INTERACTION EFFECTS IN THE WEAKLY REPULSIVE BOSE GAS: TWO STUDIES

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and approved by

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Two investigations on correlation effects in a uniform three-dimensional Weakly Interacting Bose Gas (WIBG) are presented in this thesis.

The first topic is a study of squeezing effects, in the sense of quantum optics, in the zero-temperature WIBG. After a review of relevant quantum-optics concepts (coherence and squeezing), we describe a variational investigation of squeezing in the Bose-condensed system.

The variational study reveals that squeezing in the zero-momentum (condensate) mode is not present at mean field level but comes from diagrams beyond one-loop order. On the other hand, for nonzero momenta, mixed-mode squeezing between opposite-momenta pair modes appears at mean field already. An alternate variational calculation is also formulated, to provide a more physical picture of the mixed-mode squeezing.

The second study involves the dependence of the Bose-Einstein condensation temperature ($T_c$) on the interaction. The shift of $T_c$ from the non-interacting
gas value, $T_{c}^{(0)} = (2\pi/m[\zeta(3)/2]^{2/3}) n^{2/3}$, is a long-disputed problem. We present a critique of various studies on the topic, and describe our own efforts.

Our approach to $T_c$ involves a quasiparticle description of the Bose gas in the symmetry-unbroken phase. We regulate ultraviolet divergences and rule out any effect of quasiparticle lifetime, up to second order. Our method reduces the calculation of $T_c$ to the determination of the quasiparticle spectrum at criticality. Two approaches to the quasiparticle spectrum are detailed out.

The first technique is to use the chemical potential as an explicit cutoff for regularizing critical-point infrared divergences. This procedure yields a $T_c$ shift approximately proportional to $a \sqrt{\ln a}$, where $a$ is the scattering length.

The second procedure is a self-consistent treatment of the spectrum, which enables a numeric calculation of both the quasiparticle spectrum at $T_c$, and of $T_c$ itself.
Preface

During the period spent at Rutgers, I studied several aspects of the weakly interacting Bose gas (WIBG) under the direction of my PhD advisor, Andrei E. Ruckenstein. I learned about quantized vortices precessing in trapped Bose condensates. For about two years, I probed at the “$T_c$ problem”. Later, I read about light scattering and coherence phenomena in the condensates, which eventually led to the work on “squeezing”.

Other than the WIBG work, I attempted a number of things in collaboration with my colleagues S. Pankov and I. Paul. Most didn’t work out, but the three of us published a paper on lattice structures of a Wigner crystal on liquid substrates.

Over the last year at Rutgers, I started projects on exciton physics in semiconductors, particularly on exciton condensation in biased coupled quantum wells. Some of the projects died ingloriously, but some I hope to continue later.

For the PhD thesis, it seemed appropriate to write on my work on the Bose gas. Over the decades, the Bose fluid has attracted some of the greatest minds of condensed matter physics. It has been and continues to be a fruitful source and testing-ground of many-body concepts and techniques. I am happy to be able to write something on this enduring topic.

Chapters 1 and 2 are review & survey material, background for the following chapters. They were written explicitly for this thesis.

The work described in chapter 3 has not been published, and appears here for the first time.

Chapter 4 is adapted from an article placed on the Los Alamos archives in February 2003 [1], where I reviewed the state of the $T_c$ problem (the aspects I
understood). The article was meant as a service for the community of theorists working on the $T_c$ problem, and involves analysis of existing work, rather than new results. A modified version serves in this thesis as an overview of the topic.

Chapter 5 is based on an article written with A. E. Ruckenstein. The paper is available on the Los Alamos archives [2], but not yet published.

M. Haque

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I have to thank my many friends at Rutgers, who made life away from my home country not only bearable but often delightful.

Above all, I am fortunate to have had Indranil Paul near me, who shared my joys and sorrows over the years, and with whom I explored culture and physics. I like to think that we represented the relationship between East and West Bengal, as it should be.

I spent many hours discussing physics and non-physics with Sergey Pankov. A rewarding experience!

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To those who took care of me while I was injured, far better than my mother could ever have done, I don’t quite have the words to express my gratitude: Indranil and Sahana, Sergey, Max, Subarana & Saadi, David Brookes, William, Mick, Nayana Shah, Marcello Civelli. Because of these wonderful people, having an accident far away from home and family did not seem such a bad thing!

Physics was much more fun in discussion with peers. Indranil and Sergey, in addition to being close friends, also taught me the most. I am also grateful to Craig, Ivan Skachko, Carlos Bolech, Andrei Lopatin, Harald Jeschke, Edouard and Pankaj for physics lessons, and to Rossen for teaching computing tricks. My presentations were critiqued by Craig, Indranil, Edouard, Carlos, Nayana, Rossen. I hope I am a better speaker now, thanks to these people. Craig, David Brookes and Sahana proofread my physics writings: hopefully I write better because of them!

Throughout my Ph.D. years, I received continuous emotional support from my parents and siblings in Bangladesh, from teachers at my undergraduate institution (Susanta K. Das, Yasmeen Haque, Arun K. Basak, M. Zafar Iqbal), and from my Bangladeshi friends at Rutgers, Subarna Khan and Saadi.

Finally, Banu Ilal deserves all credit for feeding, housing, and sustaining me through the difficult final months of my PhD.
Dedication

Dedicated to
All who strive for justice, equality, and a secular world
And to
Peoples of the Third World.
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<td>WIBG</td>
<td>Weakly Interacting Bose Gas</td>
</tr>
<tr>
<td>HFB</td>
<td>Hartree-Fock-Bogoliubov</td>
</tr>
<tr>
<td>BEC</td>
<td>Bose-Einstein Condensate, or Bose-Einstein Condensation</td>
</tr>
<tr>
<td>RG</td>
<td>Renormalization Group</td>
</tr>
<tr>
<td>$\int_k$</td>
<td>$\int \frac{d^3k}{(2\pi)^3}$</td>
</tr>
<tr>
<td>UV</td>
<td>Ultraviolet (high momentum)</td>
</tr>
<tr>
<td>IR</td>
<td>Infrared (low momentum)</td>
</tr>
<tr>
<td>3D</td>
<td>Three-dimensional, or three dimensions</td>
</tr>
<tr>
<td>1D (2D)</td>
<td>One-(two-)dimensional, or one (two) dimension(s)</td>
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Chapter 1
Weakly Interacting Bose Gas

The work described in this thesis involves the dilute uniform (homogeneous) Bose gas with a weak repulsive two-body interaction between the constituent bosons. We present two studies of interaction effects in the weakly interacting Bose gas (WIBG).

The first topic (chapters 2 and 3) is a study of a particular kind of coherence phenomenon, known as squeezing. Squeezed states were first studied in the context of quantum optics, in the 1970s and 1980s. It is only recently that squeezing has been discussed in the context of Bose-Einstein condensation (BEC), and our work is a contribution towards this effort. We describe a variational study of squeezing effects in the zero-temperature Bose-condensed WIBG.

The second topic is a study of the effect of the repulsive interaction on the critical temperature ($T_c$) for Bose-Einstein condensation. This is a longstanding problem that has remained unsolved for several decades. Interest in this problem has re-surfaced with the resurgence of BEC research in recent years. In chapters 4 and 5, we describe attempts to understand the $T_c$ shift in the WIBG.

Einstein’s deduction in 1924, that an ideal Bose gas at low temperatures would condense into the lowest single-particle state, was used in 1938 by Fritz London, who suggested [3] that the newly-discovered superfluid transition of $^4$He was related to the BEC phenomenon. The WIBG is a modification of the ideal Bose gas, introduced by theorists struggling to understand the superfluid physics of liquid helium. Liquid helium is a strongly interacting dense liquid rather than
a dilute weakly interacting gas; nevertheless it was expected that some of the insights from studying the WIBG would carry over to liquid helium. In the 2-3 decades after Bogoliubov’s seminal 1947 paper [4], the WIBG model became an object of intense interest in its own right. During this period, much of the early many-body theory was developed in the context of the weakly repulsive Bose gas.

Prolonged experimental efforts, directed at producing a Bose-Einstein condensate by laser-cooling a trapped atomic gas, were finally successful in 1995. The study of the WIBG received an enormous boost as a result. With new experiments being reported at an extraordinary rate, the amount of theoretical work in the field has continued to increase exponentially. Other than the physics relevant to the new experiments, older unsettled questions have received fresh attention during this period of heightened interest. The $T_c$ problem is one such question.

The idea of squeezed states developed around 1975-1985, in studying novel quantum states of light and coherence phenomena using laser fields. The associated language and concepts open up a new set of questions concerning the Bose gas. We report in chapter 3 our efforts at identifying and addressing several such questions.

This chapter is an overview of the weakly repulsive Bose gas model. In Sec. 1.1 we introduce the WIBG Hamiltonian, and give a quick historical review.

Some known results on the WIBG are summarized briefly in Secs. 1.2 and 1.3. This description serves as the background for topics discussed in later chapters.

Much of the material reviewed in these two sections can be found in the 1964 review by Hohenberg and Martin [5], or in texts from the mid-1960s onwards [6–13]. The terminology used here is more modern. Also, the material on the many-body $\mathcal{T}$-matrix and its temperature-dependence is new, about five years old at the time of writing [14–16].

In Sec. 1.4 we give an introduction to the $T_c$ problem, as a prelude to chapters 4 and 5. Since trapped atomic gases have become so important in the study of
the WIBG, in Sec. 1.5 we survey selected experiments related to BEC in the trapped-cloud systems. Finally, we give an outline of the rest of the thesis in 1.6.

1.1 The model

We first present the WIBG Hamiltonian and make some preliminary comments, before giving a historical survey of theoretical (1.1.1) and experimental (1.1.2) research on the model. In second-quantized form, the Hamiltonian is

$$\hat{H} = \sum_k \epsilon_k \hat{c}_k^\dagger \hat{c}_k + \frac{1}{2V} \sum_{p,q,k} U(k) \hat{c}_{p+k}^\dagger \hat{c}_{q-k}^\dagger \hat{c}_p \hat{c}_q.$$  (1.1)

$\epsilon_k = k^2/2m$ is the free-gas spectrum, and $\hat{c}(\hat{c}^\dagger)$ are bosonic annihilation (creation) operators. The simplest interaction to use is a momentum-independent one, $U(k) = U$, i.e., a point interaction $U(r) = U\delta(r)$ in real space.

The use of a point interaction often gives rise to unphysical ultraviolet divergences, some of which may be cured by using the two-body scattering amplitude, or the two-body $t$-matrix, instead of the interaction potential $U$. At first order, $U$ is equal to the $t$-matrix. Therefore, using the low-energy limit for $t$ [17], one finds $U = t = 4\pi \hbar^2 a/m$, where $a$ is the $s$-wave scattering length. Corrections to this may be required at higher order. This is discussed in more detail in chapter 5, where we use the correction to remove ultraviolet divergences.

An alternative way to deal with ultraviolet divergences is to use the “pseudopotential” method introduced by Huang and Yang [18], which moderates the $U(r) = U\delta(r)$ approximation with a differential operator: $U(r) = U\delta(r) \frac{\partial}{\partial r}$. We will not be using this method in the present thesis.

The scattering length $a$, compared to other lengths relevant to the system, gives dimensionless measures of the interaction. One such measure is the ratio of $a$ to the average inter-particle distance, $an^{1/3}$, where $n$ is the density. (In two dimensions, the corresponding quantity is $an^{1/2}$.) Thus a bose gas maybe
considered to be “weakly interacting,” even if $a$ is large, when the density is low enough. This is why the WIBG is often known as the *dilute* interacting Bose gas.

Using the thermal wavelength $\lambda = \sqrt{\frac{2\pi k^2}{mk_B T}}$, the ratio $a/\lambda$ may also be used as the measure of the interaction, but only at nonzero temperatures. In the discussion of the $T_c$ problem (chapters 4 and 5), both $an^{1/3}$ and $a/\lambda$ are used in the literature.

The work in this thesis concerns only the three-dimensional (3D) Bose gas. The physics of two- and one-dimensional WIBGs are interesting topics in their own right, but will not be discussed here except in passing. The uniform WIBG does not undergo Bose-Einstein condensation at lower dimension. The investigations here involve BEC (in one case the $T = 0$ condensed gas, and in the other case the temperature of condensation). Therefore our calculations pertain to 3D.

**1.1.1 Brief history**

Theoretical studies of the WIBG start with Bogoliubov [4], who used the idea of macroscopic occupancy of the $k = 0$ mode to do a mean-field approximation, replacing the $k = 0$ operators ($\hat{c}_0$, $\hat{c}_0^\dagger$) by their $c$-number expectation value $\sqrt{N_0}$. This method yields the gapless Bogoliubov spectrum for the zero-temperature WIBG, $E_k = [\epsilon_k^2 + 2Un_0\epsilon_k]^{1/2}$.

Beliaev [19, 20] introduced the formalism of Green’s functions and diagrammatics in the study of the Bose-condensed gas. Other than reformulating Bogoliubov’s work in field-theoretic language, he calculated terms in perturbation theory beyond mean field, and introduced the use of the $T$-matrix (Sec. 1.2.3). His work was later refined and extended by Popov [21], who devised methods for higher temperatures as well. A review of this line of work, in modern language, can be found in [15].

In the West, a great number of studies were reported during the early period, up to 1965. We mention here some of the most influential.
• Penrose and Onsager developed [22,23] the idea of Off-Diagonal Long Range Order (ODLRO), in terms of the factorization of density matrices, to describe Bose condensation. The ODLRO idea was later expanded by Yang [24].

• Brueckener and Sawada performed an early field-theoretic description of the Bose-condensed system, in 1957 [25]. Like Beliaev, they use the $T$-matrix. This work produced a spurious gap in the spectrum, an anomaly that torments many approximations for the WIBG.

• Hugenholtz and Pines [26] produced another early field-theoretic calculation. The celebrated Hugenholtz-Pines (HP) theorem, which we discuss in Sec. 1.2.2, was introduced and proved to all orders (for zero temperature) in this work.

• Girardeau and Arnowitt performed a variational calculation [27] emphasizing opposite-momenta pair correlations (as we do, in more detail and in a new language, in this thesis).

• Huang, Yang and collaborators did a series of calculations [18,28,29] in which they introduced their pseudopotential method of using a derivative with the $s$-wave approximation.

• The understanding of the many-boson system obtained during these early years is reviewed and formalized in the 1964 classic Hohenberg & Martin article [5].

Of the variety of theoretical work on the WIBG after the early years until around 1990, we point out as highlights the investigations on spatially non-uniform systems (development and use of the Gross-Pitaevskii equations [30-34]), vortices and vortex lattices (representative references: [35-40]), two-dimensional [12,41-47] and one-dimensional [48-50] systems, numerical work via variational
and Monte Carlo [53, 54] methods, theory of BEC in particular systems, e.g., in spin-polarized hydrogen [33, 55–58] and in excitonic systems [59–61], etc.

With the prospect of the creation of a quantum-degenerate WIBG in the laboratory, work on this model has intensified since the early 1990s, and has exploded since the actual reports [62–64] in 1995 of successful cooling to form condensates.

The theoretical literature produced during this time is vast, but the majority of these calculations concern trapped condensates, or issues related to current experiments. Trapped-gas theory has been reviewed, e.g., in [65–67]. We will omit detailed discussion of this type of theoretical work, since this thesis is concerned with interaction effects in the uniform WIBG. A survey of current-era experiments is given in Sec. 1.5.

Of studies relevant to the homogeneous WIBG performed during the current period, I point out the following: renormalization group (RG) and effective-action (functional) formulations [14, 16, 68–70], descriptions of the Bose-condensed state avoiding symmetry-breaking (number-conserving descriptions) [71–75], and the use of quantum-optics concepts to study the quantum state of condensates [76–80].

1.1.2 Physical realizations

Liquid $^4$He was the first (and for a long time the only) bosonic fluid that could be cooled down to quantum degeneracy. Below the “lambda point” (2.2 K), liquid helium goes superfluid and displays a number of remarkable properties. Helium is a dense liquid with strong interactions among the particles, very different from the ideal non-interacting gas for which Einstein had first predicted the BEC phenomenon. London’s idea [3], that $^4$He superfluid properties are related to BEC, was therefore not quite obvious. In fact, Landau’s paper on helium superfluidity [81], which explained many aspects of the phenomenon, never mentions the role of bosonic statistics.
The development and acceptance of London’s idea (of superfluid helium being a Bose condensate) took some time. The WIBG model grew as a compromise between, on the one hand, the textbook ideal Bose gas with no interactions, and on the other, liquid helium the strongly interacting liquid. The WIBG does indeed display (explain) many of the properties of liquid helium, e.g., the existence of a second-order transition, the linear spectrum at long wavelengths, quantized vortices, etc. It does not reflect certain other properties, such as the roton minimum in the superfluid helium spectrum, which occur in $^4$He because of its large density.

As the theoretical WIBG model itself became a subject of intense interest, it became natural to use liquid helium to study the model, rather than thinking of WIBG studies as a path to understanding helium superfluidity. In search of a physical realization of the WIBG, Reppy and coworkers [82–85] at Cornell used helium in Vycor (a porous glass) to produce extremely dilute liquid helium, in both two or three dimensions. (Helium will act as a WIBG if it is dilute enough, when $na^3$ is reduced far below unity.) In addition to other measurements starting from around 1980, Reppy’s group recently used this arrangement to measure the transition temperature ($T_c$) for the Bose condensation of the WIBG [85].

Superconductors and superfluid $^3$He may be regarded as a condensate of pseudo-bosonic Cooper pairs, although there are many differences with the WIBG picture of condensation. (For example, the Cooper pairs themselves break up at the temperature where the condensate vanishes). With the advent of high-$T_c$ superconductors, the picture of superconductivity as a BEC phenomenon has become important again, the idea being that in some parameter regimes there is a crossover from a momentum-space pairing (BCS picture) to real-space pairing (BEC picture). The BCS-BEC crossover idea was introduced in 1969 [86] and has received recent attention in the context of the cuprate superconductors.

Another classic context in which BEC physics has been sought for many years
is that of excitons in semiconductors. The idea is that electron-hole pairs excited by a laser beam form bound states (excitons or biexcitons) which are approximately bosonic, and might be made to condense if the density is high enough (intense laser) and the temperature is low enough. The electron-hole pair may be closely or loosely bound compared to the density, so that a BCS and a WIBG description are possible in different geometries or different parameter regimes.

Since the first suggestions in the early 1960s [87, 88], experimental attempts toward a degenerate excitonic WIBG have continued for four decades, in a number of systems and geometries. (Relatively recent reviews can be found in [89] and in the exciton-related articles in [90]). Currently, use of parallel quantum wells, in which the electrons and holes are forced by a biasing field to be spatially separated, have generated intense interest [91–94].

Spin-polarized atomic hydrogen is the system whose study led to attempts to cool alkali gases, which eventually led to the first realizations of WIBGs [62–64, 95]. Considering the current importance of these systems, we will discuss these systems separately in more detail, in 1.5.1.

1.2 Field-Theoretic Language

The Green’s function formalism has to be specialized for the case of a Bose-condensed gas, which we summarize in this section. This will allow us to discuss $U(1)$ symmetry breaking (1.2.2), and various levels of approximations (Sec. 1.3).

1.2.1 Green’s functions and diagrammatics

The peculiarity of the condensed system is the macroscopic occupancy of a particular ($k = 0$) single-particle state. The usual way to deal with this is to treat the second-quantization operators for this particular mode as commuting numbers. Propagators involving condensate ($k = 0$) bosons are therefore treated specially.
Figure 1.1: Eight different vertices are required when the mean-field prescription $\hat{c}_0, \hat{c}^\dagger_0 \rightarrow \sqrt{N_0}$ is used. (Solid line represents non-condensate propagator, dotted lines are $k = 0$ propagators or factors of $\sqrt{N_0}$, and wavy lines represent the interaction.) The first vertex goes in the calculation of the ground state. The next four, involving two condensate lines, are the ones retained in mean field treatments.

Therefore, for the interaction term in Eqn. (1.1), we have eight different kinds of vertices in the field theory, depending on the number of condensate lines (Fig. 1.1).

We want to describe the Green’s functions for both zero and finite temperatures. We will use a generic “time” argument $\tilde{t}$, which will mean, for $T = 0$, the usual time, and for $T \neq 0$, the periodic variable $\tau$ with inverse-temperature dimensions. Similarly, the variable $z$ will represent ordinary frequencies for $T = 0$ and discrete Matsubara frequencies for $T \neq 0$. Also, retarded and advanced Green’s functions can be obtained with the usual prescription $z \rightarrow \omega \pm 0^+$.

The usual Green’s function is defined as the correlator of a time ordered product, $G(r, \tilde{t}) = -i \langle T \hat{\psi}(r, \tilde{t}) \hat{\psi}^\dagger(0,0) \rangle$. To treat the Bose gas with a macroscopic occupation of one single-particle state, it becomes convenient to also consider correlators of the form $\langle \hat{\psi} \hat{\psi} \rangle$ and $\langle \hat{\psi}^\dagger \hat{\psi}^\dagger \rangle$. We therefore use the tensor $\hat{\Psi} = \begin{pmatrix} \hat{\psi} \\ \hat{\psi}^\dagger \end{pmatrix}$
to define a 2×2 matrix Green’s function

\[
G(x) = -i \langle T \hat{\Psi}(x) \hat{\Psi}^\dagger(0) \rangle = -i \begin{pmatrix}
\langle T \hat{\psi}(x) \hat{\psi}(0) \rangle & \langle T \hat{\psi}(x) \hat{\psi}(0) \rangle \\
\langle T \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(0) \rangle & \langle T \hat{\psi}^\dagger(x) \hat{\psi}(0) \rangle
\end{pmatrix},
\]

with \( x = (r, \tilde{t}) \). Hereafter we will work in Fourier space with \((k, z)\) arguments.

The Green’s function matrix actually has only two independent elements, as \( G_{22}(k, z) = G_{11}(-k, -z) \) and \( G_{21}(k, z) = G_{12}(-k, -z) \). \( G_{11} \) and \( G_{12} \) are called respectively the normal and anomalous Green’s functions.

The self-energy is similarly a 2×2 matrix with two independent elements, the normal self-energy \( \Sigma_{11} \) and the anomalous self-energy \( \Sigma_{12} \). Figs. 1.2 and 1.3 show the Green functions and self-energies for a Bose-condensed system.

Dyson’s equation, \( G = G^{(0)} + G^{(0)} \Sigma G \), is now a matrix equation, representing four equations relating the \( G_{ij} \)’s and the \( \Sigma_{ij} \)’s, two of which are independent. These are called the Dyson-Beliaev equations.

Using \( G^{(0)}_{11}(k, z) = 1/(z - \epsilon_k + \mu) \) and \( G^{(0)}_{12} = 0 \), the Dyson-Beliaev equations
As in the usual Green’s function formalism, the pole of the Green’s function gives the excitation spectrum of the system.

### 1.2.2 The Hugenholtz-Pines theorem, $U(1)$ symmetry breaking, and gapless spectrum

BEC is, of course, a classic example of spontaneous symmetry breaking. The $U(1)$ symmetry $\hat{\psi}(r) \rightarrow \hat{\psi}(r) e^{i\theta}$, present in the Hamiltonian (1.1), is broken in the condensed phase as $\hat{\psi}(r)$ develops an expectation value and chooses a particular value of the phase $\theta$.

In the language developed in 1.2.1, spontaneous symmetry breaking manifests itself as the Hugenholtz-Pines (HP) theorem:

$$\mu = \Sigma_{11}(k = 0, z = 0) - \Sigma_{12}(k = 0, z = 0)$$

(1.4)

The HP theorem was first proved by Hugenholtz and Pines [26] for $T = 0$. A more general proof, valid for all $T$ and outlined briefly below, was given by Hohenberg.
and Martin [5], from the simple requirement that the field operator $\hat{\psi}(\mathbf{r})$ acquire a nonzero expectation value.

In [5], a source term $\int \eta^*(\mathbf{r})\psi(\mathbf{r}) + \eta(\mathbf{r})\psi^\dagger(\mathbf{r})$ was first used in the Hamiltonian to generate a nonzero $\langle \hat{\psi}(\mathbf{r}) \rangle$. Using linear response and a small shift in the phase of $\eta$, one can derive $G(0,0)^{-1}\tau_3\langle \hat{\Psi} \rangle = \left( \frac{\eta}{\eta'} \right)$. (Here $G(\mathbf{k},\omega)$ is the 2x2 Beliaev matrix and $\tau_3$ is the Pauli matrix.) The condition to preserve the nonzero $\langle \hat{\psi}(\mathbf{r}) \rangle$ when the fictitious source $\eta$ vanishes is thus $G(0,0)^{-1} = 0$, which, upon use of the Dyson-Beliaev equations, leads to the HP theorem (1.4).

According to Goldstone’s theorem [96–98], the spontaneous breaking of a continuous symmetry, in the absence of coupling to a gauge field, implies the existence of a gapless mode. The spectrum of the Bose-condensed state thus needs to be gapless, since the existence of a nonzero $\hat{\psi}(\mathbf{r})$ breaks a $U(1)$ symmetry.

It is not surprising, therefore, that the same condition (1.4) can also be obtained by imposing the requirement that the spectrum be gapless. In Eqn. (1.2), setting the denominator to zero (pole of $G_{11}$ gives spectrum), and imposing the condition $z(\mathbf{k} \to 0) = 0$, gives us back the Hugenholtz-Pines theorem (1.4).

1.2.3 The two-body $t$ matrix and many-body $T$ matrix

We will introduce here two quantities, each having loosely the meaning of an “effective interaction,” which recur in WIBG theory. The first is the two-body $t$-matrix, which is the sum of all ladder diagrams. For our purposes, it is equivalent to the vacuum scattering amplitude $f$ of two-particle scattering theory, which describes the effect of repeated interactions among two particles in vacuum. The second quantity is the many-body $T$-matrix, which also incorporates the effect of the surrounding medium on the interactions.

We will denote the two quantities by $t$ and $T$ respectively. (Shi and Griffin [15] in their review use the symbols $\Gamma$ and $\bar{\Gamma}$ respectively. Stoof [16,99] uses $T^{2B}$ and $T^{MB}$.)
The diagrammatic definition of the two-body $t$ matrix:

$$
t = \frac{1}{4} (k_3 - k_1)(k_4 - k_2) + \ldots
$$

Note that the internal propagators are all non-interacting propagators (thin lines).

The corresponding equation is

$$
t(k_1, z_1; k_2, z_2; k_3, z_3; k_4, z_4) = U(k_1 - k_2) + \int \frac{d^3qdz_q}{(2\pi)^4} U(q)G(0)(k_1 - q, z_1 - z_q)G(0)(k_2 + q, z_2 + z_q) \times t(q, k_2; k_1, z_2, z_3, z_1, z_4).
$$

(1.5)

Actually, one only needs two momenta ($k_1 - k_2$ and $k_3 - k_4$) and a single complex energy to specify the $t$-matrix. The $t$-matrix is related to the bare potential by the Lippman-Schwinger equation

$$
t(k, k'; z) = U(k - k') + \int_q \frac{U(k - q)t(q, k'; z)}{z - 2\epsilon_q}
$$

In chapter 5, we will use the on-shell version of this relation to remove ultraviolet divergences from our quasiparticle description of the Bose gas.

The two-body $t$-matrix is related to the vacuum scattering amplitude $f$ by the Beliaev-Galitskii relation [20,100]; at low densities they coincide. We will not need to distinguish between the two in our work.

The quantity physically measured in a scattering experiment in vacuum is $t$ (or $f$) rather than the bare interaction $U(k)$. The zero-momentum limit of the $t$-matrix is proportional to the $s$-wave scattering length $a$:

$$
t(k_1; k_2; k_1; k_2) = t = \frac{4\pi a}{m}.
$$
The many-body $T$-matrix is also a sum of ladder diagrams; however the internal propagators in the ladders are now full propagators rather than the bare propagators summed in the two-body $t$-matrix. Eqn. 1.5 will give $T$ instead of $t$ when the $G^{(0)}$'s are replaced by $G$'s.

1.3 Approximations: Mean Field and Beyond

Having introduced the relevant quantities, in this section we describe some of the approximations used in describing the WIBG. In 1.3.1, the properties of the zero-temperature Bose gas are described at the level of various mean field approximations. This will be useful as a reference when, in chapter 3, we develop a description of the $T = 0$ BEC in terms of a squeezed coherent state, and compare our results with standard WIBG properties.

In 1.3.2, we review some finite-temperature physics of the WIBG; this is a conceptual prelude to our work on the BEC transition temperature (chapters 4 and 5). The temperature-dependence of the zero-energy $T$ matrix is discussed separately in 1.3.3, because of the importance of this quantity in current studies of the BEC transition.

Finally, a discussion of proceeding beyond mean field is given in 1.3.4. We gloss over perturbative techniques for the Bose-condensed system, and focus instead on variational treatments, which are more relevant to this thesis.

1.3.1 Hartree-Fock-Bogoliubov approximation at $T = 0$

Mean-field schemes for the WIBG were developed first by Bogoliubov [4], and later improved by Popov [21], Girardeau and Arnowitt [27], and others.

Bogoliubov’s original approximation involves the mean-field substitution $\hat{c}_0, \hat{c}_0^\dagger \rightarrow N_0^{1/2}$, along with a neglect of all terms involving more than two non-condensate operators. The Hamiltonian thus becomes quadratic and can be solved by a
canonical transformation. In the language of Green’s functions, this involves using for the normal self-energy the Hartree and Fock diagrams with condensate atoms only (Fig. 1.4).

\[
\Sigma_{11}(k, z) = n_0 [U(0) + U(k)] , \quad \Sigma_{12}(k, z) = n_0 U(k) .
\]

Using these self-energies, one obtains the Bogoliubov spectrum

\[
E_k = \sqrt{\epsilon_k^2 + 2n_0 U(k)\epsilon_k} ,
\]

which at long wavelengths has a linear phonon spectrum with sound velocity \( c = [n_0 U(0)/m]^{1/2} \).

Even at the mean field level, the Bogoliubov treatment can be improved by taking into account interactions between non-condensate bosons. In other words, we include in the normal self-energy (\( \Sigma_{11} \)) the diagrams in Fig. 1.5 in addition to the ones of Fig. 1.4. This improved mean-field theory is known as the Hartree-Fock-Bogoliubov (HFB) approximation.

Popov [21] was one of the first to have included non-condensate contributions at mean field (and beyond); so the name Popov approximation (and sometimes Girardeau-Arnovitt approximation) is also used for this level of treatment.
Figure 1.5: Diagrams included in the normal self-energy $\Sigma_{11}$ in the HFB approximation, in addition to those already included in the Bogoliubov approximation.

The Popov improvement is particularly important at non-zero temperatures, when a significant fraction of the WIBG is outside the condensate. For now we describe this approximation at $T = 0$. Assuming $k$-independent interaction $U(k) = U(0) = U$,

$$
\Sigma_{11}(k, z) = 2n_0 U + 2U \int \frac{d^3k_1dz_1}{(2\pi)^4} G^{(0)}_{11}(k_1, z_1) e^{iz_10^+} = 2nU,
$$

$$
\Sigma_{12}(k, z) = n_0 U.
$$

In general, when we refer to the $T = 0$ HFB approximation, we mean the approximations $\Sigma_{11} = 2Un$ and $\Sigma_{12} = Un_0$.

At non-zero temperatures, Popov and HFB refer to different approximations [101], but they are identical at $T = 0$ and we are not interested much in the distinctions between finite-temperature mean-field schemes (next section).

### 1.3.2 Finite temperatures

For temperatures above the condensation temperature $T_c$, the WIBG is normal, anomalous self-energies and Green’s functions vanish, and the occupancy of the lowest ($k = 0$) single-particle state, $N_0$, becomes microscopic. Perturbation theory reduces to the more familiar form with a single kind of propagator and self-energy. This is the formalism we use in our discussion analysis of $T_c$, in chapter
5, where we approach the transition from above.

The fact that the anomalous self-energies vanish at and above $T_c$ allows one to use the Hugenholtz-Pines theorem for specifying the transition point as $\mu = \Sigma(0, 0)$.

At nonzero temperatures below $T_c$, the basic structure of the theory remains the same as that for $T = 0$, but it becomes important to account for condensate depletion and for the correlations between non-condensate particles. A number of approximations have arisen to deal with such effects. Discussion and classifications of the various approximations may be found, e.g., in Refs. [5,15,101].

Fig. 1.6 shows schematically the variation of $N_0$ with temperature, for the ideal and interacting Bose gases. The interacting gas has some depletion even at $T = 0$ ($N_0(T = 0) < N$), and the low-$T$ variation is $\sim -T^2$ rather than the $\sim -T^{3/2}$ of the ideal gas [12,15]. We point out that the two $N_0(T)$ curves are made to vanish at the same temperature marked $T_c$; this reflects the facts that (1) the shift of $T_c$ in the WIBG (compared to the ideal gas $T_c^{(0)}$) is small, and
its magnitude not quite agreed upon, and (2) even the direction of the shift was under debate until a few years ago. This shift is the subject of chapters 4 and 5.

Also shown in Fig. 1.6 is the temperature-variation of the zero-energy many-body \( T \)-matrix [14–16], discussed in more detail in 1.3.3.

### 1.3.3 \( T \)-matrix near \( T_c \)

The vanishing of the low-energy \( T \)-matrix at the transition point is a dramatic many-body effect, which has never been fully accounted for in \( T_c \) calculations. We believe this to be the main limitation of quasi-particle treatments near the critical point. A renormalization group (RG) calculation [16] shows that the effective two-body interaction follows the many-body \( T \)-matrix curve rather than the temperature-independent two-body \( t \)-matrix.

The \( T \)-matrix curve is a testament to the continuing excitement of WIBG theory today: this striking feature was discovered only in 1997, by Bijlsma & Stoof [14], via a variational calculation followed by numerics. An approximate derivation has been given by Shi & Griffin [15], which we summarize here.

The zero-energy limits of the two quantities will be denoted by \( t_0 \) and \( T_0 \). Comparing definitions, one finds: \( T_0 = t_0/[1 + \alpha(T)t_0] \), with

\[
\alpha(T) = \frac{1}{\beta} \sum_n G_{11}(\mathbf{q}, i\omega_n)G_{11}(-\mathbf{q}, -i\omega_n) - \frac{1}{2\epsilon q^2}.
\]

In the \( T \)-matrix approximation, \( \Sigma_{11} = 2nT_0, \Sigma_{12} = n_0T_0 \). The Beliaev-Dyson equations, with the help of the H-P theorem, allow one to write \( G_{11}(\mathbf{k}, i\omega_n) \) as

\[
G_{11} = -\frac{i\omega_n + \epsilon_\mathbf{k} + n_0T_0}{\omega_n^2 + \epsilon_\mathbf{k}^2 + 2n_0T_0};
\]

below \( T_c \), and as \( G_{11} = -1/(i\omega_n - \epsilon_\mathbf{k} + n_0T_0) \), above \( T_c \). Using these to evaluate \( \alpha \), one can solve for \( T_0 \) both above and below \( T_c \). Close to \( T_c \), one obtains

\[
T_0 \approx \begin{cases} \frac{\gamma t_0}{(n^{1/3}a)} \left[ 1 - (T/T_c)^{3/2} \right] & \text{if } T < T_c, \\ \frac{\gamma t_0}{(n^{1/3}a)} [(T/T_c)^{3/2} - 1] & \text{if } T > T_c, \end{cases}
\]
Here $\gamma = [\zeta(3/2)]^{4/3} / 4\pi \approx 0.286$. This treatment captures the essential behavior of $T_0$ near $T_c$: decrease to zero from both sides, with sharper decrease for smaller $n^{1/3}a$.

The $T$ matrix vanishes completely at $T_c$ only for zero momenta and frequency. For nonzero momenta and frequencies, $T$ retains nonzero values at all temperatures. Some consequences were pointed out in Ref. [14].

1.3.4 Beyond mean field

Above $T_c$, perturbation theory is more straightforward (no anomalous terms). An example of second-order perturbation theory is our quasiparticle calculation of chapter 5.

In the Bose-condensed phase, perturbative calculations beyond mean field becomes quite cumbersome because of the anomalous terms. Second-order calculations were performed early in the theory of WIBG, starting with Beliaev [19,20]; details of the bookkeeping complications can be found in [15]. In recent years, a functional formulation of the WIBG has also been popular [69,102,103]; such formulations have sometimes allowed incorporation of some higher-order diagrams which are not easy to include otherwise.

Fortunately, in this thesis, we will not deal with perturbative calculations in the ordered phase. Instead, we are interested in variational formulations of the Bose-condensed phase, which is a different route to beyond-mean-field physics.

In the early days (1959-64), Valatin and Butler [104,105] and Girardeau and Arnowitt [27] both suggested wavefunctions created by operators similar to

$$\prod_k \exp \left[ \gamma_k \hat{c}_k \hat{c}_k^\dagger - \gamma_k^* \hat{c}_k^\dagger \hat{c}_k \right].$$

In the modern language of quantum optics, these are “squeezed” states. We will discuss these variational approaches in more detail in chapter 2, after introducing the quantum-optics terminology of quantum states. More recently, several studies
have been performed ( [76, 78], chapter 3 of this thesis), in the same tradition of using variational wavefunctions to account for the correlation between opposite-momenta pair excitations in the Bose-condensed WIBG.

Another variational approach to the Bose gas is a real-space one: based on the use of a wavefunction of the Jastrow (or Bijl-Dingle-Jastrow) type

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \propto \prod_{i<j} f(r_{ij}) \propto \exp \left( \sum_{i<j} u(r_{ij}) \right).$$

Such an approach has been useful for the WIBG [51, 106–113] as well as for numerical calculations on other quantum fluids ([51, 114]; also references in [107]). The method is also known as the method of correlated basis functions (CBF).

The relationship between the CBF (Jastrow) and perturbation-theoretic methods for the Bose-condensed state tends to be a difficult question. It is not always clear what classes of diagrams are accounted for in these variational procedures [107–109].

In dealing with our variational description of the Bose gas (chapter 3), we are faced with a similar issue: we find that the squeezing of the zero-momentum mode comes from some contribution beyond the Hartree-Fock-Bogoliubov level (Sec. 3.2.3). In this thesis we do not attempt to identify which diagrams are responsible for $k = 0$ squeezing; this remains a future challenge.

In a recent variational calculation [14], M. Bijlsma and H. Stoof set up a functional formulation of the theory and then minimized the thermodynamic potential, treating the normal and anomalous self-energies as variational parameters. They find that this variational procedure captures $\Sigma_{11}$ up to HFB (one-loop) order, while $\Sigma_{12}$ goes beyond mean field, and is obtained in the $T$-matrix approximation.

In our variational procedure in chapter 3, the beyond-HFB $k = 0$ squeezing appears in the anomalous self-energy; thus we also get a $\Sigma_{11}$ correct to HFB order, and a $\Sigma_{12}$ including physics from beyond mean field.
1.4 Bose-Einstein Condensation Temperature

The Bose-Einstein Condensation Temperature $T_c^{(0)}$ of a non-interacting gas is obtained from the ideal-gas relation

$$N = N_0 + \frac{V}{\lambda^3} g_{3/2}(e^{3\mu}) ,$$

by noting that, for a fixed density, the $k = 0$ state will have to be macroscopically occupied below the temperature $T_c^{(0)} = (2\pi/m[\zeta(3/2)]^{2/3}) n^{2/3}$. Here, $g_{\nu}(x)$ stands for the Bose-Einstein integral functions [115].

Once a repulsive interaction is introduced between the bosons, one is faced with the question of how much the transition temperature shifts due to the repulsive interaction. Simple as this question is, it has resisted a conclusive answer for over four decades. An early statement of the “$T_c$ problem” appears in Abrikosov, Gorkov and Dzyaloshinski’s classic many-body text [13] of 1963: “There is no general rule which allows us to determine the direction in which the transition temperature is shifted when the interaction is turned on.” (Sec. 27, chapter 5.)

To many observers, the problem appeared to be settled in 1982 when Toyoda [116] calculated that the effect of a small repulsion is to decrease $T_c$, with a shift $\Delta T_c \propto -\sqrt{a}$, where $a$ is the scattering length. A negative shift fit nicely with the observation that the helium $\lambda$-point temperature is lower than the BEC temperature for an ideal gas of the same density. Both the direction and the $a$-dependence of the shift are now known to be wrong, but it was not until the new alkali-gas era of BEC research, after 1995, that this fundamental question was re-examined seriously.

Overall, calculations on the $T_c$ problem have produced widely dissimilar results: increases and decreases of $T_c$ proportional to $a$, $\sqrt{a}$, $a \ln a$, etc. have been reported by various authors. It is only during the past several years that the community has been converging toward a consensus.

The second half of this thesis concerns the $T_c$ problem. In chapter 4, we give
a review of the diverse approaches, draw connections between them, and examine some misconceptions and fine points. In chapter 5, we analyze $T_c$ by developing a quasi-particle description of the WIBG just above the critical point.

1.5 Experiments in Atomic Clouds

1.5.1 Realizations

The fact that interactions in liquid helium drastically reduce the occupancy of the lowest one-particle state motivated the search for a WIBG system with a higher condensate fraction. Early on [117], the possibility of using spin-polarized hydrogen for this purpose was recognized, and Stwalley and Nosanow’s 1976 work [118] generated significant interest in this idea. Spin-polarized hydrogen was first stabilized by Silvera and Walraven [119], who coated the surface of the container with superfluid helium.

Surface interaction effects continued to be a deterrent for the stability of high densities, and this led a group at MIT, led by Greytak and Kleppner, to develop purely magnetic traps for atoms. Among other techniques, this group also developed evaporative cooling of magnetically trapped gases. The trapping and evaporative cooling methods developed by this group are applicable both to hydrogen and alkali gases. However, alkali gases have some added advantages, such as being amenable to highly efficient laser-cooling procedures. Efforts, therefore, were focused on alkali gases.

After two decades of development of experimental techniques, the first gases to be cooled to degeneracy temperatures and display Bose-Einstein condensation were alkali gases (rubidium [62], sodium [63] and lithium [64,120]). Condensation of spin-polarized hydrogen came later, in 1998 [95].
Other atomic species, in various hyperfine states, are also under active investigation for Bose condensation. In 2000, a different isotope of rubidium was Bose-condensed [121], and in 2001, two groups reported the condensation of metastable $^4$He atoms in an excited state [122,123] (the lowest spin-triplet hyperfine state). According to the Cornell & Wieman Nobel lecture [124], it is expected that almost any magnetically trappable species can be Bose-condensed. One thus expects a number of new quantum-degenerate WIBGs in the coming years.

1.5.2 Selective look at experiments

Although the research discussed in this thesis does not pertain to any particular trapped-gas experiment, the influence of these experimental developments on WIBG research is so great that it seems appropriate to present a brief survey.

Description of experiments exploring coherence and squeezing aspects of the WIBG (e.g., interference and four-wave mixing experiments) will be deferred to the next chapter (Sec. 2.4), until after we have discussed coherence and squeezing formally.

Excitations. Soon after the first creation of BECs, excitations involving shape oscillations of various kinds were excited and measured. Since then, a wide variety of excitation studies have been performed, such as the measurement of the quasiparticle spectrum, observation of Beliaev and Landau damping, creation of solitonic excitations, etc.

Rotating BEC: vortices. The first rotating condensed WIBGs, with a single quantized vortex precessing around the center of the trap, were created around the end of 1999. Since then, vortex lattices have been created, and excitations of the vortex lattices are also being studied.

Quantum Hall physics. It is expected that, at angular velocities close to the trapping frequency, there should be a regime where the rotating condensate is in a composite-boson “quantum hall” state. At the time of the writing of this thesis,
experiments in JILA (Boulder, Colorado) seem to be very close to achieving such a state.

**Tunable interactions and Feshbach resonances.** A magnetic field can change the interaction between the atoms in a trapped gas, and thus the scattering length of a condensate can be tuned. In particular, crossing through certain values of the magnetic field even changes the sign of the interaction. This discovery has made possible an entirely new class of studies, such as the dynamics of a many-body condensate after the interaction strength is changed rapidly.

**Lower Dimensions.** By making the traps extremely flat or extremely elongated, alkali-gas experimenters have managed to produce 2D and 1D quantum-degenerate systems, with quasi-condensates.

**Superfluid-“insulator” transition.** By trapping cold atoms in an optical lattice, and varying the strength of the lattice, it is now possible to observe a quantum phase transition between a superfluid and a localized phase. (The localization transition is similar but not identical to the freezing of superfluid helium.) Various dynamic phenomena, e.g., involving a fast transition from one phase deep into the other, have also been demonstrated.

**Light scattering, superradiance.** Light scattering for the atomic-gas condensates has the status that neutron scattering did for superfluid helium. Light scattering has been used to probe the structure factor, the phonon spectrum and other excitations. In addition, a type of highly directional scattering of light (“super-radiant” scattering), involving Bose-stimulated transfer of a large fraction of the atoms to a particular mode, has been observed: this has no analog in liquid helium physics.
1.6 Outline of Thesis

In this introductory chapter, we have reviewed aspects of the physics of the weakly repulsive Bose gas. The coverage is of course highly selective: the attempt was to try to concentrate on those aspects which have some relevance to the work described in the following chapters.

Chapters 2 and 3 will concern a description of the WIBG in terms of the quantum-optics concepts of coherence and squeezing. Chapter 2 introduces these concepts and surveys their use in the study of condensed-matter systems, in particular the interacting Bose gas. In chapter 3, our variational calculations are presented.

Chapters 4 and 5 will discuss the problem of determining the transition temperature ($T_c$) of the WIBG.

Chapter 4 is a review and critique of the many attempts to solve the problem. We also provide a re-derivation, in modern language, of a $T_c$ calculation first performed by Kanno in 1969 [125]. Most of the material in this chapter is adapted from the preprint [1].

Chapter 5 presents our $T_c$ calculations, a quasiparticle formulation which reduces the problem of the shift in $T_c$ to the problem of determining the quasiparticle spectrum at the transition point. Once the problem is formulated this way, two ways of determining the spectrum (and hence $T_c$) are pointed out. The results of these two approaches are given in chapter 5 while details are deferred to appendix A.