnitude and sign of the $s$-wave scattering length $a$ between Fermi atoms in different hyperfine states, one can go in a smooth fashion from a BCS phase with Cooper pairs immersed in a gas of fermion BCS quasiparticles to a Bose condensate phase in which all the fermion excitations have paired up to form Bose molecules. This BEC of molecules is a very promising new "Bose gas", since molecules made up of two fermions are very stable against three-body decay in a two-component Fermi gas, because of the Pauli exclusion principle. Moreover, the molecular scattering length is proportional to $a$ and hence can be very large (Petrov *et al.*, 2004, 2005) near the Feshbach resonance (where $|a| \to \infty$). As a final bonus, the creation of bosonic molecules via the destruction of two fermions is a concrete illustration of a physical process that does *not* conserve the total number of bosons and thus can be thought of as a symmetry-breaking perturbation of the type (1.7).

One can formulate the Gross–Pitaevskii and Bogoliubov approximations directly in terms of variational many-particle wavefunctions. However, such formulations are usually limited to simple mean-field approximations at $T = 0$. The explicit introduction of the broken-symmetry order parameter $\Phi(\mathbf{r}, t)$ gives a more systematic way (Beliaev, 1958a; Hohenberg and Martin, 1965; Bogoliubov, 1970; Nozières and Pines, 1990) of isolating the role of the Bose condensate within a general treatment of an interacting Bose-condensed fluid at finite temperatures. This approach was developed in order to understand the characteristic properties of a Bose superfluid such as liquid $^4$He, in spite of the fact that one could not do quantitative calculations on such a strongly interacting system. A major goal of this book is to show that the resulting formalism allows one to treat, in an easy and natural manner, questions related to damping as well as superfluidity at finite temperatures in both the collisionless and hydrodynamic regions.

As already noted, this book deals with the Bose condensate by means of the approach formalized and developed by Beliaev (1958a,b), which is based on separating out the Bose-condensate degree of freedom as an order parameter related to a broken symmetry. The finite value of the condensate order parameter leads to new correlations in space and time between the noncondensate atoms. As a result, besides using the ordinary single-particle Green's functions, it is natural to introduce anomalous ("off-diagonal") single-particle Green's functions to describe the new condensate-induced correlations between the atoms outside the condensate. In the early 1960s, it was realized that one could give a compact version of many body perturbation theory for Bose superfluids by working with a $2 \times 2$ matrix single-particle Green's function $\tilde{G}_{\alpha\beta}$ describing the noncondensate atoms. A similar scheme for BCS superconductors grew out of the related work of Gor'kov (1958). For over five decades, these Green's function techniques have been used with great success in dealing with both Bose and Fermi superfluids.

By the 1960s, it was realized that there are three paradigms for quantum fluids:

(1) Bose superfluids (associated with a Bose condensate wavefunction $\Phi$);
(2) normal Fermi fluids (associated with the key role of a Fermi surface);
(3) Fermi superfluids (associated with Cooper pairs that form a Bose condensate).

The first two kinds of quantum fluid were magnificently described in two books by Nozières and Pines written in the early 1960s, although the book on superfluid Bose liquids (Nozières and Pines, 1990) was only published decades later. One of the clearest discussions of the connection between the order parameter $\Phi(\mathbf{r}, t)$ and superfluidity in Bose fluids is given in Chapters 4 and 5 of Nozières and Pines (1990). The classic account formulating the various levels of theory for Bose superfluids is the monumental paper by Hohenberg and Martin (1965). This paper shows the central unifying role of the broken-symmetry order parameter $\Phi(\mathbf{r}, t)$, summarizes the physics involved in both the collisionless and hydrodynamic domains and gives criteria for developing and judging various microscopic approximation schemes for correlation functions, using thermal Green's function techniques. The general philosophy and approach of the present book has been strongly influenced by Hohenberg and Martin's seminal paper.

The introductory review article by Leggett (2001) and his recent book on quantum liquids (Leggett, 2006) give a thoughtful account of many basic assumptions used in current theories on ultracold gases. However, we do not share Leggett's reservations about the usefulness of the concept of a Bose order parameter arising from a broken symmetry. Treating the condensate as a new degree of freedom becomes especially convenient when one is attempting to deal with the dynamics of a trapped Bose-condensed gas at finite temperatures, as we hope to illustrate in the present book.

We have emphasized that our approach to nonequilibrium problems in Bose gases involves separating out the condensate right at the beginning, following the classic Bogoliubov–Beliaev approach. This means that the condensate and noncondensate dynamics are treated in quite different ways, $\Phi(\mathbf{r}, t)$ playing the role of the order parameter. There is an alternative approach used in the current literature in which the equations of motion for all low-energy bosonic modes (for which the occupation numbers $N_i \gg 1$) are treated classically. This "classical field" approach had its origins in the theory of lasers and quantum optics. It leads to what are called stochastic GP equations, in which an analogue of $\Phi(\mathbf{r}, t)$ describes both the condensate mode and low-energy excitations on an equal basis. We note that such stochastic GP equations have a basis completely different from that of the condensate generalized GP equation we introduce in Chapter 3. For reviews, applications and further references to such equations, see Sinatra, Lobo and Castin (2001); Davis, Morgan and Burnett (2001); Gardiner, Anglin and Fudge (2002); Bradley, Blakie and Gardiner (2004); and Brewczyk, Gajda, and Rzazewski (2007). While having advantages in certain problems, the classical field approach has not yet been extensively implemented in the study of collective modes in trapped Bose gases. Indeed, it is not clear how this approach could be used to discuss the collisional hydrodynamic region.

For a comparison of various formalisms for dealing with trapped Bose-condensed gases at finite temperatures, we refer to the proceedings of a recent workshop on this topic[2].

## 1.1 Historical overview of Bose superfluids

To put the coupled equations for the condensate and thermal cloud into context, we now briefly review some features of the theory of superfluidity in liquid $^4$He. In later chapters, we often make connections between the properties of superfluid Bose gases at finite temperatures and superfluid $^4$He.

The original discovery of superfluidity in liquid $^4$He was announced in the famous papers by Kapitza (1938) working in Moscow and by Allen and Misener (1938) based in Cambridge. These and subsequent experiments in the following years (for a review see Wilks, 1967) showed that, in comparison with classical fluids, superfluid $^4$He could exhibit very bizarre behaviour. The attempt to understand this behaviour led to the development of a two-fluid theory of the hydrodynamic behaviour of liquid $^4$He by Landau (1941). An earlier but less complete two-fluid theory based on a dilute Bose gas

[2] *Proc. Workshop on Nonequilibrium Behaviour in Superfluid Gases at Finite Temperatures*, Sandbjerg, Denmark June 10–13, 2007 ( http://www.phys.au.dk/nonequilibrium/Home.html). See also the long tutorial review by Proukakis and Jackson (2008).

was developed by Tisza in the period 1938–40. For further discussion of the history of BEC and superfluids, see Griffin (1999a) and Balibar (2007).

In this early work, superfluidity (the term was coined in 1938 by Kapitza) was entirely associated with the *relative* motion of the normal and superfluid components under a variety of conditions (Khalatnikov, 1965; Wilks, 1967). The main conclusion of this early research was that while the normal fluid exhibited the finite viscosity and thermal conductivity typical of an ordinary fluid, the superfluid component (which exhibited only irrotational flow) did not. In more recent times, an aspect of superfluidity that has been emphasized as most central (for example, see Chapter 4 of Nozières and Pines, 1990; Leggett, 2001, 2006) is that the superfluid velocity is associated with the gradient of the phase of the macroscopic wavefunction $\Phi(\mathbf{r}, t)$. However, an equally important property to understand is why superfluidity persists *even* in the presence of a dissipative normal fluid. This question can best be addressed by studying the local equilibrium region induced by strong collisions, a region described by the two-fluid hydrodynamic equations.

In essence, Landau developed his generic two-fluid hydrodynamics by generalizing the standard theory of classical hydrodynamics (see, for example, Huang, 1987) to include the equations of motion for a new "superfluid" degree of freedom. We recall that classical fluid dynamics was developed well before the existence of atoms had been demonstrated. Since the work of Maxwell and Boltzmann in the 1880s, it has been known that a "coarse-grained" hydrodynamic description of a fluid, in terms of just a few quantities such as the local density $n(\mathbf{r}, t)$ and the local velocity $\mathbf{v}(\mathbf{r}, t)$, is only valid when the collisions between atoms are strong enough to produce "local equilibrium". As a result, hydrodynamics describes only low-frequency phenomena, for which the fluid is in local equilibrium. This is defined by the condition $\omega\tau \ll 1$, where $\omega$ is the frequency of the collective mode and $\tau$ is the collisional relaxation time to reach local equilibrium.

The description of a fluid in terms of a few hydrodynamic local variables was developed by Bernoulli, Euler and others in the eighteenth century. In work which led to a microscopic basis for these hydrodynamic theories, Boltzmann introduced the key concept of a kinetic equation to describe the nonequilibrium behaviour of atoms in a dilute classical gas. He developed the idea that such a gas would approach thermal equilibrium in several distinct stages. Initially the dynamical behaviour is very complex. However, the system eventually reaches the so-called "kinetic" stage, which can be described by a single-particle distribution function $f(\mathbf{p}, \mathbf{r}, t)$. The latter is given by the solution of a kinetic equation, the structure of which (even when we generalize it to deal with a Bose-condensed gas) is usefully written