Re-examining Bogoliubov’s theory of an interacting Bose gas

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As is well-known, in the conventional formulation of Bogoliubov’s theory of an interacting Bose gas, the Hamiltonian $\hat{H}$ is written as a decoupled sum of contributions from different momenta of the form $\hat{H} = \sum_{k \neq 0} \hat{H}_k$. Then, each of the single-mode Hamiltonians $\hat{H}_k$ is diagonalized separately, and the resulting ground state wavefunction of the total Hamiltonian $\hat{H}$ is written as a simple product of the ground state wavefunctions of each of the single-mode Hamiltonians $\hat{H}_k$. While this way of diagonalizing the total Hamiltonian $\hat{H}$ may seem to be valid from the perspective of the standard, number non-conserving Bogoliubov’s method, where the $k = 0$ state is removed from the Hilbert space and hence the individual Hilbert spaces where the Hamiltonians $\{\hat{H}_k\}$ are diagonalized are disjoint from one another, we argue that from a number-conserving perspective this diagonalization method may not be adequate since the true Hilbert spaces where the Hamiltonians $\{\hat{H}_k\}$ should be diagonalized all have the $k = 0$ state in common, and hence the ground state wavefunction of the total Hamiltonian $\hat{H}$ may not be written as a simple product of the ground state wavefunctions of the $\hat{H}_k$’s. In this paper, we give a thorough review of Bogoliubov’s method, and discuss a variational and number-conserving formulation of this theory in which the $k = 0$ state is restored to the Hilbert space of the interacting gas, and where, instead of diagonalizing the Hamiltonians $\hat{H}_k$ separately, we diagonalize the total Hamiltonian $\hat{H}$ as a whole. When this is done, we find that the ground state energy is lowered below the Bogoliubov result, and the depletion of bosons is significantly reduced with respect to the one obtained in the number non-conserving treatment. We also find that the spectrum of the usual $\alpha_k$ excitations of Bogoliubov’s method changes from a gapless one, as predicted by the standard, number non-conserving formulation of this theory, to one which exhibits a finite gap in the $k \rightarrow 0$ limit. We discuss the presence of a gap in the spectrum of the $\alpha_k$’s in light of Goldstone’s theorem, and show that there is no contradiction with the latter.

Subject Index: 322, 320

§1. Introduction

There has been a lot of interest in the properties of interacting Bose systems during the past fifteen years following the experimental observation of Bose-Einstein condensation (BEC) in ultracold vapors of trapped rubidium[1] and sodium gases[2]. On the theoretical front, much of the effort to understand the properties of these systems has focused on using approaches of the Bogoliubov type at the lowest temperatures[3, 4, 5, 6, 7, 8, 9, 10, 11] and finite temperature generalizations of Bogoliubov’s theory[12, 13, 14, 15, 16, 17, 18, 19, 20] at higher temperatures. At a fundamental level, theories of the Bogoliubov type are based on two major approximations. The first approximation is the so-called Bogoliubov prescription (BP), which consists in replacing the creation and annihilation operators of the condensate with a $c$-number. The Hamiltonian which is obtained from that procedure does not commute with the operator $\hat{N}$ describing the total number of particles in the system, which implies that

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the total number of particles is not conserved. The second approximation, sometimes
called \(22), 23)\), the Bogoliubov truncation (BT), consists in truncating the Hamiltonian
of the system, keeping only enough terms to allow the truncated Hamiltonian to be
exactly diagonalizable with the help of a “canonical transformation.” The question
then arises as to whether the physics of Bose condensed systems is correctly de-
scribed by Bogoliubov type theories, given these two major approximations that are
made, and given also a number of other, lesser and mainly technical approximations
having to do with the choice of self-energies in the field-theoretic formulation of these
theories. Over the years, many authors have tried to shed light on these kinds of
questions using different degrees of mathematical rigor (see References \(23)-24)\) for
an overview and a list of relevant references). Yet, and despite considerable activity,
a closer look reveals that several aspects of Bogoliubov type theories are still not
fully understood.\(23), 24), 25), 26), 27), 28), 29), 30)\)

In this paper, we will examine Bogoliubov’s theory at zero temperature in quite
some detail, shedding more light on the validity and accuracy of the Bogoliubov pre-
scription at a microscopic level, and raising a few issues with this theory which have
been overlooked in the past, and which in the author’s view still need to be clarified.
Chief among these new issues that we want to address is the question of trying to
understand how the decoupled way in which the Hamiltonian is diagonalized in Bo-
goliubov’s theory affects the nature of the Bogoliubov ground state. Indeed, and as
is well-known, in the standard formulation of Bogoliubov’s theory, after the creation
and annihilation operators of the condensate, \(a^\dagger_0\) and \(a_0\) respectively, are replaced
by the c-number \(\sqrt{N}\) (\(N\) being the total number of bosons in the system), the
Hamiltonian \(\hat{H}\) can be written as a decoupled sum of contributions from differ-
ent momenta of the form \(\hat{H} = \sum_{k \neq 0} \hat{H}_k\), where each Hamiltonian \(\hat{H}_k\) describes
the interaction of bosons in the condensed \(k = 0\) state with bosons in the momentum
modes \(\pm k\). Then, each of the single-mode Hamiltonians \(\hat{H}_k\) is diagonalized sep-
arately and the ground state (GS) wavefunction of \(\hat{H}\) is obtained as the product
of the GS wavefunctions of the \(\hat{H}_k\)’s. Here we shall argue that, while this way of
diagonalizing the total Hamiltonian \(\hat{H}\) may seem to be valid from the perspective
of the conventional, number non-conserving Bogoliubov’s method, where the \(k = 0\)
state is removed from the Hilbert space and hence the individual Hilbert spaces
where the Hamiltonians \(\{\hat{H}_k\}\) are diagonalized are disjoint from one another, from a
number-conserving perspective this diagonalization method is not appropriate, since
the true Hilbert spaces where the Hamiltonians \(\{\hat{H}_k\}\) should be diagonalized all have
the \(k = 0\) state in common, and hence the ground state wavefunction of the Hamil-
tonian \(\hat{H}\) may not be written as a simple product of the ground state wavefunctions
of the \(\hat{H}_k\)’s. We then shall discuss a variational, number-conserving generalization
of Bogoliubov’s theory in which the \(k = 0\) state is restored into the Hilbert space of the
interacting gas, and where, instead of diagonalizing the Hamiltonians \(\hat{H}_k\) separately,
we diagonalize the total Hamiltonian \(\hat{H}\) as a whole. When this is done, we find that
the ground state energy is lowered below the Bogoliubov result, and the depletion
of bosons is significantly reduced with respect to the number non-conserving treat-
ment. Moreover, the spectrum of excitations of the system changes from a gapless
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The rest of this article consists of two main parts. The first part is almost entirely devoted to assessing the accuracy of Bogoliubov’s prescription, and consists of Secs. 2 through 6. In the second part of the paper, consisting mainly of Sec. 7, we go beyond the conventional formulation of Bogoliubov’s theory by trying to enforce the conservation of the number of bosons in the system, making sure we keep an accurate count of the number of bosons in the \( k = 0 \) state. As mentioned above, when this is done, the results of Bogoliubov’s theory are changed both in quantitative and qualitative ways, and these changes are discussed in quite some detail in Sec. 8.

We now want to give the reader a more detailed overview of the contents of each one of the remaining eight Sections of this article. In Sec. 2 we shall start by reviewing the standard Bogoliubov treatment of an interacting Bose gas. As we mentioned above, after the BP is performed the total number of bosons is not conserved, which leads to a number of unphysical features. As an example, the average number of bosons \( N_k \) in the single-particle state of momentum \( k \) is found to diverge like \( 1/k \) as \( k \to 0 \), which does not of course make much sense for a system with a fixed number of bosons \( N \). In Sec. 3 we discuss this and other similar unphysical predictions of Bogoliubov’s method, and their consequence on the evaluation of expectation values of physical observables in the Bogoliubov ground state. To be able to formulate Bogoliubov’s theory within a number-conserving framework and get rid of the aforementioned unphysical features, in Sec. 4 we proceed to derive a number-conserving version of Bogoliubov’s Hamiltonian, which we show can be written as a sum of decoupled Hamiltonians \( \hat{H}_k \) for each momentum mode \( k \), \( \hat{H} = \sum_{k \neq 0} \hat{H}_k \). Then, in order to substantiate the claim made above according to which each one of the single-mode Hamiltonians \( \hat{H}_k \) corresponding to a given momentum mode \( k \) is diagonalized independently in Bogoliubov’s theory, in Sec. 5 we present a detailed analysis of a variational, number-conserving approach to the single-mode Hamiltonian \( \hat{H}_k \), and show explicitly that the results obtained from the diagonalization of this single-mode Hamiltonian perfectly coincide with the results of Bogoliubov’s method in the thermodynamic \( N \to \infty \) limit. At this point, and in order to assess the accuracy of the above diagonalization of the single-mode Hamiltonian \( \hat{H}_k \), in Sec. 6 we perform an exact numerical diagonalization of this Hamiltonian. Our numerical results corroborate the variational approach of Sec. 5 which is found to be surprisingly accurate. The main conclusion of the analysis carried out in Secs. 5 and 6 is that the treatment of the truncated many-body Hamiltonian carried out in Bogoliubov’s theory amounts to diagonalizing each one of the Hamiltonians \( \hat{H}_k \) (representing the kinetic energy plus the interaction energy of bosons having a momentum \( +k \) or \( -k \) with the condensate) independently from the other momentum contributions \( \hat{H}_{k'}(\neq k) \), and is in fact exceedingly good at predicting the ground state energy of each one of these single-mode Hamiltonian \( \hat{H}_k \) taken separately. While this would be perfectly legitimate if the various Hilbert spaces used to diagonalize the Hamiltonians \( \hat{H}_k \) were disjoint, in our case all these Hilbert spaces have the single-particle state with \( k = 0 \) in common, and so the above
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decoupled diagonalization procedure, strictly speaking, is mathematically not valid.

In the second part of the paper, and in order to assess the quantitative accuracy of diagonalizing the $\hat{H}_k$’s in the decoupled way described above, we generalize the variational approach of Sec. 5 for the single-mode Hamiltonian $\hat{H}_k$ to the total Hamiltonian $\hat{H} = \sum_{k \neq 0} \hat{H}_k$ in Sec. 7 and we do that in such a way as to keep an accurate count of the number of bosons in the $k = 0$ state, and with the requirement that the total number of bosons in all momentum modes be conserved. This leads, quite surprisingly, to an excitation spectrum of bosons which presents a gap as $k \to 0$, by contrast to the usual Bogoliubov method in which the spectrum of excitations is gapless. In Section 8 we give a discussion of our results, in view of their apparent violation of Goldstone’s theorem, and in Section 9 we present our conclusions.

§2. Review of the standard, number non-conserving formulation of Bogoliubov’s theory

We shall begin by reviewing the standard, number non-conserving formulation of Bogoliubov’s theory. To this end, let us consider the Hamiltonian of a gas of $N$ spinless bosons, interacting through a two-body potential $v(r)$:

$$\hat{H} = \int dr \hat{\Psi}^\dagger(r) \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\Psi}(r) + \frac{1}{2} \int dr dr' \hat{\Psi}^\dagger(r) \hat{\Psi}^\dagger(r') v(r-r') \hat{\Psi}(r') \hat{\Psi}(r), \quad (2.1)$$

where $\hat{\Psi}(r)$ is a boson field operator in second quantized language, which has the Fourier decomposition $\hat{\Psi}(r) = \sum_k a_k e^{ikr}/\sqrt{V}$ (periodic boundary conditions will be assumed throughout this paper), $a_k$ being a boson annihilation operator, and $V$ being the volume of the system. In Fourier space, the Hamiltonian $\hat{H}$ has the following expression:

$$\hat{H} = \sum_{k \neq 0} \varepsilon_k a_k^\dagger a_k + \frac{1}{2V} \sum_{k,k'} \sum_q v(q)[a_k^\dagger a_{k+q}^\dagger a_{k'-q} a_{k'}], \quad (2.2)$$

where $v(k)$ is the Fourier transform of $v(r)$ and $\varepsilon_k = \hbar^2 k^2/2m$ is the kinetic energy of bosons with wavevector $k$.

According to Bogoliubov’s prescription[9][10] one replaces the creation and annihilation operators $a_0^\dagger$ and $a_0$ of the $k = 0$ state by $\sqrt{\frac{N_0}{V}}$, where $N_0$ is the number of bosons in the condensate, upon which the above Hamiltonian takes the form $\hat{H} = \hat{H}_0 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4$, with $(n_0 = N_0/V$ is the density of condensed bosons):

$$\hat{H}_0 = \frac{1}{2} V n_0^2 v(0), \quad (2.3a)$$

$$\hat{H}_2 = \sum_{k \neq 0} \left\{ \xi_k a_k^\dagger a_k + \frac{1}{2} n_0 v(k)[a_k^\dagger a_{-k}^\dagger + a_k a_-] \right\} \quad (2.3b)$$

$$\hat{H}_3 = \sqrt{\frac{n_0}{V}} \sum_{q,k} v(q)[a_{k+q}^\dagger a_k a q + a_k^\dagger a_q a_{k+q}], \quad (2.3c)$$
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\[
\hat{H}_4 = \frac{1}{2V} \sum_{q,k,k'} v(q) a_{k+q}^\dagger a_{k'}^\dagger a_q a_k. \tag{2.3d}
\]

In Eq. (2.3b), \( \xi_k \) is the shifted boson energy:

\[
\xi_k = \varepsilon_k + n_0 \left[ v(\mathbf{k}) + v(\mathbf{0}) \right], \tag{2.4}
\]

and it is understood that no creation and annihilation operators of the condensate \( (a_0^\dagger \text{ and } a_0) \) appear on the rhs of Eqs. (2.3c) and (2.3d).

As it can be seen, the new expression of the Hamiltonian after the Bogoliubov prescription is performed does not conserve the number of bosons. To deal with this unphysical artifact of Bogoliubov’s prescription, Bogoliubov suggests that one should work with the “grand canonical Hamiltonian” \( \hat{H} = \hat{H} - \mu \hat{N} \), \( \mu \) being the chemical potential and the operator \( \hat{N} = \sum_k a_k^\dagger a_k \) being the total number of bosons. This amounts to replacing \( \hat{H}_0 \) and \( \hat{H}_2 \) in Eqs. (2.3) by \( \hat{H}_0' = \hat{H}_0 - \mu \hat{N}_0 \) and \( \hat{H}_2' = \hat{H}_2 - \mu \hat{N}_1 \), respectively, where \( \hat{N}_1 = \sum_{k \neq 0} a_k^\dagger a_k \) is the operator counting the total number of bosons outside the condensate. The ground state energy is then found by diagonalizing \( \hat{H}_2' \), which is done by introducing a new set of creation and annihilation operators, \( \alpha_k^\dagger \) and \( \alpha_k \), such that:

\[
\alpha_k = u_k a_k + v_k a_{-k}^\dagger, \quad \alpha_k^\dagger = u_k a_k^\dagger + v_k a_{-k}. \tag{2.5}
\]

These expressions can easily be inverted, with the result:

\[
a_k = u_k \alpha_k - v_k \alpha_{-k}^\dagger, \quad a_k^\dagger = u_k \alpha_k^\dagger - v_k \alpha_{-k}. \tag{2.6}
\]

In Eqs. (2.5) and (2.6), \( u_k \) and \( v_k \) are assumed to be real, spherically symmetric functions of the wavevector \( \mathbf{k} \). For the newly defined operators \( \alpha_k \) and \( \alpha_k^\dagger \) to describe boson excitations, it is required that they should obey bosonic commutation relations:

\[
[\alpha_k, \alpha_{k'}^\dagger] = [\alpha_k^\dagger, \alpha_{k'}] = 0, \quad [\alpha_k, \alpha_{k'}] = \delta_{k,k'}, \tag{2.7}
\]

which results in the condition:

\[
u_k^2 - v_k^2 = 1. \tag{2.8}
\]

If we now use Eq. (2.6) to rewrite the Hamiltonian \( \hat{H}_2' \) in terms of the operators \( \alpha_k \) and \( \alpha_k^\dagger \), and if in addition we require that the resulting expression not contain products of the form \( \alpha_k \alpha_{-k} \) or \( \alpha_k^\dagger \alpha_k^\dagger \), we obtain the following expressions of the so-called “coherence factors” \( u_k \) and \( v_k \):

\[
u_k^2 = \frac{1}{2} \left( \frac{\xi_k - \mu}{E_k} + 1 \right), \quad v_k^2 = \frac{1}{2} \left( \frac{\xi_k - \mu}{E_k} - 1 \right), \tag{2.9}
\]

where \( E_k \) is the energy spectrum:

\[
E_k = \sqrt{(\xi_k - \mu)^2 - n_0^2 v(\mathbf{k})^2}. \tag{2.10}
\]
The Hamiltonian $\tilde{H}_2$ then takes the quadratic form:

$$\tilde{H}_2 = \tilde{E}_2 + \sum_{k \neq 0} E_k \alpha_k^\dagger \alpha_k,$$

(2.11)

where we denote by $\tilde{E}_2$ the following quantity:

$$\tilde{E}_2 = \frac{1}{2} \sum_{k \neq 0} [E_k - \varepsilon_k - n_0 v(k)].$$

(2.12)

Requiring the spectrum $E_k$ of Eq. (2.10) to be gapless as $k \to 0$ results in the following expression of the chemical potential:

$$\mu = n_0 v(0),$$

(2.13)

upon which $E_k$ takes the celebrated Bogoliubov form:

$$E_k = \sqrt{\varepsilon_k [\varepsilon_k + 2n_0 v(k)]}.$$  

(2.14)

Using Eq. (2.13) into Eq. (2.9), one finds:

$$u_k^2 = \frac{1}{2} \left( \frac{\varepsilon_k + n_0 v(k)}{E_k} + 1 \right), \quad v_k^2 = \frac{1}{2} \left( \frac{\varepsilon_k + n_0 v(k)}{E_k} - 1 \right).$$

(2.15)

The Bogoliubov ground state (BGS) of the interacting boson gas, which we shall denote by the symbol $|\Psi_B\rangle$, is defined as the vacuum state for the $\alpha_k$ operators, and satisfies the condition:

$$\alpha_k |\Psi_B\rangle = 0, \quad \text{for all } k \neq 0.$$  

(2.16)

With this definition, it is easy to verify that $\tilde{E}_2$ is the expectation value of the Hamiltonian $\tilde{H}_2$ in the BGS, i.e. $\tilde{E}_2 = \langle \Psi_B | \tilde{H}_2 | \Psi_B \rangle$.

We now pause for a moment to emphasize the distinction which is usually done in Bogoliubov’s theory between the operators $a_k^\dagger$ and $a_k$ on one hand, and the operators $\alpha_k^\dagger$ and $\alpha_k$ on the other. For while the former create and annihilate actual bosons, the latter are thought to create and annihilate “quasiparticles”, which are identified as collective “phonon” modes, mainly because the corresponding excitation spectrum $E_k$ has a linear behavior at long wavelengths:

$$E_k \sim s \hbar k,$$

(2.17)

where

$$s = \sqrt{n_B v(0)/m}.$$  

(2.18)

is identified as the speed of sound (here and in the rest of this paper, $n_B = N/V$ is the density of bosons). We will come back to this identification in Sec. [8.3] below. For the moment, we want to have a more detailed look at a number of problematic features of Bogoliubov’s theory. These being more or less known features of this method, our main objective here is to provide a motivation for the variational formulations of Bogoliubov’s theory that will be studied in Secs. [5] through [7]. This will be the subject of the following Section.
§3. Issues with Bogoliubov’s theory

As mentioned above, in this Section we want to discuss a few questionable aspects of the number non-conserving formulation of Bogoliubov’s method as a way to motivate the variational treatment that will be presented in Secs. 5 and 7. We will start by looking at the ground state expectation values of quadratic combinations of creation and annihilation operators.

3.1. Divergence of the depletion $N_k = \langle a_k^\dagger a_k \rangle$ and of the anomalous average $\langle a_k a_{-k} \rangle$ in the $k \to 0$ limit

The first quantity we will discuss is the expectation value:

$$N_k = \langle a_k^\dagger a_k \rangle = \langle \Psi_B | a_k^\dagger a_k | \Psi_B \rangle,$$

which gives the average number of bosons in the single-particle state of momentum $k$. In the standard formulation of Bogoliubov’s theory, this quantity is given by:

$$N_k = \frac{\tilde{\epsilon}_k^2}{\tilde{v}_k^2} = \frac{1}{2} \left( \frac{\tilde{\epsilon}_k + n_0 v(k)}{E_k} - 1 \right).$$

Using the expression of $E_k$ given in Eq. (2.14), it is not difficult to see that $N_k$ diverges like $1/k$ as $k \to 0$, which is of course unphysical, given that we started from a system of fixed number $N$ of bosons.

The divergence of $N_k$ as $k \to 0$ will have important ramifications, as it will affect the expectation value of one-body operators. Indeed, if we consider a given physical observable which is described by a one-body operator $\hat{O}$ of the form $\hat{O} = \sum_k O_k a_k^\dagger a_k$, then the expectation value of $\hat{O}$ in the Bogoliubov ground state is given by:

$$\langle \hat{O} \rangle = \sum_k O_k N_k.$$

Since the result for $N_k$ is unphysical near $k = 0$, we see that the result for the expectation value $\langle \hat{O} \rangle$ includes terms whose contribution is unphysical near $k = 0$ as well. As an example, let us consider the Fock part of the Hamiltonian $H_F = \sum_{k \neq 0} n_0 v(k) a_k^\dagger a_k$. The contribution of any particular $k$ mode in this last expression to the ground state energy is given by $n_0 v(k) N_k$, which diverges like $1/k$ as $k \to 0$. This divergence cannot of course be taken at face value, because it originates in the unphysical divergence of the quantity $N_k$, which should be finite and bounded by the total number $N$ of bosons in the system for all values of the wavevector $k$.

A closely related problematic feature of Bogoliubov’s theory has to do with the divergence of the anomalous averages $\langle a_k a_{-k} \rangle = \langle \Psi_B | a_k a_{-k} | \Psi_B \rangle$ and $\langle a_k^\dagger a_{-k}^\dagger \rangle = \langle \Psi_B | a_k^\dagger a_{-k}^\dagger | \Psi_B \rangle$ in the $k \to 0$ limit. Following an argument made by de Gennes for the BCS ground state of superconductors, one can argue that an average such as $\langle a_k a_{-k} \rangle$ can be given a sense, from a number-conserving perspective, if it is understood as:

$$\langle a_k a_{-k} \rangle = \langle \Psi(N - 2) | a_k a_{-k} | \Psi(N) \rangle,$$
where we denote by $|\Psi(N)\rangle$ the normalized ground state wavefunction of a system of $N$ bosons. Written in this form, $\langle a_k a_{-k}\rangle$ can be interpreted as the probability amplitude for finding the system in the ground state $|\Psi(N-2)\rangle$ when a pair of bosons $(k,-k)$ is removed from the ground state $|\Psi(N)\rangle$. Following this line of thought, if we think of $\langle a_k a_{-k}\rangle$ as a probability amplitude, then it should be a bounded quantity, and should not diverge for any value of the wavevector $k$. Unfortunately, in the standard Bogoliubov theory, the expression of the anomalous average is given by:

$$\langle a_k a_{-k}\rangle = \langle a^\dagger_k a^\dagger_{-k}\rangle = -\frac{n_0 v(k)}{2E_k} \rightarrow -\infty \text{ as } k \rightarrow 0,$$

and diverges (negatively) as $k \rightarrow 0$, which is of course incompatible with an interpretation of $\langle a^\dagger_k a^\dagger_{-k}\rangle$ in terms of probabilities. The divergence of the anomalous average $\langle a_k a_{-k}\rangle$ will also have major consequences on the evaluation of expectation values of quantities involving quadratic products of operators of the form $a_k a_{-k}$ or $a^\dagger_k a^\dagger_{-k}$. Again, as an example, if we consider the so-called “pairing” part of the Bogoliubov Hamiltonian, $\hat{H}_P = \frac{1}{2} \sum_{k \neq 0} n_0 v(k) (a^\dagger_k a^\dagger_{-k} + a_k a_{-k})$, then the contribution of any particular term in $\hat{H}_P$ corresponding to a given wavevector $k$ to the ground state energy is given by $-\frac{n_0 v(k)}{2E_k}$, and again diverges like $-1/k$ as $k \rightarrow 0$. This divergence is again not to be taken too seriously, since it originates solely from the unphysical divergence of the anomalous average $\langle a_k a_{-k}\rangle$ in Eq. (3.5). We will look at these divergences in more detail below (see Sec. 5). For the moment, we want to have a closer look at the physical meaning of the operator $\hat{H}$ in Bogoliubov’s method.

**3.2. Physical meaning of the operator $\hat{H}$ in Bogoliubov’s method**

We now want to discuss the physical meaning of the Hamiltonian $\hat{H}$ in the standard formulation of Bogoliubov’s method in view of the fact that the ground state energy of the system is the expectation value of the “grand-canonical” Hamiltonian $\tilde{\hat{H}} = \hat{H} - \mu \hat{N}$, and not of the Hamiltonian $\hat{H}$ itself. As an aside, we shall observe that the use of the term “grand-canonical Hamiltonian” to describe the operator $\tilde{\hat{H}}$ is quite misleading, given that the term “grand-canonical” has a very specific meaning in ensemble theory of statistical mechanics, and refers to a very specific statistical ensemble which only has a meaning at nonzero temperatures. We also would like to remind the reader that, in ensemble theory, various operators have the same physical meaning in the grand-canonical ensemble as in any other statistical ensemble. In particular, the operator describing the total energy in the grand-canonical ensemble is the Hamiltonian $\hat{H}$, not the combination $\hat{H} - \mu \hat{N}$, which in fact describes the grand-potential at $T = 0$. It is therefore extremely surprizing that in Bogoliubov’s theory the ground state energy is found by taking the expectation value of $\tilde{\hat{H}} = \hat{H} - \mu \hat{N}$ instead of the expectation value of the Hamiltonian $\hat{H}$ itself.

In what follows, we want to go further and show that the use of the Hamiltonian $\tilde{\hat{H}}$ instead of $\hat{H}$ can even lead, in certain situations, to nonsensical results, which will allow us to argue that the Hamiltonian $\hat{H}$ has no physical meaning in the standard formulation of Bogoliubov’s theory. To this end, let us consider states that are
generated by successive action of the “quasiparticle” operator $\alpha_k^\dagger$ on the BGS. It is easy to verify that these states are eigenstates of the “grand-canonical” Hamiltonian $\tilde{H}_2$. For example, one can show that the normalized state defined by:

$$|\Phi_k^{(n)}\rangle = \left(\alpha_k^\dagger\right)^n |\Psi_B\rangle,$$

and corresponding to the excitation of $n$ “quasiparticles” of wavevector $k$ is an eigenstate of $\tilde{H}_2$ with eigenvalue $[\tilde{E}_2 + nE_k]$:

$$\tilde{H}_2|\Phi_k^{(n)}\rangle = [\tilde{E}_2 + nE_k]|\Phi_k^{(n)}\rangle.$$

Similarly, a state of the form:

$$|\Phi_{k_1,\ldots,k_n}\rangle = \alpha_{k_1}^\dagger \cdots \alpha_{k_n}^\dagger |\Psi_B\rangle,$$

and corresponding to the excitation of $n$ “quasiparticles” with distinct wavevectors $k_1,k_2,\ldots,k_n$, is an eigenstate of the grand canonical Hamiltonian $\tilde{H}_2$ with eigenvalue $[\tilde{E}_2 + E_{k_1} + \cdots + E_{k_n}]$:

$$\tilde{H}_2|\Phi_{k_1,\ldots,k_n}\rangle = [\tilde{E}_2 + E_{k_1} + \cdots + E_{k_n}]|\Phi_{k_1,\ldots,k_n}\rangle.$$

Let us focus for simplicity on the state with one “quasiparticle” of momentum $k$. This is the state given by:

$$|\Phi_k\rangle = \alpha_k^\dagger |\Psi_B\rangle.$$

Such a state is believed to have an excitation energy which is gapless in the $k \to 0$ limit. This belief originates in Eq. (2.11), where $E_k$ is identified as the excitation energy of the $\alpha_k$ “quasiparticles”. Indeed, if we calculate the excess free energy with respect to the Bogoliubov ground state of the state $|\Phi_k\rangle$ using the “grand canonical” Hamiltonian $\tilde{H}_2$, we find:

$$\langle \Phi_k| [H_0 + \tilde{H}_2]|\Phi_k\rangle - \langle \Psi_B| [H_0 + \tilde{H}_2]|\Psi_B\rangle = E_k.$$

At this stage, it is useful to remember that the true quadratic part of the original Hamiltonian $\tilde{H}$ is $\tilde{H}_2$, not $\tilde{H}_2$. Consequently, in evaluating the excitation energy (not the excitation grand potential!) $\Delta E_k^{ex,\alpha}$ of a “quasiparticle” $\alpha_k^\dagger$, one should use the Hamiltonian $\tilde{H}_2$ instead of $\tilde{H}_2$, and define $\Delta E_k^{ex,\alpha}$ as follows (we here use the superscript $\alpha$ to indicate that we are calculating the excitation spectrum of the $\alpha_k$ “quasiparticles”):

$$\Delta E_k^{ex,\alpha} = \langle \Phi_k|[H_0 + \tilde{H}_2]|\Phi_k\rangle - \langle \Psi_B|[H_0 + \tilde{H}_2]|\Psi_B\rangle.$$

Performing the calculation, we find:

$$\Delta E_k^{ex,\alpha} = E_k + n_0 v(0)\left[u_k^2 + v_k^2\right],$$

$$= E_k + n_0 v(0)\frac{\epsilon_k + n_0 v(k)}{\sqrt{\epsilon_k^2 + 2n_0 v(k)}}.$$


As it can be seen, the energy cost to excite a “quasiparticle” $\alpha_k^\dagger$, when calculated using $\hat{H}_2$, is no longer given by the gapless expression $E_k$. There is now an additional term, which furthermore diverges like $1/k$ as $k \to 0$. We are therefore faced with the bizarre situation where the operator $\hat{H}_2$ has no physical meaning of its own whatsoever, and where the energy observable rather mysteriously is no longer represented by this last operator, but by the combination $\hat{H}_2 = \hat{H}_2 - \mu \hat{N}_1$, which, in principle, represents the grand-potential of the system at zero temperature. Because of the non-conservation of particle number, the use of the true energy operator $\hat{H}_2$ in the formulation of Bogoliubov’s theory given in Sec. 2 can lead to non-sensical results, as we have seen above with the excitation spectrum of the $\alpha_k$ “quasiparticles”.

3.3. Ad hoc nature of the canonical transformation from the $a_k$’s to the $\alpha_k$’s

We now turn our attention to another questionable aspect of Bogoliubov’s method, having to do with the physical content of the canonical transformation from the $a_k$’s to the $\alpha_k$’s, and the rather ad hoc fashion in which the commutation relations between the excitation operators $\alpha_k$ and $\alpha_k^\dagger$ are introduced. Taking note of the fact that these operators, in the standard formulation of Bogoliubov’s theory, do not conserve the number of bosons, below we will show that, in a number-conserving approach, the canonical commutation relations between the $\alpha_k$’s are not at all exact, but only approximate, and are only valid if the depletion of the ground state is small. For situations where this condition is violated, such as for liquid Helium at low temperatures, where the number of bosons in the condensate is only about 10% of the total number of bosons in the system, the canonical commutation relations are no longer valid, and should be replaced by more involved expressions. For more details, the reader is referred to Sec. 5 where the commutation relations between the $\alpha_k$’s will be obtained from first principles, and not imposed a priori, within a number-conserving variational approximation.

3.4. Diagonalizing the various Hamiltonians $\hat{H}_k$ corresponding to different momentum modes independently from one another

Perhaps one of the less obvious criticisms one can make of Bogoliubov’s method, and possibly one with the most far-ranging ramifications, has to do with the fact that, in this theory, the total “grand-canonical” Hamiltonian $\hat{H} = \hat{H} - \mu \hat{N}$ is not diagonalized as a whole, but rather, each momentum contribution $\hat{H}_k$ to $\hat{H}$ is diagonalized separately and independently from the other momentum contributions. One way to see this is by writing the total Hamiltonian $\hat{H}$ as a sum of contributions from different wavevectors $k$ of the form $\hat{H} = \sum_{k \neq 0} \hat{H}_k$. Then it is easy to convince oneself that the canonical transformation method of Sec. 2 is in fact a diagonalization of each one of the Hamiltonians $\hat{H}_k$ independently from the other Hamiltonians $\hat{H}_k'(\neq k)$. This process of diagonalizing each of the single-mode Hamiltonians $\hat{H}_k$ separately would be absolutely sound if the Hilbert spaces in which these Hamiltonians are diagonalized were totally disjoint from one another. This is unfortunately not the case here, with all these Hilbert spaces having the $k = 0$ state in common. Of course, from the perspective of Bogoliubov’s method, where the dynamic properties of the condensate are ignored and the $k = 0$ state is summarily removed from the
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Hilbert space, this is thought to be a perfectly legitimate way to proceed. However, in this paper, we shall challenge this view, and explicitly show that, when the conservation of particle number is properly taken into account, and the $k = 0$ is restored as an essential part of the Hilbert space used to describe the system, then the direct diagonalization of the full Hamiltonian $H$ gives very different results from diagonalizing each of the momentum components $H_k$ separately, as is done in the standard Bogoliubov formulation.

Since the non-conservation of particle number in the standard formulation of Bogoliubov’s theory is at the core of most of the conceptual difficulties discussed throughout this Section, it seems worthwhile to try to eliminate these difficulties by reformulating the theory within a number-conserving framework. This will be done in Sections 5 through 7. But, before we do so, we want to present a rather detailed derivation of Bogoliubov’s Hamiltonian in a number-conserving approach. This will be done next.

§4. Derivation of Bogoliubov’s Hamiltonian within a number-conserving approach

We now want to derive, within a number-conserving framework, a simplified version of the Hamiltonian (2.2) which is simple enough to allow for a straightforward evaluation of expectation values of physical observables, and at the same time captures the essential physics of a translationally invariant system of interacting bosons at zero temperature. Throughout this paper, it will be assumed, without loss of generality, that the bosons are confined in a cubic box of size $L$, and we shall use periodic boundary conditions, implying that momenta will be quantized with the following wavevectors:

\[ k = \frac{2\pi}{L} (n_x, n_y, n_z), \]

where the $n_i$’s are integers such that $-\infty \leq n_x, n_y, n_z \leq \infty$.

We shall start by specifying the Hilbert space we will use to describe our system. In the occupation number representation, a system of $N$ bosons can in general be in any one of the states

\[ |\psi_{n_1, \ldots, n_\infty}^{m_1, \ldots, m_\infty} \rangle = |N - \sum_{i=1}^{\infty} (n_i + m_i); n_1, m_1; \ldots; n_\infty, m_\infty \rangle, \]

having $n_i$ bosons in the single-particle state of wavevector $k_i$ and $m_i$ bosons in the single-particle state of wavevector $-k_i$ (for all $i$ such that $1 \leq i \leq \infty$), and $[N - \sum_{i=1}^{\infty} (n_i + m_i)]$ bosons in the single-particle state with wavevector $k = 0$. More formally, if we denote by $|0\rangle$ the vacuum state for bosons, then $|\psi_{n_1, \ldots, n_\infty}^{m_1, \ldots, m_\infty} \rangle$ is the ket defined by:

\[ |\psi_{n_1, \ldots, n_\infty}^{m_1, \ldots, m_\infty} \rangle = \frac{\left( a_{0}^\dagger \right)^{N - \sum_{i=1}^{\infty} (n_i + m_i)} \prod_{i=1}^{\infty} (a_{k_i}^\dagger)^{n_i} \left( a_{-k_i}^\dagger \right)^{m_i}}{\sqrt{[N - \sum_{i=1}^{\infty} (n_i + m_i)]!} \prod_{i=1}^{\infty} \sqrt{n_i!} \sqrt{m_i!}} |0\rangle. \]
It then follows that the most general expression of the wavefunction $|\Psi(N)\rangle$ of a system of $N$ bosons in the occupation number representation is given by:

$$|\Psi(N)\rangle = \sum_{n_1,m_1} \cdots \sum_{n_\infty,m_\infty} C_{n_1\ldots,n_\infty}^{m_1\ldots,m_\infty} |\psi_{n_1\ldots,n_\infty}\rangle. \quad (4.4)$$

In the above equation, the $C_{n_1\ldots,n_\infty}^{m_1\ldots,m_\infty}$’s are complex numbers to be determined by diagonalization of the Hamiltonian $\hat{H}$ of the system. The summations extend over the range $0 \leq n_i, m_i \leq N$, subject to the constraint that the number of bosons in the state $|\mathbf{k} = 0\rangle$ in any ket of the basis must be positive:

$$N - (n_1 + m_1) \cdots - (n_\infty + m_\infty) \geq 0. \quad (4.5)$$

Now, it can be easily verified that the total momentum operator $\hat{P} = \sum_{\mathbf{k}} \hbar \mathbf{k} a_\mathbf{k}\dagger a_\mathbf{k}$ commutes with the Hamiltonian $\hat{H}$. This implies that $\hat{H}$ and $\hat{P}$ can be diagonalized simultaneously, and that eigenstates of $\hat{H}$ can be labeled by a definite value of the total momentum operator $\hat{P}$. In particular, for a system of bosons at rest, the ground state is the translationally invariant state corresponding to the eigenvalue $P = 0$ of the total momentum $\hat{P}$.

$$\hat{P}|\Psi(N)\rangle = 0. \quad (4.6)$$

This condition imposes a rather cumbersome constraint on the coefficients $C_{n_1\ldots,n_\infty}^{m_1\ldots,m_\infty}$, namely:

$$\sum_{n_1,m_1} \cdots \sum_{n_\infty,m_\infty} C_{n_1\ldots,n_\infty}^{m_1\ldots,m_\infty} \left[ \hbar \mathbf{k}_1(n_1 - m_1) + \cdots + \hbar \mathbf{k}_\infty(n_\infty - m_\infty) \right] |\psi_{n_1\ldots,n_\infty}\rangle = 0. \quad (4.7)$$

The easiest way to satisfy the above constraint is to restrict the Hilbert space to one where there are as many bosons with momentum $\mathbf{k}_i$ as there are bosons with momentum $-\mathbf{k}_i$, i.e. we choose to work in the restricted Hilbert space such that $n_i = m_i$, for all values of the index $i$. Eq. (4.4) then becomes:

$$|\Psi(N)\rangle = \sum_{n_1} \cdots \sum_{n_\infty} C_{n_1\ldots,n_\infty} |\psi_{n_1\ldots,n_\infty}\rangle \quad (4.8)$$

where now $|\psi_{n_1\ldots,n_\infty}\rangle$ is given by:

$$|\psi_{n_1\ldots,n_\infty}\rangle = |N - 2n_1 \cdots - 2n_\infty; n_1, n_1; \ldots; n_\infty, n_\infty\rangle, \quad (4.9a)$$

$$= \frac{1}{\sqrt{[N - 2\sum_{i=1}^{\infty} n_i]^{n_1} \prod_{i=1}^{\infty} (a_{\mathbf{k}_i}\dagger)^{n_i} (a_{-\mathbf{k}_i})^{n_i}}} \left( a_{\mathbf{k}_1}\dagger \right)^{n_1} \left( a_{-\mathbf{k}_1}\right)^{n_1} |0\rangle. \quad (4.9b)$$

We now want to isolate those terms in the Hamiltonian which will give significant contributions to the ground state energy in states of the form $|4.8\rangle$. For definiteness, let us rewrite the interaction part $\hat{V}$ of the many-body Hamiltonian, which is given by:

$$\hat{V} = \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{q}} v(\mathbf{q}) a_{\mathbf{k}+\mathbf{q}} a_{\mathbf{k}'-\mathbf{q}} a_{\mathbf{k}} a_{\mathbf{k}'}^\dagger. \quad (4.10)$$
In the above expression, we shall first separate the Hartree terms, corresponding to \( k + q = k' \), i.e. to \( q = 0 \); and the Fock (or exchange) terms, which correspond to \( k + q = k' \) and \( k' - q = k \), i.e. to \( q = k' - k \). Hence, we shall write the interaction term \( \hat{V} \) in the form:

\[
\hat{V} = \hat{V}_H + \hat{V}_F + \frac{1}{2V} \sum_{k,k',q \neq 0,k'-k} v(q) a_{k+q}^\dagger a_{k'}^\dagger a_{q}^\dagger a_{k},
\]

where the Hartree and Fock contributions, \( \hat{V}_H \) and \( \hat{V}_F \) respectively, are given by:

\[
\hat{V}_H = \frac{v(0)}{2V} \sum_{k,k'} a_k^\dagger a_{k'}^\dagger a_{k'} a_k,
\]

\[
\hat{V}_F = \frac{v(0)}{2V} \hat{N} (\hat{N} - 1),
\]

\[
\hat{V}_F = \frac{1}{2V} \sum_k \sum_{k' \neq k} v(k' - k) a_k^\dagger a_{k'} a_{k} a_{k'}^\dagger.
\]

We next consider the so-called “pairing” terms. These are obtained by letting \( k' = -k \) both in \( \hat{V}_F \) and in the last term of Eq. (14.11). This allows us to write:

\[
\hat{V} = \hat{V}_H + \hat{V}_F' + \hat{V}_P + \frac{1}{2V} \sum_k \sum_{k' \neq k} \sum_{q \neq 0,k'-k} v(q) a_{k+q}^\dagger a_{k'-q}^\dagger a_{q}^\dagger a_{k},
\]

where we defined:

\[
\hat{V}_F' = \frac{1}{2V} \sum_k \sum_{k' \neq k} v(k' - k) a_k^\dagger a_{k'}^\dagger a_{k'} a_k,
\]

\[
\hat{V}_P = \frac{1}{2V} \sum_k \sum_{q \neq 0} v(q) a_{k+q}^\dagger a_{-(k+q)}^\dagger a_{q} a_{-k}.
\]

It can be shown that the last term on the rhs of Eq. (14.13) has zero expectation value in the state \(|\Psi(N)| \) of Eq. (14.8), and hence it shall be discarded. Moreover, in keeping with the spirit of Bogoliubov’s method, both in \( \hat{V}_F' \) and \( \hat{V}_P \) we shall only retain terms in which either \( k \) or \( k' \) is zero, an approximation which is believed to be valid if the depletion of the condensate is small. Hence, we shall write:

\[
\hat{V} \equiv \hat{V}_H + \hat{V}_F' + \hat{V}_P,
\]

with:

\[
\hat{V}_F' \simeq \frac{1}{V} \sum_{k \neq 0} v(k) a_k^\dagger a_0 a_k^\dagger a_k,
\]

\[
\hat{V}_P \simeq \frac{1}{2V} \sum_{k \neq 0} v(k) [a_0 a_k a_k^\dagger a_0^\dagger - a_0^\dagger a_0 a_k^\dagger a_k].
\]

Now, if we take the origin of energies at the Gross-Pitaevskii value \( v(0)N(N-1)/2V \) (which, it should be noted, is an exact eigenvalue of the operator \( \hat{V}_H \) in the state
of Eq. (4.8)), then the Hamiltonian can be written as a sum of independent contributions from different values of \( k \):

\[
\hat{H} \simeq \sum_{k \neq 0} \hat{H}_k,
\]

(4.17)

where:

\[
\hat{H}_k = \frac{1}{2} \varepsilon_k (a_k^{\dagger} a_k + a_{-k}^{\dagger} a_{-k}) + \frac{v(k)}{2V} (a_0^{\dagger} a_0 a_k^{\dagger} a_k + a_0^{\dagger} a_{-k} a_{-k}^{\dagger} a_k + a_k^{\dagger} a_{-k}^{\dagger} a_0 a_0 + a_0^{\dagger} a_{-}^{\dagger} a_k a_k). \tag{4.18}
\]

In the next Section, we shall restrict our attention to the single-mode Hamiltonian \( \hat{H}_k \). We shall see that the ground state of \( \hat{H}_k \) can be found quite easily using a number-conserving variational ansatz,[34] leading to results for the ground state energy and excitation spectrum that are very similar to those of the standard (number non-conserving) Bogoliubov theory. The implications of the diagonalization of \( \hat{H}_k \) on the diagonalization of the full many-body Boson Hamiltonian \( \hat{H} \) will be discussed in more detail in Sec. 7.

### §5. Number-conserving approach: variational formulation of Bogoliubov’s theory

In view of the conceptual difficulties of the number non-conserving formulation of Bogoliubov’s theory reviewed in Section 3, we now want to study an alternative formulation of this theory in which the number of bosons is conserved, and which therefore should be free of many of the problems encountered in the number non-conserving version. This formulation, which has already been presented in slightly different form in the literature,[7][34] consists in using a variational ansatz to find the ground state wavefunction of each single-mode Hamiltonian \( \hat{H}_k \) independently from the Hamiltonians \( \hat{H}_{k'}(\neq k) \) of the other momentum modes and writing the ground state wavefunction of the total Hamiltonian \( \hat{H} \) as a tensor product of all these separate single-mode ground states. However, since the previous expositions of this method are not widely in use, we here shall present a comprehensive review, which will allow us to assess the validity of several aspects of the standard, number non-conserving Bogoliubov formulation.

#### 5.1. Ground state energy of the single-mode Hamiltonian \( \hat{H}_k \)

We now proceed to diagonalize the Hamiltonian \( \hat{H}_k \) independently of the remaining contributions \( \hat{H}_{k'}(\neq k) \) to the total Hamiltonian \( \hat{H} \) of the system; in other words, we consider a fictitious system where bosons are only allowed to be in one of the three single particle states with wavevector \( 0, +k \) or \( -k \). We shall therefore restrict our attention to trial states of the form (without loss of generality, throughout this paper it will be assumed that the total number of bosons \( N \) is even):

\[
|\psi_k\rangle = \sum_{n=0}^{N/2} C_n |N - 2n, n, n\rangle, \tag{5.1}
\]
where each basis state $|N - 2n, n, n\rangle$ has $(N - 2n)$ bosons in the condensate, and $n$ bosons in each one of the two momentum states $\pm k$. To clarify what we mean exactly by the notation $|N - 2n, n, n\rangle$ in the present context, if $|0\rangle$ designates the vacuum state for bosons, the normalized general state $|N - n - m, n, m\rangle$ can be defined as:

$$|N - n - m, n, m\rangle = \frac{(a_l^\dagger)^{N-n-m}}{\sqrt{(N-n-m)!}} \frac{(a_k^\dagger)^n (a_{-k}^\dagger)^m}{\sqrt{n!} \sqrt{m!}} |0\rangle. \tag{5.2}$$

The expectation value of $\hat{H}_k$ in the un-normalized state $|\psi_k\rangle$ of Eq. (5.1) is given by:

$$\langle \hat{H}_k \rangle_k = \frac{\langle \psi_k | \hat{H}_k | \psi_k \rangle}{\langle \psi_k | \psi_k \rangle}. \tag{5.3}$$

Let us calculate the above expectation value. To simplify the notation, in the following we shall denote by $|n\rangle$ the ket $|N - 2n, n, n\rangle$. We then can write:

$$a_k^\dagger a_k |n\rangle = a_{-k}^\dagger a_{-k} |n\rangle = n |n\rangle, \tag{5.4a}$$
$$a_l^\dagger a_0 a_k^\dagger a_{-k} |n\rangle = a_l^\dagger a_0 a_{-k}^\dagger a_{-k} |n\rangle = n(N - 2n) |n\rangle, \tag{5.4b}$$
$$a_k^\dagger a_{-k}^\dagger a_0 a_0 |n\rangle = (n + 1) \sqrt{(N - 2n)(N - 2n - 1)} |n + 1\rangle, \tag{5.4c}$$
$$a_k a_{-k} a_0 a_0^\dagger |n\rangle = n \sqrt{(N - 2n + 1)(N - 2n + 2)} |n - 1\rangle. \tag{5.4d}$$

Using the above equations, one can easily show, after a few manipulations, that:

$$\hat{H}_k |\psi_k\rangle = \sum_{n=0}^{N/2} C_n \left[ n \xi_k + \frac{v(k)}{V} n(N - 2n) \right] |n\rangle + \frac{v(k)}{2V} \sum_{m=1}^{N/2} m C_{m-1} \sqrt{(N - 2m + 2)(N - 2m + 1)} |m\rangle + \frac{v(k)}{2V} \sum_{l=0}^{(N/2) - 1} (l + 1) C_{l+1} \sqrt{(N - 2l - 1)(N - 2l)} |l\rangle. \tag{5.5a}$$

Now, it is not difficult to see that the second sum on the rhs of the above equation can be extended to $m = 0$, since the factor $m C_{m-1}$ in the summand will make the extra term vanish. Also, the third sum can be extended to $l = N/2$, because the factor $(N - 2l)$ inside the square root will make this term vanish. This allows us to write:

$$\hat{H}_k |\psi_k\rangle = \sum_{n=0}^{N/2} \left\{ C_n \left[ n \xi_k + \frac{v(k)}{V} n(N - 2n) \right] \right\} + \frac{v(k)}{2V} n C_{n-1} \sqrt{(N - 2n + 2)(N - 2n + 1)} + \frac{v(k)}{2V} (n + 1) C_{n+1} \sqrt{(N - 2n - 1)(N - 2n)} |n\rangle. \tag{5.6}$$
Using this last result, we obtain that the expectation value \( \langle \psi_k | \hat{H}_k | \psi_k \rangle \) is given by:

\[
\langle \psi_k | \hat{H}_k | \psi_k \rangle = \sum_{n=0}^{N/2} \left\{ |C_n|^2 \left[ n \varepsilon_k + \frac{v(k)}{V} n(N-2n) \right] + \frac{v(k)}{2V} n C_n^* C_{n-1} \sqrt{(N-2n+2)(N-2n+1)} + \frac{v(k)}{2V} (n+1) C_n^* C_{n+1} \sqrt{(N-2n-1)(N-2n)} \right\}.
\]

Let us assume, for simplicity, that the coefficients \( C_n \) are real. Then, for \( v(k) > 0 \), we see that the expectation value \( \langle \psi_k | \hat{H}_k | \psi_k \rangle \) will be lowered if the coefficients \( C_n \) have alternating positive and negative signs. In this case, the terms on the second and third line will be negative, making the expectation value lower than what one would obtain if consecutive coefficients have the same sign, in which case products of the form \( C_n C_{n-1} \) and \( C_n C_{n+1} \) will be positive. Below, we will show that Bogoliubov’s theory corresponds to the following geometric ansatz\(^7\),\(^34\) for the coefficients \( C_n \):

\[
C_n = C_0 (-c_k)^n,
\]

where the constant \( c_k \) is to be determined variationally (\( C_0 \) will turn out to be an overall constant which cancels out in the normalization of \( |\psi_k\rangle \) and whose value is hence unimportant for the evaluation of expectation values of physical observables). Note that, for the \( C_n \)'s to have alternating positive and negative signs, \( c_k \) has to be positive. On the other hand, we expect on physical grounds that the coefficients \( C_n \) will decrease with increasing values of \( n \), or, in other words, that the probability amplitude of states \( |n\rangle \) with a large number \( n \gg 1 \) of bosons outside the condensate will be small. This implies that the constant \( c_k \) must be less than unity. It then follows that \( c_k \) is subject to the following constraint:

\[
0 < c_k < 1.
\]

Inserting the variational ansatz \((5.8)\) into Eq. \((5.7)\), and making use of the approximation:

\[
\sqrt{N(N+1)} = N \sqrt{1 + \frac{1}{N}} \approx N + \frac{1}{2},
\]

which is valid for \( N \gg 1 \), we can rewrite Eq. \((5.7)\) in the form:

\[
\langle \psi_k | \hat{H}_k | \psi_k \rangle \approx C_0^2 \sum_{n=0}^{N/2} \left\{ (c_k)^{2n} [n \varepsilon_k + \frac{v(k)}{V} n(N-2n)] + \frac{v(k)}{2V} n (c_k)^{2n-1} \left( N - 2n + \frac{3}{2} \right) + \frac{v(k)}{2V} (n+1) (c_k)^{2n+1} \left( N - 2n - \frac{1}{2} \right) \right\}.
\]

The summations in the above equation can be calculated analytically by taking successive derivatives with respect to the variable \( x \) of the finite geometric sum:

\[
\sum_{n=0}^{N/2} x^n = \frac{1 - x^{N+1}}{1 - x},
\]
hence obtaining the following results:

\[
\sum_{n=1}^{N/2} nx^n = x \left[ \frac{1 - x^{N/2+1}}{(1-x)^2} - \left( \frac{N}{2} + 1 \right) \frac{x^{N/2}}{1-x} \right], \tag{5.13a}
\]

\[
\sum_{n=1}^{N/2} n^2 x^n = x \left[ \frac{1 - x^{N/2+1}}{(1-x)^2} - \left( \frac{N}{2} + 1 \right) \frac{x^{N/2}}{1-x} \right]
+ x^2 \left[ \frac{2(1 - x^{1+N/2})}{(1-x)^3} - 2 \left( \frac{N}{2} + 1 \right) \frac{x^{N/2}}{(1-x)^2} \right]
- \frac{N}{2} \left( \frac{N}{2} + 1 \right) x^{N/2-1}, \tag{5.13b}
\]

Now, it would be highly impractical to use the full expressions on the rhs of Eqs. (5.13) in the evaluation of the sums on the rhs of Eq. (5.11). Luckily, these expressions simplify considerably for \(N \to \infty\) and \(0 < x < 1\), in which case we can write:

\[
\sum_{n=1}^{N/2} nx^n \simeq \frac{x}{(1-x)^2}, \tag{5.14a}
\]

\[
\sum_{n=1}^{N/2} n^2 x^n \simeq \frac{x}{(1-x)^2} + \frac{2x^2}{(1-x)^3}. \tag{5.14b}
\]

Using these last two equations in Eq. (5.11), we obtain (we remind the reader that \(n_B = N/V\) is the density of bosons in the system):

\[
\langle \psi_k | \hat{H}_k | \psi_k \rangle = |C_0|^2 \left[ \varepsilon_k + v(k)n_B \left( 1 - \frac{1}{c_k} \right) \right] \sum_{n=0}^{N/2} n c_k^{2n}, \tag{5.15a}
\]

\[
= |C_0|^2 \left\{ \frac{c_k^2}{(1-c_k^2)^2} \left[ \varepsilon_k + v(k)n_B \right] - v(k)n_B \frac{c_k}{(1-c_k^2)^2} \right\}. \tag{5.15b}
\]

On the other hand, from Eq. (5.1), we easily see that the norm \(\langle \psi_k | \psi_k \rangle\) of the wavefunction \(|\psi_k\rangle\) is given by:

\[
\langle \psi_k | \psi_k \rangle = \sum_{n=0}^{N/2} |C_n|^2 = |C_0|^2 \sum_{n=0}^{N/2} c_k^{2n}, \tag{5.16a}
\]

\[
\simeq |C_0|^2 \frac{1}{1-c_k^2}, \tag{5.16b}
\]

where, in going from the first to the second line, use has been made of the asymptotic form of Eq. (5.12), namely:

\[
\sum_{n=0}^{N/2} x^n \simeq \frac{1}{1-x}, \quad N \to \infty, \ 0 < x < 1. \tag{5.17}
\]
Now, if we divide Eq. (5.15b) by Eq. (5.16b), we can write for the expectation value \( \langle \hat{H}_k \rangle_k \) of Eq. (5.3) the following expression (notice that \(|C_0|^2\) cancels out in the division):

\[
\langle \hat{H}_k \rangle_k \simeq \frac{c_k^2}{1 - c_k^2} \left[ \varepsilon_k + v(k)n_B \right] - v(k)n_B \frac{c_k}{1 - c_k^2}. \tag{5.18}
\]

Minimization of the above expectation value with respect to \( c_k \) leads to the following quadratic equation:

\[
c_k^2 - 2 \left( \frac{\mathcal{E}_k}{v(k)n_B} \right) c_k + 1 = 0, \tag{5.19}
\]

where we defined

\[
\mathcal{E}_k = \varepsilon_k + v(k)n_B. \tag{5.20}
\]

The above quadratic equation has the following two roots:

\[
c_k^\pm = \left( \frac{\mathcal{E}_k}{v(k)n_B} \right) \pm \sqrt{\left( \frac{\mathcal{E}_k}{v(k)n_B} \right)^2 - 1}. \tag{5.21}
\]

Of these two roots, only the one with the minus sign obeys the constraint \( 0 < c_k < 1 \) of Eq. (5.9) for arbitrary values of \( \mathcal{E}_k \). We shall therefore write:

\[
c_k = \frac{1}{v(k)n_B} \left[ \mathcal{E}_k - \sqrt{\mathcal{E}_k^2 - v(k)^2n_B^2} \right]. \tag{5.22}
\]

This result for the constant \( c_k \), which is plotted as a function of the wavevector \( k \) in Fig. 1, fully determines the coefficients \( C_n = C_0(-c_k)^n \) of the variational ground state wavefunction \( |\psi_k\rangle \) of the Hamiltonian \( \hat{H}_k \) (apart, of course, from the overall constant \( C_0 \)). This, in turn, will allow us to determine the expectation values of physical observables in the ground state \( |\psi_k\rangle \). In particular, the expectation value of \( \hat{H}_k \) in the ground state \( |\psi_k\rangle \) can readily be found if we use the result (5.22) for \( c_k \) in Eq. (5.18), upon which we obtain:

\[
\langle \hat{H}_k \rangle_k = -\frac{1}{2} \left( \varepsilon_k + n_Bv(k) - E_k \right) < 0, \tag{5.23}
\]

with the definition:

\[
E_k = \sqrt{\varepsilon_k \left[ \varepsilon_k + 2n_Bv(k) \right]}. \tag{5.24}
\]

The result (5.23) is exactly the result one obtains in the standard, number non-conserving Bogoliubov approach for the expectation value of a given contribution \( \hat{H}_k \) to the Bogoliubov ground state energy. We shall discuss the meaning of this observation in more detail below. For the moment, we want to use our result for the variational wavefunction \( |\psi_k\rangle \) to explore the properties of the ground state.
5.2. Variational result for the depletion of the condensate

We now turn our attention to the depletion of the condensate. The average number of bosons $N_k$ in the single-particle state of momentum $k$ is given by:

$$N_k \equiv \langle a_k^{\dagger} a_k \rangle_k = \frac{\langle \psi_k | a_k^{\dagger} a_k | \psi_k \rangle}{\langle \psi_k | \psi_k \rangle}.$$

(5.25)

Now, it is easy to see that:

$$\langle \psi_k | a_k^{\dagger} a_k | \psi_k \rangle = |C_0|^2 \sum_{n=0}^{N/2} n |C_n|^2 = |C_0|^2 \sum_{n=0}^{N/2} n c_k^2 n,$$

(5.26a)

$$= |C_0|^2 \frac{c_k^2}{1 - c_k^2},$$

(5.26b)

where, in going from the first to the second line, use has been made of Eq. (5.14a). Then, using expression (5.16b), we finally obtain:

$$\langle a_k^{\dagger} a_k \rangle_k = \frac{c_k^2}{1 - c_k^2}.$$  

(5.27)

If we now use the expression of $c_k$ in Eq. (5.22), we find after a few manipulations:

$$N_k = \frac{1}{2} \left[ \frac{\epsilon_k + n_B v(k)}{E_k} - 1 \right].$$

(5.28)

This is again the same result one obtains in Bogoliubov’s standard, number non-conserving approach. Unfortunately, and as we have already discussed in Sec. 3.1, the above expression of $N_k$ diverges for $k \to 0$, which does not make much sense for a system of $N$ bosons. It is indeed quite easy to see that, $N_k$ being the ratio of two finite sums:

$$N_k = \frac{\sum_{n=1}^{N/2} n (c_k^2)^n}{\sum_{n=0}^{N/2} (c_k^2)^n},$$

(5.29)
with $0 < c_k < 1$, the ratio must remain finite for all values of $c_k$ in the range $(0,1)$. Luckily, the origin of the divergence in Eq. (5.28) can easily be elucidated, and has to do with our use of the approximate limiting expressions of the sums (5.14a) and (5.17) (which both diverge as $c_k \to 1$) when evaluating the average $\langle a_k^\dagger a_k \rangle_k$. If we use the full expressions (5.13a) and (5.12) instead, we find the result:

$$N_k = \frac{c_k^2}{1 - c_k^2} - \left( \frac{N}{2} + 1 \right) \frac{c_k^{2+N}}{1 - c_k^{2+N}}. \quad (5.30)$$

It can be verified that the above result, which to the best of the author’s knowledge has not been derived previously, is finite for all values of $c_k$. In particular, as $k \to 0$, $c_k \to 1$, and a Taylor expansion in $x = c_k^2$ near $x = 1$ shows that $N_k \to N/4$. This behaviour is shown in Fig. 2 where we plot the depletion $N_k$ from Eq. (5.30) as a function of the wavevector $k = |\mathbf{k}|$ for a number of values of the total number of bosons $N$.

The result of Eq. (5.30) allows us to obtain more meaningful results for expectation values of one-body operators of the form $\hat{O} = \sum_k O_k a_k^\dagger a_k$ than were obtained within the standard, number non-conserving Bogoliubov approximation. To revisit the example given in Sec. 3.1 let us consider the Fock part of the Hamiltonian $\hat{H}_F \approx \frac{1}{2} \sum_{k \neq 0} n_0 v(k) (a_k^\dagger a_k + a_{-k}^\dagger a_{-k})$, where for simplicity we made use of Bogoliubov’s approximation $a_0 = a_0^\dagger \approx \sqrt{N_0}$. While in the standard Bogoliubov approach the expectation value of a given mode $\mathbf{k}$ of $\hat{H}_F$ in the Bogoliubov ground state diverges like $1/k$ as $k \to 0$ (which, as we discussed earlier, is problematic), in the variational Bogoliubov method this expectation value is finite for all values of the wavevector $\mathbf{k}$, and is given by the usual expression involving the product of the number $N_0$ of bosons in the mode $\mathbf{k} = 0$ by the number $N_k$ of depleted bosons in each of the modes $\mathbf{k}$ and $-\mathbf{k}$ (since these are the only modes kept in $\hat{H}_F$), times...
the interaction energy \( v(k)/V \). The fact that all quantities involved are well-defined and finite within the variational approach is reassuring, and constitutes a significant improvement with respect to the standard, number non-conserving Bogoliubov approximation.

5.3. Variational result for the anomalous averages \( \langle a_k a_{-k} \rangle \) and \( \langle a_k^\dagger a_{-k}^\dagger \rangle \)

We now want to investigate the anomalous average \( \langle a_k a_{-k} \rangle \) in the variational formulation of Bogoliubov’s method. In order to do so, we note that for \( N \gg 1 \) the coefficients \( C_n \) of the variational wavefunction \( |\psi_k(N)\rangle = \sum_{n=0}^{N/2} C_n |n\rangle \) do not explicitly depend on the number of bosons \( N \), and are given to a very good approximation by the ansatz expression \( C_n = C_0 (-ck)^n \), regardless of the specific value of \( N \) (in other words, the constant \( c_k \) is independent of \( N \) for \( N \to \infty \)). Under these circumstances, we shall write for the wavefunction of a system of \( (N-2) \) bosons the following variational ansatz:

\[
|\psi_k(N-2)\rangle = \sum_{n=0}^{(N-2)/2} C_n (N-2 - 2n, n, n).
\] (5.31)

It is now easy to verify that:

\[
\langle \psi_k(N-2)|a_k^\dagger a_{-k}^\dagger|\psi_k(N-2)\rangle = \sum_{n=1}^{N/2} n C_{n-1} C_n^* \tag{5.32a}
\]

and hence that:

\[
\langle \psi_k(N)|a_k^\dagger a_{-k}^\dagger|\psi_k(N-2)\rangle = \sum_{n=1}^{N/2} n C_{n-1} C_n^* \tag{5.33a}
\]

Using the limiting form (5.14a) for the geometric sum as \( N \to \infty \), we obtain:

\[
\langle \psi_k(N)|a_k^\dagger a_{-k}^\dagger|\psi_k(N-2)\rangle \approx -C_0^2 \frac{ck}{(1-c_k^2)^2} \tag{5.34}
\]

On the other hand, the limiting form (5.12) as \( N \to \infty \) of the norm of the wavefunctions \( |\psi_k(N)\rangle \) and \( |\psi_k(N-2)\rangle \) is given by:

\[
\langle \psi_k(N)|\psi_k(N)\rangle = \langle \psi_k(N-2)|\psi_k(N-2)\rangle = C_0^2 \frac{1}{1-c_k^2} \tag{5.35}
\]

If we use the normalized ground state wavefunctions \( |\tilde{\psi}_k(N)\rangle \) such that:

\[
|\tilde{\psi}_k(N)\rangle = \frac{|\psi_k(N)\rangle}{\sqrt{\langle \psi_k(N)|\psi_k(N)\rangle}} \tag{5.36}
\]
then the anomalous average $\langle a_k^\dagger a_{-k}^\dagger \rangle_k$ can be defined in the following way:

$$\langle a_k^\dagger a_{-k}^\dagger \rangle_k = \langle \tilde{\psi}_k(N)|a_k^\dagger a_{-k}^\dagger|\tilde{\psi}_k(N-2)\rangle.$$  \hspace{1cm} (5.37)

Using Eqs. (5.34) and (5.35), we find:

$$\langle a_k^\dagger a_{-k}^\dagger \rangle_k \simeq -\frac{c_k}{1-c_k^2}.$$ \hspace{1cm} (5.38)

Given the expression (5.22) of $c_k$, we obtain, after a few manipulations:

$$\langle a_k^\dagger a_{-k}^\dagger \rangle_k = \frac{n_B v(k)}{2E_k},$$ \hspace{1cm} (5.39)

which is nothing but the standard Bogoliubov result of Eq. (3.5) above, which diverges negatively like $-1/k$ as $k \to 0$.

We now show that the divergence of the rhs of Eq. (5.39) as $k \to 0$ is also a direct consequence of using asymptotic forms as $N \to \infty$ of geometric sums, and that, if the finite $N$ results are used throughout, then a completely different result will be obtained which remains finite for all values of the wavevector $k$. Indeed, using the notation $x = c_k^2$, we can write:

$$\langle \psi_k(N)|a_k^\dagger a_{-k}^\dagger|\psi_k(N-2)\rangle = -\frac{C_0}{c_k} \sum_{n=1}^{N/2} n x^n,$$

$$= -\frac{C_0}{c_k} x \left[ \frac{1-x^{1+N/2}}{(1-x)^2} - \left( \frac{N}{2} + 1 \right) \frac{x^{N/2}}{1-x} \right].$$ \hspace{1cm} (5.40)
In a similar fashion, we obtain for the norm of the wavefunctions $|\psi_k(N)\rangle$ and $|\psi_k(N-2)\rangle$ the following expressions:

\[
\langle\psi_k(N)|\psi_k(N)\rangle = C_0^2 \frac{1 - x^{1+N/2}}{1 - x},
\]

\[
\langle\psi_k(N-2)|\psi_k(N-2)\rangle = C_0^2 \frac{1 - x^{N/2}}{1 - x}.
\]

Combining Eqs. (5.40) and (5.41) allows us to write the final expression:

\[
\langle\tilde{\psi}_k(N)|a_k^\dagger a_{-k}^\dagger|\tilde{\psi}_k(N-2)\rangle = -c_k \sqrt{(1 - c_k^N)(1 - c_k^{N+2})} \left[ \frac{1 - c_k^N}{1 - c_k^2} - \left( \frac{N}{2} + 1 \right) c_k^N \right],
\]

(5.42)

an expression which again has not been derived before, and which can be shown to be bounded for all values of $c_k$ in the range $(0, 1)$ (see Fig. 3).

The result of Eq. (5.42) allows us again to obtain more meaningful results for expectation values of one-body operators of the form $\hat{O} = \sum_k \tilde{O}_k a_k a_{-k}$ or $\hat{O} = \sum_k \tilde{O}_k a_k^\dagger a_{-k}^\dagger$ than were obtained within the standard, number non-conserving Bogoliubov approximation. To revisit the example given in Sec. 3.1, let us consider the pairing part of the Hamiltonian $\hat{H}_P \approx \frac{1}{2} \sum_{k \neq 0} n_B v(k) (a_k^\dagger a_{-k}^\dagger + a_{-k} a_k)$, where for simplicity we again made use of Bogoliubov’s approximation $a_0 = a_0^\dagger \approx \sqrt{N}$. While in the standard Bogoliubov approximation the expectation value of a given mode $k$ of $\hat{H}_P$ in the Bogoliubov ground state is given by $-\left[ n_B v(k) \right]^2 / (2E_k)$ and diverges like $-1/k$ as $k \to 0$, in the variational Bogoliubov method this expectation value is finite for all values of the wavevector $k$, and this even in lower spatial dimensions.

5.4. Elementary excitations: variational approach for the single-mode Hamiltonian $\hat{H}_k$

We now introduce the following operator:

\[
\alpha_k = \tilde{u}_k a_k a_0^\dagger + \tilde{v}_k a_0 a_{-k}^\dagger.
\]

(5.43)

We want to choose the constants $\tilde{u}_k$ and $\tilde{v}_k$ in such a way that acting on $|\psi_k\rangle$ with $\alpha_k^\dagger$ creates an excited state of the Hamiltonian $\hat{H}_k$. A necessary condition for that to happen is that $\alpha_k^\dagger |\psi_k\rangle$ has to be orthogonal to $|\psi_k\rangle$, i.e., that:

\[
\langle \psi_k | (\alpha_k^\dagger | \psi_k \rangle) = 0.
\]

(5.44)

Taking the adjoint of the above equation, we obtain the condition

\[
\langle \psi_k | \alpha_k | \psi_k \rangle = 0,
\]

(5.45)

which will always be satisfied if we require that

\[
\alpha_k | \psi_k \rangle = 0.
\]

(5.46)
Let us calculate the effect of the action of $\alpha_k$ on $|\psi_k\rangle$. We have:

$$\alpha_k|\psi_k\rangle = \sum_{n=0}^{N/2} C_n \left[ \tilde{u}_k \sqrt{n(N-2n+1)} |N-2n+1, n-1, n\rangle 
+ \tilde{v}_k \sqrt{(n+1)(N-2n)} |N-2n-1, n, n+1\rangle \right].$$  \hspace{1cm} (5.47)

Noting that the $n = 0$ term in the first summation and the $n = N/2$ term in the second summation vanish, we relabel $n \rightarrow n - 1$ in the second sum, hence obtaining:

$$\alpha_k|\psi_k\rangle = \sum_{n=1}^{N/2} \left[ C_n \tilde{u}_k \sqrt{n(N-2n+1)} 
+ C_{n-1} \tilde{v}_k \sqrt{n(N-2n+2)} |N-2n+1, n-1, n\rangle \right].$$  \hspace{1cm} (5.48)

Requiring that $\alpha_k|\psi_k\rangle = 0$ leads to the following condition:

$$\frac{C_n}{C_{n-1}} = -\frac{\tilde{v}_k}{\tilde{u}_k} \sqrt{\frac{N-2n+2}{N-2n+1}}.$$  \hspace{1cm} (5.49)

For $N \gg 1$, the square root is very close to unity for most values of $n$ such that $1 \leq n \leq N/2$, and so we obtain that, to a very good approximation, the condition $\alpha_k|\psi_k\rangle = 0$ is equivalent to:

$$\frac{\tilde{v}_k}{\tilde{u}_k} = -\frac{C_n}{C_{n-1}}.$$  \hspace{1cm} (5.50)

Using the fact that $C_n = C_0 (-c_k)^n$, we finally obtain:

$$\frac{\tilde{v}_k}{\tilde{u}_k} = c_k.$$  \hspace{1cm} (5.51)

Hence, we obtain that the operator $\alpha_k$ annihilates the variational ground state $|\psi_k\rangle$ of the Hamiltonian $\hat{H}_k$ if the constants $\tilde{v}_k$ and $\tilde{u}_k$ have the ratio specified in Eq. (5.51). This result is quite important, given that the equation $\alpha_k|\psi_k\rangle = 0$ in effect ensures that the state $\alpha_k^\dagger |\psi_k\rangle$ is orthogonal to $|\psi_k\rangle$, and is hence an excited state as we discussed earlier in this Subsection.

We now want to establish that the operator $\alpha_k^\dagger$ creates an excited state of momentum $k$. To this end, let us find the average momentum in the state $\alpha_k^\dagger |\psi_k\rangle$, which is defined as:

$$\langle \hat{P}_k \rangle_{\text{exc}} = \frac{\langle \psi_k | \alpha_k \hat{P} \alpha_k^\dagger |\psi_k\rangle}{\langle \psi_k | \alpha_k \alpha_k^\dagger |\psi_k\rangle},$$  \hspace{1cm} (5.52)

with $\hat{P} = \sum_k \hbar k a_k^\dagger a_k$ the total momentum operator. Noting that the commutator $[\hat{P}, \alpha_k^\dagger]$ is given by:

$$[\hat{P}, \alpha_k^\dagger] = \hbar k \alpha_k^\dagger,$$  \hspace{1cm} (5.53)

and that $\hat{P} |\psi_k\rangle = 0$, we can easily write:

$$\langle \psi_k | \alpha_k \hat{P} \alpha_k^\dagger |\psi_k\rangle = \hbar k \langle \psi_k | \alpha_k \alpha_k^\dagger |\psi_k\rangle,$$  \hspace{1cm} (5.54)
from which we finally obtain:
\[
\langle \hat{P} \rangle^\text{exc}_k = \hbar k,
\] (5.55)
thus proving that the state \( \alpha_k^\dagger |\psi_k\rangle \) has an average momentum \( \hbar k \).

Let us recapitulate what we have done so far. We have defined a new operator \( \alpha_k \) such that the state \( \alpha_k^\dagger |\psi_k\rangle \) is (i) orthogonal to \( |\psi_k\rangle \) and (ii) has an average momentum of \( \hbar k \). These two properties allow us to identify the state \( \alpha_k^\dagger |\psi_k\rangle \) as an an excited state of the Hamiltonian \( \hat{H}_k \) with momentum \( \hbar k \). At this point, we make the observation that, while the requirement \( \alpha_k |\psi_k\rangle = 0 \) allowed us to determine the ratio of \( \tilde{v}_k \) to \( \tilde{u}_k \), Eq. (5.51), these constants are otherwise still arbitrary. In order to determine their actual values, we shall require that the excited state \( \alpha_k^\dagger |\tilde{\psi}_k\rangle \) be normalized to unity, i.e. that:
\[
\langle \tilde{\psi}_k | \alpha_k \alpha_k^\dagger |\tilde{\psi}_k\rangle = 1,
\] (5.56)
where we remind the reader that \( |\tilde{\psi}_k\rangle \) denotes the normalized ground state of the single-mode Hamiltonian \( \hat{H}_k \). Using the fact that \( \alpha_k \alpha_k^\dagger = [\alpha_k, \alpha_k^\dagger] + \alpha_k^\dagger \alpha_k \), the condition (5.56) becomes:
\[
\langle \tilde{\psi}_k | [\alpha_k, \alpha_k^\dagger] |\tilde{\psi}_k\rangle = 1,
\] (5.57)
where we used the fact that \( \alpha_k |\tilde{\psi}_k\rangle = 0 \). An immediate way to satisfy this last condition is to require that the commutator \([\alpha_k, \alpha_k^\dagger]\) be equal to unity:
\[
[\alpha_k, \alpha_k^\dagger] = 1.
\] (5.58)
We thus see that the canonical commutation relation \([\alpha_k, \alpha_k^\dagger] = 1 \), which is imposed \textit{a priori} in the standard textbook formulation of Bogoliubov’s theory, emerges as a natural requirement that we need to satisfy in order for the excited state \( \alpha_k^\dagger |\tilde{\psi}_k\rangle \) to be normalized to unity.

Now, if we calculate the commutator \([\alpha_k, \alpha_k^\dagger]\), given the definition (5.50), we find, after a few manipulations:
\[
[\alpha_k, \alpha_k^\dagger] = (\tilde{u}_k^2 - \tilde{v}_k^2) a_0^\dagger a_0 - \tilde{v}_k^2 a_k^\dagger a_k + \tilde{v}_k^2 a_{-k}^\dagger a_{-k}.
\] (5.59)
While in Bogoliubov’s theory the commutator \([\alpha_k, \alpha_k^\dagger]\) is a c-number, the fact that the \textit{rhs} of the above equation is an operator makes it impossible to satisfy the constraint \([\alpha_k, \alpha_k^\dagger] = 1 \) exactly in the number-conserving formalism. However, we can try to satisfy this constraint in an averaged sense in the ground state \( |\tilde{\psi}_k\rangle \) by imposing the condition given in Eq. (5.57), which can be rewritten in the form:
\[
\langle [\alpha_k, \alpha_k^\dagger] \rangle_k = (\tilde{u}_k^2 - \tilde{v}_k^2) \langle a_0^\dagger a_0 \rangle_k - \langle a_k^\dagger a_k \rangle_k,
\] (5.60)
where we denote by \( \langle \cdots \rangle_k \) the quantum average \( |\tilde{\psi}_k \rangle \cdots |\tilde{\psi}_k\rangle \), and where we used the fact that \( \langle a_k^\dagger a_k \rangle_k = \langle a_{-k}^\dagger a_{-k} \rangle_k \). Now, the normalization condition (5.57) leads to the following constraint on the constants \( \tilde{u}_k \) and \( \tilde{v}_k \):
\[
\tilde{u}_k^2 - \tilde{v}_k^2 = \gamma_k^2,
\] (5.61)
where, for compactness of notation, we defined the quantity $\gamma_k$ such that:

$$\gamma_k^2 = \frac{1}{\langle a_0^\dagger a_0 \rangle_k - \langle a_k^\dagger a_k \rangle_k}$$  \hspace{1cm} (5.62a)

$$\simeq \frac{1}{\langle a_0^\dagger a_0 \rangle_k},$$  \hspace{1cm} (5.62b)

In going from the first to the second line of Eq. (5.62) we assumed that $\langle a_k^\dagger a_k \rangle_k \ll \langle a_0^\dagger a_0 \rangle_k$, i.e. that the depletion of the condensate into the single-particle state with momentum $k$ is small. Note that this is not always the case, as in the standard formulation of Bogoliubov’s theory the quantity $N_k = \langle a_k^\dagger a_k \rangle_k$ diverges in the $k \to 0$ limit. This, incidentally, gives us another reason why it is important to be able to formulate a version of the theory in which the expectation value $\langle a_k^\dagger a_k \rangle$ always remains finite. As mentioned above, in the number non-conserving formulation of Bogoliubov’s theory, $\langle a_k^\dagger a_k \rangle$ diverges as $k \to 0$, and taking this result at face value would lead to a completely different result for $\gamma_k^2$ in Eq. (5.62b), which would in turn affect the evaluation of the excitation energies given below, Eq. (5.67).

Using Eqs. (5.51) and (5.61), we now can determine the values of the constants $\tilde{u}_k$ and $\tilde{v}_k$. These can be written in the form:

$$\tilde{u}_k = \gamma_k u_k, \hspace{0.5cm} \tilde{v}_k = \gamma_k v_k,$$  \hspace{1cm} (5.63a)

$$u_k = \frac{1}{\sqrt{1 - c_k^2}}, \hspace{0.5cm} v_k = \frac{c_k}{\sqrt{1 - c_k^2}}.$$  \hspace{1cm} (5.63b)

Using the result (5.22) for $c_k$, we finally obtain:

$$u_k^2 = \frac{1}{2} \left( \frac{\varepsilon_k + n_{B\nu}(k)}{E_k} + 1 \right),$$  \hspace{1cm} (5.64a)

$$v_k^2 = \frac{1}{2} \left( \frac{\varepsilon_k + n_{B\nu}(k)}{E_k} - 1 \right).$$  \hspace{1cm} (5.64b)

Note that these are the same expressions for the quantities $u_k$ and $v_k$ defined in the conventional formulation of Bogoliubov’s theory. The above results, Eqs. (5.63) and (5.64), allow us to rewrite the expression of $\alpha_k$, Eq. (5.43), in the form:

$$\alpha_k = \gamma_k \left( u_k a_k a_0^\dagger + v_k a_0 a_0^\dagger \right).$$  \hspace{1cm} (5.65)

If in the above expression we replace $a_0$ and $a_0^\dagger$ by $\sqrt{N_0}$, and then use the fact that $\gamma_k \simeq 1/\sqrt{N_0}$ as indicated by Eq. (5.62b), we recover the usual expression, Eq. (2.52), of $\alpha_k$ in terms of $a_k$ and $a_0^\dagger$, used in the standard, number non-conserving formulation of Bogoliubov’s method.

We now are finally in a position to find the energy of the excited state $\alpha_k^\dagger$, which is given by the expression:

$$\Delta E_{exc}^{(1)}(k) = \frac{\langle \tilde{\psi}_k | \alpha_k \hat{H}_k | \alpha_k^\dagger \rangle \langle \tilde{\psi}_k \rangle}{\langle \tilde{\psi}_k | \alpha_k \hat{H}_k | \tilde{\psi}_k \rangle} - \frac{\langle \tilde{\psi}_k | \hat{H}_k | \tilde{\psi}_k \rangle}{\langle \tilde{\psi}_k | \alpha_k \hat{H}_k | \tilde{\psi}_k \rangle},$$  \hspace{1cm} (5.66a)
Here, in going from the first to the second line, we used the fact that the excited state \( |\tilde{\psi}_k\rangle \) is normalized to unity, i.e. that \( \langle \tilde{\psi}_k | a_k a_k^\dagger | \tilde{\psi}_k \rangle = 1 \). In Appendix A we show that, for weak perturbation, the Hamiltonian \( \hat{H}_k \) can be written in the form:

\[
\hat{H}_k \simeq -\frac{1}{2} [\varepsilon_k + n_{B\nu}(k)] - E_k + \frac{1}{2} E_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}),
\]

where \( E_k \) is the Bogoliubov spectrum given in Eq. (5.24). This last result, when used in conjunction with Eq. (5.66) and the commutation relations for the \( a_k \)'s, Eqs. (A.17)-(A.19) of Appendix A, leads to the conclusion that the excitation energy of the Hamiltonian \( \hat{H}_k \) from the ground state \( |\tilde{\psi}_k\rangle \) to the excited state \( a_k^\dagger |\tilde{\psi}_k\rangle \) of momentum \(+k\) is given by the following result:

\[
\Delta E_{\text{exc}}^{(1)}(k) = \frac{1}{2} E_k = \frac{1}{2} \sqrt{\varepsilon_k [\varepsilon_k + 2 n_{B\nu}(k)]}.
\]

Here we would like to emphasize that this is the excitation energy of the Hamiltonian \( \hat{H}_k \). The full Hamiltonian \( \hat{H} = \sum_k \hat{H}_k \) contains identical contributions from \( \hat{H}_k \) and \( \hat{H}_{-k} \), and hence one can easily see that the total energy cost \( \Delta E_{\text{exc}}^{\text{tot}}(k) \) of the excitation \( a_k^\dagger |\tilde{\psi}_k\rangle \), accounting for contributions from \( \hat{H}_k \) as well as \( \hat{H}_{-k} \), is twice the amount given by Eq. (5.68), and is given by the standard Bogoliubov result, namely:

\[
\Delta E_{\text{exc}}^{\text{tot}}(k) = \Delta E_{\text{exc}}^{(1)}(k) + \Delta E_{\text{exc}}^{(1)}(-k) = E_k.
\]

Before we end this Section, we briefly comment on why we define the excitation operator \( a_k \) by the expression (5.43), and why we find it useful to impose the condition (5.46) as a way to fix the value of the constants \( \hat{u}_k \) and \( \hat{v}_k \). As a matter of fact, it is not difficult to verify that the operator \( a_k^\dagger a_0 \) also creates a state which is orthogonal to the ground state \( |\psi_k\rangle \) of the operator \( \hat{H}_k \), and could therefore be a possible choice for an excited state of the Hamiltonian \( \hat{H}_k \). Indeed, the action of the operator \( a_k^\dagger a_0 \) on \( |\psi_k\rangle \) gives:

\[
a_k^\dagger a_0 |\psi_k\rangle = \sum_{n=0}^{N/2} C_n \sqrt{(N-2n-1)(n+1)} |N-2n-1, n+1, n\rangle.
\]

Now, the rhs of the above equation belongs to the Hilbert space spanned by kets of the form \( |N-2n-1, n+1, n\rangle \), which is totally disjoint from the Hilbert space spanned by states of the form \( |N-2n, n, n\rangle \) and to which the ground state belongs, hence the orthogonality of the state \( a_k^\dagger a_0 |\psi_k\rangle \) and the ground state \( |\psi_k\rangle \) of the Hamiltonian \( \hat{H}_k \). By the same token, \( \langle \tilde{\psi}_k | a_k^\dagger a_0 \rangle \) is automatically zero, and so \( a_k^\dagger |\tilde{\psi}_k\rangle \) is automatically orthogonal to \( |\tilde{\psi}_k\rangle \). So, why do we choose the special combination \( a_k = \hat{u}_k a_0^\dagger + \hat{v}_k a_{-k}^\dagger a_0 \) instead of simply \( a_k = a_k^\dagger a_0 \)? And why do we go through the trouble of requesting that \( a_k |\tilde{\psi}_k\rangle \) itself has to vanish?

To answer the first question, we note that the operator \( a_k^\dagger = \hat{u}_k a_0^\dagger + \hat{v}_k a_{-k}^\dagger a_0 \) increases the momentum of the system by an amount \(+\hbar k\). The expression of \( a_k^\dagger \)
simply emphasizes the fact that this can be done in two different ways. The first way consists in removing a boson from the condensate and adding a boson in the single-particle state of wavevector $k$, hence the term $\tilde{u}_k a_k a_0^\dagger$ in the expression of $\alpha_k^\dagger$. The second way consists in removing a boson of wavevector $-k$ from the system and adding a boson to the condensate, hence the term $\tilde{v}_k a_{-k} a_0^\dagger$ in the expression of $\alpha_k^\dagger$. The use of the special combination $\tilde{u}_k a_k a_0^\dagger + \tilde{v}_k a_{-k} a_0^\dagger$ allows us to combine the two types of processes into one excitation operator, and also allows us to choose values for the constants $\tilde{u}_k$ and $\tilde{v}_k$ such that the ket $\alpha_k^\dagger |\psi_k\rangle$ is automatically normalized to unity. As for the second question, the reason we impose the condition (5.46) is in fact to ensure that all states obtained by successive application of the operator $\alpha_k^\dagger$ are orthogonal to the ground state. Indeed, without the condition (5.46), there is no guarantee that a state of the form $(\alpha_k^\dagger)^n |\psi_k\rangle$ is orthogonal to the ground state $|\psi\rangle$ of the Hamiltonian $\hat{H}_k$, a fact that can be easily verified by taking the adjoint of the expression $\langle \psi_k | (\alpha_k^\dagger)^n |\psi_k\rangle$ (It can in fact be shown that the condition (5.46) ensures that states of the form $(\alpha_k^\dagger)^n |\psi_k\rangle$ and $(\alpha_k^\dagger)^m |\psi_k\rangle$ are orthogonal to each other if $n \neq m$. The proof, which is quite straightforward, will not be presented here.)

§6. Exact numerical diagonalization of the single-mode Hamiltonian $\hat{H}_k$

Having discussed a number-conserving variational approach to the single-mode Hamiltonian $\hat{H}_k$ of Eq. (4.18), we now proceed to perform an exact numerical diagonalization of this Hamiltonian. Such a numerical treatment, which to the best of the author’s knowledge has not been attempted before, will allow us to assess the validity of the variational treatment of the previous Section, and possibly point to areas where the variational approach may need improvement. We shall again use the complete basis $|n\rangle \equiv |N - 2n, n, n\rangle$ formed by states with $(N - 2n)$ bosons in the $k = 0$ state, and $n$ bosons in each of the states $k$ and $-k$. Since $n$ can only take values between 0 and $N/2$, the basis $\{|n\rangle\}$ has $(1+N/2)$ kets, and hence diagonalizing $\hat{H}_k$ requires the diagonalization of an $(1+N/2) \times (1+N/2)$ matrix. For a system of 1000 bosons, this would be a $501 \times 501$ matrix, which is not a prohibitively large matrix size to diagonalize numerically given the capabilities of modern day computers.

Using Eqs. (5.1), we can easily write the following matrix elements:

$$
\langle m | \hat{H}_k | n \rangle = \left[ n \varepsilon_k + \frac{v(k)}{V} n(N - 2n) \right] \delta_{nm} \\
+ \frac{v(k)}{2V} \left[ (n + 1) \sqrt{(N - 2n)(N - 2n - 1)} \delta_{m,n+1} \\
+ n \sqrt{(N - 2n + 1)(N - 2n + 2)} \delta_{m,n-1} \right]. \tag{6.1}
$$

We now introduce dimensionless units, where we measure energies in units of
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\[v(0)n_B = v(0)N/V.\]

Hence, we shall write:

\[
\langle m|\hat{H}_k|n\rangle = \left[ n\tilde{\varepsilon}_k + \tilde{v}(k)\frac{n}{N}(N - 2n) \right]\delta_{nm} + \frac{1}{2}\tilde{v}(k)\left[ \frac{(n + 1)}{N}\sqrt{(N - 2n)(N - 2n - 1)}\delta_{m,n+1} \right] + \frac{n}{N}\sqrt{(N - 2n + 1)(N - 2n + 2)}\delta_{m,n-1},
\]

(6.2)

where we denote by \(\tilde{\varepsilon}_k\) and \(\tilde{v}(k)\) the dimensionless quantities:

\[
\tilde{\varepsilon}_k = \frac{\varepsilon_k}{v(0)n_B},
\]

(6.3a)

\[
\tilde{v}(k) = \frac{v(k)}{v(0)}.
\]

(6.3b)

Having in mind an interaction potential of the form \(v(r) = g\delta(r)\), whereby \(v(k) = g\), throughout this Section we shall present numerical results using for \(\tilde{v}(k)\) the value \(\tilde{v}(k) = 1\).

(6.4)

Now, using the dimensionless matrix elements in Eq. (6.2), it is a relatively easy task to diagonalize the Hamiltonian \(\hat{H}_k\) for a given value of the total number of bosons \(N\) and for various values of the dimensionless variable \(\tilde{\varepsilon}_k\). In the following, we shall present plots of physical quantities of interest as a function of the dimensionless wavevector \(\tilde{k}\) such that:

\[
\tilde{k} = \frac{k}{k_0},
\]

(6.5)

where we defined:

\[
k_0 = \sqrt{\frac{2mn_Bv(0)}{\hbar}}.
\]

(6.6)

6.1. Ground state energy

The first quantity we shall be interested in is the ground state energy of the Hamiltonian \(\hat{H}_k\). Numerically, the ground state energy \(E^0_k(N)\) of the single-mode Hamiltonian \(\hat{H}_k\) is defined as the smallest eigenvalue of \(\hat{H}_k\). In Bogoliubov’s method, the ground state energy of \(\hat{H}_k\) is the expectation value of this last quantity in the normalized ground state \(|\tilde{\psi}_k\rangle\), and is given by Eq. (5.23). Fig. 4 shows plots of \(E^0_k(N)\) obtained by numerical diagonalization of \(\hat{H}_k\) for \(N = 200\) bosons on one hand, and by using the Bogoliubov expression for \(\langle \hat{H}_k \rangle_k\), Eq. (5.23), on the other. The agreement between Bogoliubov’s method and the exact numerical treatment is quite impressive. The Bogoliubov results are practically indistinguishable from the exact numerical ones for all values of \(k\), except in a narrow interval near \(k = 0\), where there is a small deviation between the two results. Here, we shall not spend too much time trying to understand this (rather small) deviation. Suffice it to say that it is near \(k = 0\) where \(c_k \rightarrow 1\) that we previously found that the standard Bogoliubov theory breaks down, leading to unphysically diverging results for the averages \(\langle a_k^\dagger a_k \rangle_k\) and
Fig. 4. Upper panel: Ground state energy of the Hamiltonian $\hat{H}_k$ for $N = 200$ bosons as a function of the wavevector $k$. The solid line represents the exact result obtained by numerical diagonalization of the Hamiltonian $\hat{H}_k$, while the dashed line is the result of the standard and of the variational Bogoliubov formulations. Lower panel: Detail from the above figure at small wavevectors showing that the exact numerical result (solid line) very slightly deviates from the results of Bogoliubov’s theory (dashed line) near $k = 0$.

$\langle a_k a_{-k} \rangle_k$. Here, we speculate that the deviation of Bogoliubov’s result from the exact one for $E^k_0(N)$ may be due to similar reasons; in other words, this small deviation may be due to the ground state energy being evaluated using the truncated version of the sums (5.14a)-(5.14b) and (5.17) instead of the complete ones in Eqs. (5.13a)-(5.13b) and (5.12).

6.2. Ground state wavefunction and depletion of the condensate

While Bogoliubov’s theory gives results for the ground state energy $E^k_0(N)$ that are in excellent agreement with the exact diagonalization of the single-mode Hamiltonian $\hat{H}_k$, there is only limited agreement between the exact results for the properties of the ground state wavefunction itself and the results of Bogoliubov’s method. This is a well-known feature of variational methods in general, which may, with a judicious choice of trial wavefunctions, give excellent approximations to the ground state energy of the system, but quite often only produce tentative agreement as far as the
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Fig. 5. Upper panel: Coefficients $\tilde{C}_n$ of the normalized ground state wavefunction $|\tilde{\psi}_k\rangle$ of the Hamiltonian $\hat{H}_k$ vs. the index $n$ for $N = 20$ bosons and $k = 0.1$. The circles are the results of the exact numerical diagonalization, and the stars are the result of the variational approach. The triangles show the ratio $\tilde{C}_{n+1}/\tilde{C}_n$ vs. $n$. Contrarily to the variational formulation of Bogoliubov’s theory where this ratio is found to be a constant given by $c_k$ (see the constant line of squares in the figure), in the exact treatment the ratio $\tilde{C}_{n+1}/\tilde{C}_n$ is an increasing function of $n$ and goes to zero as $n \to N/2$. Lower panel: Same as the upper panel for $N = 200$ bosons.

spatial properties of the wavefunction itself are concerned. In the case at hand, and as it can be seen in Fig. 5, we find that the coefficients $\tilde{C}_n$ of the normalized ground state function $|\tilde{\psi}_k\rangle$, as obtained by exact diagonalization of $\hat{H}_k$, do alternate in sign between positive and negative values as predicted by the variational formulation of Bogoliubov’s method. However, the ratio $\tilde{C}_{n+1}/\tilde{C}_n$ does not assume a constant value as the latter theory predicts, which indicates that Bogoliubov’s method produces good qualitative but only approximate quantitative agreement with the exact treatment as far as the ground state wavefunction $|\tilde{\psi}_k\rangle$ itself is concerned. More specifically, we find that the ratio $\tilde{C}_{n+1}/\tilde{C}_n$ goes to zero at large values of the index $n$ in the numerical treatment, which indicates that in the exact solution the highly depleted states $|N-2n,n,n\rangle$ with $n \sim N/2$ are much more strongly suppressed than in the variational Bogoliubov method. This in turn will have a pronounced effect on the depletion of the condensate.
In Fig. 6 we plot the depletion $N_k$ vs. wavevector $k$ that is obtained for $N = 200$ bosons using three different methods. The circles show the exact result:

$$N_k = \langle a_k^\dag a_k \rangle_k = \frac{N}{2} \sum_{n=1}^{N/2} n |\tilde{C}_n|^2.$$  (6.7)

where the $\tilde{C}_n$’s are obtained by exact numerical diagonalization of $\hat{H}_k$. The stars on the other hand, show the result obtained from the number-conserving variational formulation of Bogoliubov’s method, Eq. (5.30), while the solid line shows the result of the standard (number non-conserving) Bogoliubov treatment, Eq. (5.28). It is seen that, while the latter result diverges near $k \to 0$ and is therefore unphysical, the variational result is finite for all values of $k$, and goes to the limiting value $N/4 = 50$ near $k = 0$. It is also seen that the variational method overestimates the depletion of the condensate near $k = 0$ by a factor of about 7 for the particular value of $N$ chosen. As we mentioned earlier in this paragraph, this is due to the overestimation in Bogoliubov’s variational treatment of the coefficients $\tilde{C}_n$ for large values of the index $n$, which also contribute to the calculation of the depletion of the condensate according to Eq. (6.7).

In Fig. 7 we plot the depletion that is obtained by exact numerical diagonalization of the Hamiltonian $\hat{H}_k$ for a number of values of the total number of bosons $N$. Again, comparison with the results shown in Fig. 2 shows that the variational method consistently overestimates the depletion near $k = 0$ for all the values of $N$ considered by about one order of magnitude. The depletion obtained by exact numerical diagonalization of the Hamiltonian $\hat{H}_k$ is seen to be extremely small, and is in fact much smaller than what the standard Bogoliubov theory predicts in the $|k| \to 0$ limit.
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6.3. Elementary excitations

The exact numerical diagonalization of $\hat{H}_k$ described in the two previous Sub-sections gives access not only to the ground state energy, but also to all excited eigenvalues and eigenfunctions of the system in the Hilbert space spanned by the kets $|n\rangle = |N - 2n, n, n\rangle$, where $0 \leq n \leq N/2$. Such excited states can typically be generated by successive application of the operator $\alpha_k^\dagger \alpha_{-k}$ (to be specific, here the $\alpha_k$'s are the operators defined in the number-conserving version of Bogoliubov’s theory, Eq. (5.43)). Indeed, if we calculate the quantity $\alpha_k^\dagger \alpha_{-k} |\psi_k\rangle$, where $|\psi_k\rangle$ is of the form $|\psi_k\rangle = \sum_{n=0}^{N/2} C_n |N - 2n, n, n\rangle$, we find successively:

$$\alpha_k^\dagger |\psi_k\rangle = \sum_{n=1}^{N/2} A_n |N - 2n + 1, n, n - 1\rangle,$$

$$A_n = C_{n-1} \tilde{u}_k \sqrt{n(N - 2n + 2)} + C_n \tilde{v}_k \sqrt{n(N - 2n + 1)},$$

then:

$$\alpha_{-k}^\dagger \alpha_k^\dagger |\psi_k\rangle = \sum_{n=0}^{N/2} B_n |N - 2n, n, n\rangle,$$

$$B_n = A_n \tilde{u}_k \sqrt{n(N - 2n + 1)} + A_{n+1} \tilde{v}_k \sqrt{(n + 1)(N - 2n)},$$

where, in the last equation, it is understood that $A_{1+N/2} = 0$. Eq. (6.9a) shows that the doubly excited state $\alpha_k^\dagger \alpha_{-k}^\dagger |\psi_k\rangle$ belongs to the Hilbert space spanned by the kets $|n\rangle \equiv |N - 2n, n, n\rangle$, and hence is accessible through the numerical diagonalization of the Hamiltonian $\hat{H}_k$.

Let us step back for a moment and try to calculate the analytical expression of the energy required to excite the system from the ground state $|\psi_k\rangle$ to the doubly...
excited state $\alpha^+_k \alpha^+_k |\psi_k\rangle$. This is the quantity:

$$
\Delta E^{(2)}_{\text{exc}}(k) = \frac{\langle \tilde{\psi}_k | \alpha_k \alpha^+_k \hat{H}_k \alpha^+_k \alpha^+_k | \tilde{\psi}_k \rangle}{\langle \tilde{\psi}_k | \alpha_k \alpha^+_k \alpha^+_k \alpha^+_k | \tilde{\psi}_k \rangle} - \langle \tilde{\psi}_k | \hat{H}_k | \tilde{\psi}_k \rangle. \tag{6.10}
$$

Using the diagonalized expression of $\hat{H}_k$ in terms of the $\alpha_k$‘s, Eq. (5.67), we find, after a straightforward calculation (in which the approximation $[\alpha_k, \alpha^+_k] = \gamma_k^2 a_0^\dagger a_0 \approx 1$, see Eq. (A.19) from Appendix A, is used throughout) that $\Delta E^{(2)}_{\text{exc}}(k)$ is given by:

$$
\Delta E^{(2)}_{\text{exc}}(k) = E_k. \tag{6.11}
$$

This is not at all surprising. Indeed, since the excitation energy for a singly excited state with respect to the Hamiltonian $\hat{H}_k$ was found to be $E_k/2$, here for a doubly excited state we expect an excitation energy $2 \times (E_k/2) = E_k$.

We now go back to the numerics, and show that the energy of the first excited state in our numerical treatment coincides with the energy of the double excitation given in Eq. (6.11). As we mentioned in the opening paragraph of this Subsection, dealing with doubly excited states of the form $\alpha^+_k \alpha^+_k |\psi_k\rangle$ has the advantage of keeping us inside the same Hilbert space we used to diagonalize the Hamiltonian $\hat{H}_k$.

Hence, in our numerical diagonalization procedure, if we extract the ground state energy $E_k^{(0)}(N)$ and the energy of the first excited state $E_k^{(1)}(N)$, then the difference $\Delta E^{(2)}_{\text{exc}}(k) = E_k^{(1)}(N) - E_k^{(0)}(N)$ should correspond to the energy of a doubly excited state of the form $\alpha^+_k \alpha^+_k |\psi_k\rangle$ and should be given by the rhs of Eq. (6.11). The upper panel of Fig. 8 shows a comparison between the Bogoliubov result (6.11) and the excitation energy $\Delta E^{(2)}_{\text{exc}}(k)$ as a function of $k$ for $N = 200$ bosons. The agreement is again excellent for most values of $k$, except for small $k$ where the lower panel of that same figure reveals a deviation from linear behavior and the existence of a small energy gap near $k = 0$, where the excitation energy goes to a finite value as $k \to 0$. To probe whether this gap, which it should be noted is much smaller than the gap predicted by Hartree-Fock theory, is due to a finite-size effect, in Fig. 9 we plot the excitation energy obtained numerically at $k = 0.001$ for increasing values of the total number of bosons $N$ in the system. The results obtained show that the value of the gap monotonically decreases as the number $N$ of bosons increases, which in turn suggests that the gap will go to zero as $N$ grows infinitely large in the thermodynamic limit.

§7. Generalization: full Bogoliubov Hamiltonian

Having studied in detail the number-conserving variational formulation of Bogoliubov’s method for the single-mode Hamiltonian $\hat{H}_k$, we now are in a position to tackle the more involved case of the full Hamiltonian $\hat{H} = \sum_{k \neq 0} \hat{H}_k$ of the interacting Bose system. However, before we do so, we want to examine the relationship between what we did so far and previously published work on this system. This will be done next.
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Fig. 8. Upper panel: Plot of the excitation energy $\Delta E_{(2)}^{(2)}(k)$ vs. wavevector $k$ for $N = 200$ bosons. The solid line is the exact diagonalization result, and the dashed line is the result of the variational Bogoliubov method for the Hamiltonian $\hat{H}_k$. For the most part, these two lines are indistinguishable. The dotted line indicates the asymptotic form of Bogoliubov’s result, $\sqrt{2k}$ in dimensionless units, as $k \to 0$. Lower panel: Detail of the region near $k = 0$, where $\Delta E_{(2)}^{(2)}(k)$ goes to a finite limiting value as $k \to 0$, signaling the existence of a small energy gap at low momenta, which is most likely due to finite size effects.

7.1. Connection to previous work

Up till now, we have been discussing the variational approach to the Hamiltonian $\hat{H}_k$ describing the interaction of the condensate with states of momentum $k$ and $-k$. At this point, we will observe that it is quite remarkable that most of the results we derived by diagonalizing $\hat{H}_k$ perfectly coincide with the results of the standard Bogoliubov theory, implying that the latter is effectively a theory in which each one of the Hamiltonians $\hat{H}_k$ which contribute to the total Hamiltonian $\hat{H} = \sum_{k \neq 0} \hat{H}_k$ is diagonalized independently from the other Hamiltonians $\hat{H}_{k'(\neq k)}$ in essentially disjoint Hilbert spaces. For example, the ground state energy of the system in Bogoliubov’s theory is given by (note that we still take the origin of energies to be
Fig. 9. Plot of the excitation energy $\Delta E^{(2)}(k)$ at $\tilde{k} = 0.001$ obtained from the exact numerical diagonalization of the single-mode Hamiltonian $\hat{H}_k$ as a function of the number of bosons $N$. The fact that the excitation energy decreases with increasing values of $N$ suggests that the small gap seen in the lower panel of Fig. 8 is due to finite-size effects and vanishes in the thermodynamic limit $N \to \infty$.

the Gross-Pitaevskii value $N(N-1)v(0)/2V$:

$$E_{\text{Bog}} = -\frac{1}{2} \sum_{k \neq 0} (\varepsilon_k + n_Bv(k) - E_k),$$  \hspace{1cm} (7.1)

and it can be verified that this quantity is nothing but:

$$E_{\text{Bog}} = \sum_{k \neq 0} \langle \tilde{\psi}_k(N)|\hat{H}_k|\tilde{\psi}_k(N)\rangle,$$  \hspace{1cm} (7.2)

where we remind the reader that $|\tilde{\psi}_k(N)\rangle$ is the normalized ground state of the single-mode Hamiltonian $\hat{H}_k$. This is rather surprising, since we expect the ground state energy of the system to be given by an expression of the form:

$$E_{\text{Bog}} = \langle \Psi(N)|\hat{H}|\Psi(N)\rangle,$$  \hspace{1cm} (7.3a)

$$= \sum_{k \neq 0} \langle \Psi(N)|\hat{H}_k|\Psi(N)\rangle,$$  \hspace{1cm} (7.3b)

where $|\Psi(N)\rangle$ is the normalized ground state wavefunction of the total Hamiltonian $\hat{H}$. In what follows, we want to examine how, within the standard formulation of Bogoliubov’s theory, one can go from Eqs. (7.3) to the result in Eq. (7.2), which will entail uncovering how the ground state wavefunction $|\Psi(N)\rangle$ for the total Hamiltonian $\hat{H}$ has been constructed in the literature from the ground state functions $|\tilde{\psi}_k(N)\rangle$ of the single-mode Hamiltonians $\hat{H}_k$.

The main argument allowing one to construct the ground state $|\Psi(N)\rangle$ of the total Hamiltonian $\hat{H}$ from the single-mode ground state wavefunctions $|\tilde{\psi}_k(N)\rangle$ is based on the following reasoning. As we have already seen in Sec. 2 in the standard formulation of Bogoliubov’s method the creation and annihilation operators of bosons

$$E_{\text{Bog}} = \sum_{k \neq 0} \langle \tilde{\psi}_k(N)|\hat{H}_k|\tilde{\psi}_k(N)\rangle,$$  \hspace{1cm} (7.2)
in the condensate, $a_0^\dagger$ and $a_0$, are replaced by the c-number $\sqrt{N_0} \approx \sqrt{N}$. After this replacement is made, the various Hilbert spaces where the single-mode Hamiltonians $\hat{H}_k$ act are totally disjoint from each other. This in turn implies that the single-mode Hamiltonians $\{\hat{H}_k\}$ can be diagonalized independently from one another, and that the ground state wavefunction of the system can be written as the product of the ground state wavefunctions of each of the single-mode Hamiltonians $\hat{H}_k$:

$$|\Psi(N)\rangle = \prod_{i=1}^{\infty} |\tilde{\psi}_{k_i}(N)\rangle.$$ (7.4)

Now, it can be shown that, even though the operators $a_0$ and $a_0^\dagger$ have been replaced by $\sqrt{N}$ in the expression of the Hamiltonian $\hat{H}$, minimization of the expectation value of the single-mode Hamiltonian $\hat{H}_k$ in the single-mode ground state $|\tilde{\psi}_k(N)\rangle \approx \sqrt{1 - c_k^2} \sum_{n=0}^{N/2} |(-c_k)^n n\rangle$ leads to the same variational coefficients $c_k$ as in Eq. (5.22). This leads, in the notation of the classic work of Lee, Huang and Yang\(^\text{37}\) to the following expression of the normalized ground state $|\Psi(N)\rangle$ of the Hamiltonian $H$ (see also Ref. \[^{41}\]):

$$|\Psi(N)\rangle = Z \sum_{n_1=0}^{\infty} \cdots \sum_{n_{\infty}=0}^{\infty} (-c_{k_1})^{n_1} \cdots (-c_{k_{\infty}})^{n_{\infty}} |n_1, n_1; \ldots; n_{\infty}, n_{\infty}\rangle,$$ (7.5)

where:

$$|n_1, n_1; \ldots; n_{\infty}, n_{\infty}\rangle = \prod_{i=1}^{\infty} \frac{(a_{k_i}^\dagger)^{n_i}}{\sqrt{n_i!}} \frac{(a_{-k_i})^{n_i}}{\sqrt{n_i!}} |0\rangle.$$ (7.6)

In the above equations, $n_i$ is the number of bosons in the states $\pm k_i$, and the coefficient $C_{n_1, \ldots, n_{\infty}} = (-c_{k_1})^{n_1} (-c_{k_2})^{n_2} \cdots (-c_{k_{\infty}})^{n_{\infty}}$ represents the probability amplitude of finding the system in the many-body state $|n_1, n_1; \ldots; n_{\infty}, n_{\infty}\rangle$. In principle, we would like the coefficients $C_{n_1, \ldots, n_{\infty}}$ of the wavefunction $|\Psi(N)\rangle$ to vanish if $n_1 + n_2 + \cdots + n_{\infty} \geq N/2$:

$$C_{n_1, \ldots, n_{\infty}} = 0 \quad \text{if} \quad n_1 + n_2 + \cdots + n_{\infty} \geq N/2.$$ (7.7)

However, enforcing the above constraint is not expected to give rise to any significant change in the value of the ground state energy in the thermodynamic $N \to \infty$ limit. Going back to Eq. (7.5), the quantity $Z$ defined in that equation is the normalization constant:\(^{41}\)

$$Z \approx \prod_{i=1}^{\infty} \sqrt{1 - \frac{c_k^2}{k_i}}.$$ (7.8)

With the definitions (7.5) and (7.8), one can verify that the ground state energy $E_0(N) = \langle \Psi(N) | H | \Psi(N) \rangle$ is given by the $rhs$ of Eq. (7.1), which is again the same as the $rhs$ of Eq. (7.2). One can also verify that the depletion of the condensate is still given by an expression of the form (5.24), namely:

$$\langle \Psi(N) | a_k^\dagger a_k | \Psi(N) \rangle = \frac{c_k^2}{1 - \frac{c_k^2}{k}}.$$ (7.9)
Finally, if we forego the number conserving expression of the operators \( \alpha_k \) and \( \alpha_k^\dagger \) derived in Sec. 5.3 above, and use the number non-conserving approximations of Eq. (7.5),

\[
\alpha_k = u_k a_k + v_k a_{-k}^\dagger, \quad \alpha_k^\dagger = u_k a_k^\dagger + v_k a_{-k},
\]

with \( u_k \) and \( v_k \) the quantities defined in Eq. (2.13), one can easily verify that the action of the operator \( \alpha_k \) on \( |\Psi(N)\rangle \) yields zero, and that the excitation spectrum generated by the \( \alpha_k^\dagger \) operator is indeed given by the Bogoliubov spectrum \( E_k = \sqrt{\varepsilon_k(v_k + 2nBV(k))} \).

At this juncture, we would like to attract the reader’s attention to the fact that in the expression (7.3) of the wavefunction \( |\Psi(N)\rangle \), the number of bosons in the \( k = 0 \) state is not explicitly specified (this is indeed how Lee et al. write the ground state wavefunction in their work, Ref. 7)). One may correctly observe that the number of condensed bosons is automatically known and is given by \( (N - 2 \sum n_i) \). But in fact the reason Lee et al. do not specify the number of bosons in the \( k = 0 \) state is a more trivial one, and has to do with the fact that these authors use Bogoliubov’s approximation of replacing the operators \( a_0 \) and \( a_0^\dagger \) by the c-number \( \sqrt{N} \) (one place where this is made obvious is the expressions of the excitation operators they use, \( \alpha_k \) and \( \alpha_k^\dagger \), which does not contain any trace of the operators \( a_0 \) and \( a_0^\dagger \)).

Unlike to the \( \alpha_k \)’s used by Leggett in Ref. 34, which are similar to those we used in Sec. 5.3 above, and hence their calculation is one where the \( k = 0 \) state is removed altogether from the Hilbert space used to describe the system. A major question that therefore arises is to know if and how the standard results that were derived using the expression (7.5) of \( |\Psi(N)\rangle \) will change if we put the \( k = 0 \) back into the Hilbert space, and we keep a more accurate tally of how many bosons are present in this \( k = 0 \) state, hence enforcing the conservation of boson number. This will be the subject of the next Subsection.

7.2. Variational treatment of the full Hamiltonian \( \hat{H} = \sum_{k \neq 0} \hat{H}_k \)

We now want to generalize the variational approach of Sec. 5 to treat the full Hamiltonian \( \hat{H} = \sum_{k \neq 0} \hat{H}_k \) of the interacting Bose system. To this end, we shall use for \( |\Psi(N)\rangle \) an expression of the form (we here denote by \( M \) the total number of momentum modes kept in the calculation, which will eventually be sent to infinity):

\[
|\Psi(N)\rangle = Z \sum_{n_1, n_2, \ldots, n_M=0}^{n_M=\max} C_{n_1} C_{n_2} \cdots C_{n_M} |N - 2 \sum_{i=1}^{M} n_i; n_1, n_1, \ldots, n_M, n_M\rangle,
\]

(7.11)

where the normalized basis wavefunctions are given by (compare with Eq. (7.6)):

\[
|N - 2 \sum_{i=1}^{M} n_i; n_1, n_1, \ldots, n_M, n_M\rangle = \frac{(a_0^\dagger)^{N-2 \sum_{i=1}^{M} n_i} \prod_{i=1}^{M} (a_{k_i}^\dagger)^{n_i} (a_{-k_i}^\dagger)^{n_i}}{\sqrt{[N - 2 \sum_{i=1}^{M} n_i]!} \sqrt{n_1!} \sqrt{n_2!} \cdots \sqrt{n_M!}} |0\rangle.
\]

(7.12)
Note that the ground state wavefunction in Eq. (7.11) is not a simple product of ground state wavefunctions of the single-mode Hamiltonians $\hat{H}_k$, as in Eq. (7.4), and that, even though the $\hat{H}_k$’s may seem to be decoupled, the presence of all the $n_i$’s in the number of condensed bosons $(N - 2\sum_{i=1}^{M} n_i)$ acts like an implicit and rather nontrivial coupling between all these single-mode Hamiltonians. Note also that the summations over the $n_i$’s in Eq. (7.11) extend from 0 to a value $n_{i,\text{max}}$, emphasizing the constraint that the number of bosons in the $k = 0$ state in each of the basis wavefunctions has to be greater than or equal to zero, i.e., $\sum_{i=1}^{M} n_i \leq N/2$ (see Eq. (7.7)). A possible (but, by no means, unique) choice for the values $n_{i,\text{max}}$ is given by:

$$n_{1,\text{max}} = N/2,$$

$$n_{2,\text{max}} = N/2 - n_1,$$

$$\ldots$$

$$n_{M,\text{max}} = N/2 - n_1 - \cdots - n_{M-1}.$$  

(7.13a)

(7.13b)

(7.13c)

It can be verified that the above parametrization of the $n_{i,\text{max}}$’s exhausts all possible states compatible with the constraint (7.7). In what follows, however, we shall place ourselves in the thermodynamic limit $N \to \infty$ where it can be shown that it is not important to keep track of the constraints (7.13), and in the evaluation of physical expectation values we shall for simplicity extend the summations to infinity, as is done in the standard Bogoliubov theory of Eq. (7.5). However, we shall find it essential to keep track of the number of bosons in the $k = 0$ state, as this significantly modifies some important results of the standard Bogoliubov approach, changing the nature of the excitation spectrum from a gapless one to one which has a finite energy gap as $k \to 0$.

As we mentioned above, although it may appear at first glance that the wavefunction given in Eq. (7.11) should allow us to reproduce the salient features of Bogoliubov’s theory, a careful analysis shows that, in fact, different results are obtained for the ground state energy and for the energy of elementary excitations, since now the number of particles in the condensate is not given by $(N - 2n_i)$ as was the case in the variational approach for the single-mode Hamiltonian $\hat{H}_k$, but is given by the more complicated expression $(N - 2\sum_{i=1}^{M} n_i)$ involving all momentum modes. In particular, in Appendix B we show that the expectation value of the Hamiltonian $\hat{H}_{kj}$ in the state $|\Psi(N)\rangle$ is no longer given by Eq. (5.18), but by the following expression:

$$\langle \Psi(N)|\hat{H}_{kj}|\Psi(N)\rangle \simeq \frac{c_{kj}^2}{1 - c_{kj}^2} \left[ \varepsilon_{kj} + \bar{v}(k_j)n_B \right] - \bar{v}(k_j)n_B \frac{c_{kj}^2}{1 - c_{kj}^2},$$  

(7.14)

where $\bar{v}(k_j)$ is given by:

$$\bar{v}(k_j) = v(k_j) \left( 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{c_{ki}^2}{1 - c_{ki}^2} \right).$$  

(7.15)
If it were not for the term between parenthesis in this last equation, the result in
Eq. (7.14) would be perfectly identical to the expectation value obtained within
the single-mode approach, Eq. (5.18). Minimization of the expectation value of the
total Hamiltonian \( \langle \Psi(N)|\hat{H}|\Psi(N) \rangle \) with respect to the variational parameters \( \{c_k\} \)
would then give the same values for these parameters as in the single-mode case,
Eq. (5.22), and hence everything we discussed in Sec. 5 would remain pretty much
unchanged. Below we will show that minimization of \( \langle \Psi(N)|\hat{H}|\Psi(N) \rangle \) as given by
Eq. (7.14), i.e. with \( v(k) \) replaced by \( \bar{v}(k) \), leads to a very different solution for the
c_k’s, leading in turn to some important changes for the ground state properties of
the interacting Bose system.

Going back to the result of Eq. (7.14), if we now minimize the expectation value
of the total Hamiltonian \( \hat{H} = \sum_{j=1}^{M} \hat{H}_{kj} \), which is given by:
\[
\langle \Psi(N)|\hat{H}|\Psi(N) \rangle = \sum_{j=1}^{M} \left\{ \left[ \varepsilon_{kj} + n_B \bar{v}(k_j) \right] \frac{c_{kj}}{1 - c_{kj}} - n_B \bar{v}(k_j) \frac{c_{kj}}{1 - c_{kj}} \right\}, \tag{7.16}
\]
with respect to the constants \( c_{kj} \), instead of Eq. (5.19) we now obtain the following
equation (see Appendix C):
\[
c_{kj}^2 - 2 \left( \frac{\tilde{\varepsilon}_{kj}}{n_B \bar{v}(k_j)} \right) c_{kj} + 1 = 0. \tag{7.17}
\]
In the above equation, \( \tilde{\varepsilon}_{kj} \) now denotes the quantity:
\[
\tilde{\varepsilon}_{kj} = \varepsilon_{kj} + n_B \bar{v}(k_j) + \sigma_{kj}, \tag{7.18a}
\]
with \( \sigma_{kj} = \frac{2}{N} \sum_{i=1(\neq j)}^{M} n_B v(k_i) \frac{c_{ki}}{1 + c_{ki}}. \tag{7.18b}
\]
Solving Eq. (7.17) for \( c_k \), we obtain:
\[
c_k = \left( \frac{\tilde{\varepsilon}_k}{n_B \bar{v}(k)} \right) - \sqrt{\left( \frac{\tilde{\varepsilon}_k}{n_B \bar{v}(k)} \right)^2 - 1}. \tag{7.19}
\]
where again the sign of the second term has been chosen so that \( 0 < c_k < 1 \).
Expressions (7.19) for the ground state expectation value of the Hamiltonian and
(7.19) for the coefficients of the ground state wavefunction are the main results of
this paper. In the rest of this Section we want to explore how these expressions,
which, to the best of the author’s knowledge, have not been studied previously,
alter the description of interacting Bose systems given in the standard Bogoliubov
formulation.

We now rewrite the quantity \( \sigma_{kj} \) of Eq. (7.18b) in the form:
\[
\sigma_{kj} = \frac{2}{N} \sum_{i=1}^{M} n_B v(k_i) \frac{c_{ki}}{1 + c_{ki}} - \frac{2}{N} n_B v(k_j) \frac{c_{kj}}{1 + c_{kj}}. \tag{7.20}
\]
Using the fact that \( n_B = N/V \), and neglecting the second term on the rhs of this last equation, (which is of order \((1/N)\)) we obtain:

\[
\sigma_{kj} \simeq \frac{2}{V} \sum_{i=1}^{M} v(k_i) \frac{c_{k_i}}{1 + c_{k_i}}.
\]  (7.21)

Transforming the sum into an integral, we obtain (notice that the factor of 2 disappears because the summation in Eq. (7.21) is over half of phase space only – notice also that the number of momentum modes \( M \) has been sent to infinity):

\[
\sigma_k \simeq \int v(k') \frac{c_k}{1 + c_{k'}}.
\]  (7.22)

As it can be seen, the quantity on the rhs of the above equation does not depend on \( k \), and we shall henceforth drop the subscript \( k \) from \( \sigma_k \), and rewrite Eq. (7.18b) in the form:

\[
\tilde{\varepsilon}_{kj} = \varepsilon_{kj} + n_B \bar{v}(k_j) + \sigma,
\]  (7.23a)

with \( \sigma = \int v(k) \frac{c_k}{1 + c_k} \).  (7.23b)

In the particular case where \( v(k) = g \), corresponding to \( v(r) = g\delta(r) \) in real space, it is not difficult to see that the integral in Eq. (7.23b) has an ultraviolet divergence in three dimensions, since \( c_k \) as given in Eq. (7.19) behaves like \( 1/k^2 \) as \( k \to \infty \). To circumvent this difficulty, instead of the interaction potential \( v(r) = g\delta(r) \) we shall use:

\[
v(r) = \frac{ge^{-r^2/(2\lambda^2)}}{(2\pi\lambda^2)^{3/2}}, \]

(7.24)

where \( \lambda \) is a positive quantity having the dimensions of length. This expression of the interaction potential has been chosen to ensure that we recover the form \( v(r) = g\delta(r) \) in the limit \( \lambda \to 0 \). In Fourier space, the interaction potential of Eq. (7.24) is given by:

\[
v(k) = ge^{-k^2\lambda^2/2}.
\]  (7.25)

With this expression of \( v(k) \), the integral on the rhs of Eq. (7.23b) converges. Going back to this last equation, we see that the integral on the rhs depends on \( \sigma \) through \( c_k \), and hence we see that Eq. (7.23b) can be seen as a self-consistent equation for \( \sigma \). In the following, we shall solve this self-consistent equation and find the value of \( \sigma \) for a given value of the parameters \( g, n_B \) and \( \lambda \). But, before we do that, we want to go back and re-examine the quantity \( \bar{v}(k) \) we introduced in Eq. (7.15).

Let us rewrite the rhs of Eq. (7.15) in the form:

\[
\bar{v}(k_j) = v(k_j) \left( 1 - \frac{2}{N} \sum_{i=1}^{M} \frac{c_{k_i}^2}{1 - c_{k_i}^2} + \frac{2}{N} \frac{c_{k_j}^2}{1 - c_{k_j}^2} \right).
\]  (7.26)
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The last term between brackets in the above equation is of order \(1/N\), and hence can be neglected in the thermodynamic \(N \to \infty\) limit. On the other hand, the sum

\[
\sum_{i=1}^{M} \frac{c_{k_i}^2}{1 - c_{k_i}^2}
\]

is recognized as the expectation value

\[
\langle \Psi(N) | \sum_{i=1}^{M} a_{k_i}^\dagger a_{k_i} | \Psi(N) \rangle,
\]

where the summation extends over half of the wavevectors \(k\) in phase space. Hence, we can write:

\[
\bar{v}(k) = v(k) \left(1 - \frac{N_d}{N}\right), \tag{7.27}
\]

where \(N_d\) is the total number of depleted bosons:

\[
N_d = 2 \sum_{i=1}^{M} \frac{c_{k_i}^2}{1 - c_{k_i}^2} \tag{7.28a}
\]

\[
= \sum_{k \neq 0} \frac{c_{k}^2}{1 - c_{k}^2} \tag{7.28b}
\]

For ease of notation, we shall introduce a new symbol \(C_d\), which we shall dub the “depletion factor”, such that:

\[
C_d = 1 - \frac{N_d}{N}. \tag{7.29}
\]

Then, Eq. (7.27) can be rewritten in the form:

\[
\bar{v}(k) = C_d v(k), \tag{7.30}
\]

We now are ready to tackle the self-consistent equation for \(\sigma\). To this end, we will again use dimensionless units, where energies are measured in units of \(n_Bv(0) = gn_B\), and wavevectors are measured in units of \(k_0 = \sqrt{2mn_Bg}/h\), and we will find it convenient to express the interaction strength \(g\) in terms of the s-wave scattering length \(a\), such that:

\[
4\pi a^2 \frac{h}{m} = g. \tag{7.31}
\]

Then we can write for \(c_k\) the following expression:

\[
c_k = 1 + \frac{1}{C_d} (\tilde{k}^2 + \tilde{\sigma}) e^{4\pi n_B a^2 \tilde{k}^2} - \sqrt{\left[1 + \frac{1}{C_d} (\tilde{k}^2 + \tilde{\sigma}) e^{4\pi n_B a^2 \tilde{k}^2}\right]^2 - 1}, \tag{7.32}
\]

where we denote by \(\tilde{k}\) and \(\tilde{\sigma}\) the dimensionless quantities:

\[
\tilde{k} = \frac{k}{k_0}, \tag{7.33a}
\]

\[
\tilde{\sigma} = \frac{\sigma}{gn_B}. \tag{7.33b}
\]

If we use this last expression of \(c_k\) in Eq. (7.23b), and change the variable of integration from \(k\) to the dimensionless quantity \(\tilde{k}\), we can write for the dimensionless quantity \(\tilde{\sigma}\) the following self-consistent equation:

\[
\tilde{\sigma} = \frac{8\sqrt{2}}{\sqrt{\pi}} (n_B a^3)^{\frac{1}{2}} \int_0^\infty d\tilde{k} \tilde{k}^2 e^{-4\pi (n_B a^2) \tilde{k}^2} \frac{1 + Q^2 - \sqrt{(1 + Q^2)^2 - 1}}{2 + Q^2 - \sqrt{(1 + Q^2)^2 - 1}}, \tag{7.34}
\]
where we used the shorthand notation:

\[ Q^2 = C_d^{-1}(\tilde{k}^2 + \tilde{\sigma})e^{4\pi(n_Ba\lambda^2)\tilde{k}^2}. \tag{7.35} \]

A numerical solution to the above equation for \( \tilde{\sigma} \) can be found by iteration in the following way. First, one starts with an initial guess for \( \tilde{\sigma} \). Using this initial guess, one computes the ratio \( \frac{N_d}{N} \) using Eq. (7.42) below, which allows us to find the depletion factor \( C_d = 1 - \frac{N_d}{N} \). This value of \( C_d \) is then used to solve Eq. (7.34) for \( \tilde{\sigma} \). This computed value of \( \tilde{\sigma} \) is then used again as an input to find a better estimate of the ratio \( \frac{N_d}{N} \) using Eq. (7.42), and the process is henceforth repeated until convergence and a stable solution for \( C_d \) and \( \tilde{\sigma} \) is found.

In the following, we shall be mostly interested in dilute Bose gases, for which \( n_Ba^3 \ll 1 \). There indeed seems to be a broad consensus in the physics community\(^{36}\) that Bogoliubov’s theory is not adequate for describing the properties of denser systems such as, e.g., superfluid liquid Helium near zero temperature. For the particular case of liquid Helium, this belief stems from the fact that Bogoliubov’s theory fails to capture a few major features of this system, most notably the fact that the depletion, even at the lowest temperatures, is quite substantial (the number of bosons in the condensate not representing more than 10% of the total number of bosons \( N \) in the system), as well as the appearance of a roton minimum in the excitation spectrum at higher values of the wavevector \( k \). Given the above, we shall restrict ourselves to the situation of a dilute Bose gas, the ground state properties of which are believed to be properly captured by the Bogoliubov Hamiltonian.

For simplicity, we shall take the characteristic length scale \( \lambda \) which governs the range of the interaction potential \( v(\mathbf{r}) \) to be the scattering length \( a \). Under these circumstances, a numerical solution of the self-consistency equation (7.34) for \( n_Ba^3 = 10^{-3} \) yields the following values for the quantities \( \tilde{\sigma} \) and \( C_d \) (the reader will note that similar results are obtained using other numerical values of the parameter \( n_Ba^3 \) as well):

\[ \tilde{\sigma} = 0.3899 \simeq 0.39, \tag{7.36a} \]
\[ C_d = 0.9762 \simeq 0.98. \tag{7.36b} \]

With the knowledge of \( \tilde{\sigma} \) and \( C_d \), we now are in a position to determine the coefficients \( c_k \), and hence find the depletion and the ground state energy of the gas. Going back to Eq. (7.32), we see that the exponential factor \( \exp(k^2\lambda^2/2) \) for \( \lambda = a \) is given by \( \exp(4\pi n_Ba^3k^2) \), and for small values of \( k \) this quantity can be approximated by unity (since \( n_Ba^3 = 10^{-3} \ll 1 \)). The expression of \( c_k \) can therefore be approximated by:

\[ c_k \simeq 1 + C_d^{-1}(\tilde{k}^2 + \tilde{\sigma}) - \sqrt{\left[1 + C_d^{-1}(\tilde{k}^2 + \tilde{\sigma})\right]^2 - 1}. \tag{7.37} \]

Notice that this expression of \( c_k \) reduces to the expression we found before in the single-mode model, Eq. (7.22), in the limit \( \tilde{\sigma} = 0 \) and \( C_d = 1 \). Fig. 10 shows a plot of \( c_k \) as a function of the dimensionless wavevector \( \tilde{k} \) for \( \tilde{\sigma} \simeq 0.39 \) and \( C_d \simeq 0.98 \).
7.3. Depletion of the condensate in presence of many momentum modes

With the knowledge of $c_k$, it is easy to find the number of depleted bosons $N_k$ in the single momentum state $k$, which is given by:

$$N_k = \langle \Psi(N)|a_k^\dagger a_k|\Psi(N)\rangle = \frac{c_k^2}{1 - c_k^2}.$$  (7.39)

In the case of the single mode theory, the coefficient $c_k$ as given by Eq. (5.22) goes to unity as $k \to 0$, leading to a divergence of the quantity $N_k$ at small wavevectors. This happens, as we have shown in detail in Sec. 5.2 when we work in the $N \to \infty$ limit and extend summations over the coefficients of the wavefunction to infinity; but otherwise if we insist on working with finite sums, the depletion does not diverge as $k \to 0$. Here, by contrast, $c_k$ goes to a limit which is smaller than 1 as $k \to 0$, and hence $N_k$ does not diverge at small values of $k$ even though the geometric summations (over the coefficients $C_n$ of the wavefunction) in the derivation of Eq. (7.39) are extended to infinity. Fig. 11 shows a plot of the depletion $N_k$ as a function of the dimensionless wavevector $\tilde{k}$ for the single-mode theory where $c_k$ is given by Eq. (5.22) (upper curve), and for the multi-mode approach where $c_k$ is given by Eq. (7.37), with $\tilde{\sigma} = 0.39$ and $C_d = 0.98$ (lower curve).

The total depletion is given by the following expression:

$$N_d = \sum_{k \neq 0} \frac{c_k^2}{1 - c_k^2}.$$  (7.40)
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Fig. 11. Plot of the depletion of the condensate \( N_k = c_k^2/(1 - c_k^2) \) as a function of the dimensionless wavevector \( \tilde{k} \). The dashed line shows the depletion obtained using the coefficients \( c_k \) obtained in the single-mode theory, Eq. (5.22). The solid line, on the other hand, shows the depletion obtained using the coefficients \( c_k \) obtained from the multi-mode variational treatment of the present section, Eq. (7.19), with \( \tilde{\sigma} = 0.39 \) and \( C_d = 0.9762 \).

The summand, after a few manipulations, can be written in the form:

\[
\frac{c_k^2}{1 - c_k^2} = \frac{1}{2} \left( \frac{1 + Q^2}{\sqrt{Q^2(2 + Q^2)}} - 1 \right).
\]  

(7.41)

Transforming the sum in Eq. (7.40) into an integral, we can write the ratio \( N_d/N \) of the number of depleted bosons \( N_d \) to the total number of bosons \( N \) in the form:

\[
\frac{N_d}{N} = \frac{4\sqrt{2}}{\sqrt{\pi}} (n_B \alpha^3)^{\frac{1}{2}} \int_0^\infty \, \tilde{k}^2 \left( \frac{1 + Q^2}{\sqrt{Q^2(2 + Q^2)}} - 1 \right).
\]  

(7.42)

In the standard formulation of Bogoliubov’s theory, which corresponds to setting \( \tilde{\sigma} = 0, \, C_d = 1 \) and \( \lambda = 0 \) in the above expression, the integral in the above equation can be evaluated exactly, and has a value of \( (\sqrt{2}/3) \approx 0.4714 \). For non-zero values of \( \tilde{\sigma} \), it is straightforward to evaluate the integral numerically. For example, for \( \tilde{\sigma} = 0.39 \) and \( \lambda = 0 \), the integral evaluates to 0.3276, which translates into a reduction in the number of depleted bosons by about a third (0.3276/0.4714 ≈ 0.695) with respect to the result of the standard Bogoliubov method.

7.4. Ground state energy in presence of many momentum modes

We are now in a position to find the ground state energy \( \langle \hat{H} \rangle = \langle \Psi(N) | \hat{H} | \Psi(N) \rangle \) of the system, which is given by:

\[
\langle \hat{H} \rangle = \sum_{k \neq 0} \frac{1}{1 - c_k^2} \left\{ [\epsilon_k + n_B \vec{v}(k)] c_k^2 - n_B \vec{v}(k) c_k \right\}.
\]  

(7.43)

Using the expression (7.37) of the coefficients \( c_k \) into this last equation leads to an ultraviolet divergence at large \( k \), much like in the standard Bogoliubov approach.
To circumvent this difficulty, we here shall use the “regularized” expression (7.32) of $c_k$, which takes into account the fact that the interaction potential between bosons falls off at large $k$. Then, if we transform the sum into an integral, we obtain (in three dimensions):

$$
\frac{E}{V} = -\frac{1}{2} g n_B^2 \left\{ 8 \sqrt{2} \frac{(n_B a^3)^{3/2}}{\sqrt{\pi}} \int_0^\infty dk \ k^2 \left[ C_d e^{-4 \pi n_B a \lambda^2 k^2} (1 + Q^2 - \sqrt{Q^2 (Q^2 + 2)}) + \tilde{\sigma} \left( \frac{1 + Q^2}{\sqrt{Q^2 (Q^2 + 2)}} - 1 \right) \right] \right\}.
$$

(7.44)

Numerical evaluation of the above integral for $\lambda = a$ and $n_B a^3 = 0.001$ yields, for $\tilde{\sigma} = 0$ (the corresponding value of $C_d$, evaluated using Eq. (7.42), is given by $C_d = 0.9642$),

$$
\frac{E}{V} \bigg|_{\tilde{\sigma} = 0} \simeq \frac{1}{2} g n_B^2 \cdot (13.02) (n_B a^3)^{3/2},
$$

(7.45a)

$$
\simeq \frac{1}{2} g n_B^2 \cdot (0.412),
$$

(7.45b)

while for $\tilde{\sigma} = 0.39$ and $C_d = 0.9762$, we obtain:

$$
\frac{E}{V} \bigg|_{\tilde{\sigma} = 0.39} \simeq \frac{1}{2} g n_B^2 \cdot (13.20) (n_B a^3)^{3/2},
$$

(7.46a)

$$
\simeq \frac{1}{2} g n_B^2 \cdot (0.417).
$$

(7.46b)

We hence see that the solution with $\tilde{\sigma} \neq 0$ for the coefficients $c_k$ leads a lower overall energy than a solution with $\tilde{\sigma} = 0$ when the depletion factor $C_d$ is used in the calculation (we remind the reader that this factor emerges when we keep an accurate count of the number of bosons in the condensed state $k = 0$, see Eq. (7.13)), which constitutes a direct verification of the validity of our variational method. The fact that the solution with $\tilde{\sigma} \neq 0$ has a lower energy than the solution with $\tilde{\sigma} = 0$ can best be visualized in Fig. 12, where we plot the quantity $\tilde{k}^2 \langle \hat{H}_k | \Psi(N) \rangle$ that appears when we integrate over momentum modes in the calculation of the total energy $E$. It appears that the area enclosed by the curve with $\tilde{\sigma} = 0.39$ is greater than the area enclosed by the curve with $\tilde{\sigma} = 0$, hence showing that the value $\tilde{\sigma} = 0.39$ leads to a lower ground state energy of the system.

One may wonder at this point if the above results for the ground state energy are not simply an artifact of the special choice we made for the interaction potential between bosons, which has a Gaussian dependence on $\tilde{k}$ in Fourier space. To clarify this point, in the upper panel of Fig. 13 below we plot the ground state expectation value of $\hat{H}_k$ as a function of the wavevector $\tilde{k}$ from Eq. (7.14) using $\lambda = 0$ (corresponding to $v(r) = g \delta(r)$) and with a different value of the parameter $n_B a^3$, $n_B a^3 = 0.01$ (more precisely, we plot the product $\tilde{k}^2 \langle \hat{H}_k | \Psi(N) \rangle$ vs. $k$, the factor $\tilde{k}^2$ representing the Jacobian of the integral over wavevectors in three dimensions that appears in the calculation of the ground state energy $E = \langle \Psi(N) | \hat{H} | \Psi(N) \rangle$).
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Fig. 12. Plot of the quantity $\tilde{k}^2 \langle \Psi(N) | \hat{H}_k | \Psi(N) \rangle$ (where the factor $\tilde{k}^2$ comes from the Jacobian of the integral over wavevectors in three dimensions) that appears in the calculation of the ground state energy $E = \langle \Psi(N) | \hat{H} | \Psi(N) \rangle$. The dashed curve corresponds to $\tilde{\sigma} = 0$ and $C_d = 0.9642$, while the solid curve corresponds to $\tilde{\sigma} = 0.39$ and $C_d = 0.9762$.

In this last figure, the solid line shows the result for $\tilde{k}^2 \langle \hat{H}_k \rangle$ one obtains by plugging the coefficients $c_k$ of the single-mode theory, Eq. (5.22), into Eq. (7.14). The dotted lines, on the other hand, show the results for this same quantity one obtains using the coefficients $c_k$ from Eq. (7.37) for three nonzero values of $\tilde{\sigma}$. It is again seen that the expectation values $\langle \hat{H}_k \rangle$ that are obtained using the coefficients $c_k$ from Eq. (7.37) with $\tilde{\sigma} \neq 0$ are consistently lower than the one calculated using the single mode coefficients from Eq. (5.22), which gives further credence to our minimization procedure in which the number of bosons in the condensate $(N - 2 \sum_i n_i)$ is kept throughout the calculation. Conversely, in the lower panel of Fig. (13) we plot the quantity $\tilde{k}^2 \langle \tilde{\psi}_k | \hat{H}_k | \tilde{\psi}_k \rangle$ from Eq. (5.18) using the Bogoliubov result (5.22) for $c_k$ (solid line), and using the result (7.37) for various nonzero values of $\tilde{\sigma}$. It is seen that for the single-mode model the standard result for $c_k$ (which corresponds to setting $\tilde{\sigma} = 0$ and $C_d = 1$ in Eq. (7.37)) is always smaller in energy than the result obtained by using a non-zero value of $\tilde{\sigma} = 0$ in the expression of $c_k$ from Eq. (7.37). We therefore conclude that both our minimizations, in Sec. 5.1 and in the present Section, produce correct functional forms for the constants $c_k$ that minimize the ground state energy of the system, with Eq. (5.22) representing the correct functional form of $c_k$ when we consider the single-mode Hamiltonian $\hat{H}_k$ (or, equivalently, when we use the Bogoliubov prescription $a_0 \simeq \sqrt{N}$ and remove the $k = 0$ mode from the Hilbert space, so that all the single-mode Hamiltonians $\hat{H}_k$ are decoupled), and Eq. (7.37) representing the functional form that minimizes the ground state energy when we do not use Bogoliubov’s prescription and keep the correct expression $(N - 2 \sum_i n_i)$ of the number of bosons in the $k = 0$ state throughout the calculation.

7.5. Elementary excitations in presence of many momentum modes

We now want to examine the elementary excitations of the Bose system in presence of many momentum modes. By contrast to the situation of Sec. 5.4 where we
studied the elementary excitations of the single-mode Hamiltonian $\hat{H}_k$, and where the only possible excitations increasing the momentum of the system by an amount $\hbar k$ were $a_k^\dagger a_0$ and $a_0^\dagger a_{-k}$, here since we are dealing with the total Hamiltonian $\hat{H}$, there are an infinite number of excitations of the form $a_k^\dagger a_{k+q}^\dagger a_q$ which increase the momentum the system by $\hbar k$. The most general excitation of momentum $\hbar k$ can be written in the form:

$$\tilde{\alpha}_k^\dagger = \sum_q \beta_q a_{k+q}^\dagger a_q,$$

(7.47)

with the $\beta_q$'s being arbitrary complex numbers. In principle, the possibility that the $\beta_q$'s may be chosen in such a way that the excitation energies of the operators $\tilde{\alpha}_k$ are lower than the excitation energies of the usual operators $\alpha_k$ cannot be ruled out.
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(49)

(this is because the diagonalization of $\hat{H}$ in terms of the $\alpha_k$ is not exact, but only approximate). However, since we here want to draw a comparison with the standard formulation of Bogoliubov’s theory, we shall proceed to study the diagonalization of $\hat{H}$ in terms of the simple $\alpha_k$ operators, instead of the cumbersome form defined in Eq. (7.47) above, which is not easy to work with.

Let us again define the operators $\alpha_k$ and $\alpha_k^\dagger$ as follows:

$$
\alpha_k = \tilde{u}_k a_k a_0^\dagger + \tilde{v}_k a_0 a_{-k}^\dagger,
$$

(7.48a)

$$
\alpha_k^\dagger = \tilde{u}_k a_k^\dagger a_0 + \tilde{v}_k a_0^\dagger a_{-k}.
$$

(7.48b)

It is easy to verify that the action of $\alpha_k^\dagger$ on the ket $|\Psi(N)\rangle$ gives the following result:

$$
\alpha_k^\dagger |\Psi(N)\rangle = Z \sum_{n_1=1}^\infty \sum_{n_2}^\infty \cdots \sum_{n_M}^\infty C_{n_2} \cdots C_{n_M} \left[ C_{n_1} \tilde{u}_k \right] \left[ \sum_{i=1}^M n_i \right] \left[ N + 1 - 2 \sum_{i=1}^M n_i \right] \langle \Psi(N) | a_{-k}^\dagger a_0 \rangle.
$$

(7.49)

Requiring that $\alpha_k^\dagger |\Psi(N)\rangle = 0$ gives the condition:

$$
\frac{\tilde{u}_k}{\tilde{v}_k} = - \frac{C_{n_1}}{C_{n_1}^*} \sqrt{\frac{\sum_{i=1}^M n_i}{N - 1 - 2 \sum_{i=1}^M n_i}}.
$$

(7.50)

Approximating the square root with unity, we obtain:

$$
\frac{\tilde{v}_k}{\tilde{u}_k} \simeq - \frac{C_{n_1}}{C_{n_1}^*},
$$

(7.51a)

which is the same condition obtained previously for the single-mode case, Eq. (5.49). Proceeding in the same way as in Sec. 5.4, we can determine the constants $\tilde{u}_k$ and $\tilde{v}_k$ by using Eq. (7.51) and the requirement that the excited state $\alpha_k^\dagger |\Psi(N)\rangle$ be normalized to unity, i.e. that:

$$
\langle \Psi(N) | \alpha_k a_k^\dagger |\Psi(N)\rangle = 1.
$$

(7.52)

The above condition leads to the following result for the quantity $\tilde{u}_k^2 - \tilde{v}_k^2$:

$$
\tilde{u}_k^2 - \tilde{v}_k^2 = \gamma_k^2,
$$

(7.53)

where now the quantity $\gamma_k$ is given by (compare with Eq. (5.62)):

$$
\gamma_k^2 = \frac{1}{\langle a_k^\dagger a_0 \rangle - \langle a_k^\dagger a_k \rangle} \approx \frac{1}{\langle a_k^\dagger a_0 \rangle},
$$

(7.54a)

(7.54b)
In the above equations, we denote by \( \langle \cdots \rangle \) the expectation value in the ground state \( | \Psi(N) \rangle \), i.e., \( \langle \cdots \rangle = \langle \Psi(N) | \cdots | \Psi(N) \rangle \). (In Sec. 5.1, \( \gamma_k \) was defined in terms of expectation values in the normalized ground state \( | \tilde{\psi}_k \rangle \) of the single-mode Hamiltonian \( \hat{H}_k \).) Note also that, in going from the first to the second line of Eq. (5.62) we again assumed that \( \langle a_k^\dagger a_k \rangle \ll \langle a_0^\dagger a_0 \rangle \), i.e., that the depletion of the condensate into any single-particle state with momentum \( k \) is small. Using Eqs. (7.51) and (7.53), we now can determine the values of the constants \( \tilde{u}_k \) and \( \tilde{v}_k \). These can be written in the form:

\[
\tilde{u}_k = \gamma_k u_k, \quad \tilde{v}_k = \gamma_k v_k, \tag{7.55a}
\]

\[
u_k = \frac{1}{\sqrt{1 - c_k^2}} \quad v_k = \frac{c_k}{\sqrt{1 - c_k^2}}. \tag{7.55b}
\]

Using the new result (7.19) for \( c_k \) derived in presence of many momentum modes, we finally obtain:

\[
u_k^2 = \frac{1}{2} \left( \frac{\varepsilon_k + n B v(k) + \sigma}{E_k} + 1 \right), \tag{7.56a}
\]

\[
u_k^2 = \frac{1}{2} \left( \frac{\varepsilon_k + n B v(k) + \sigma}{E_k} - 1 \right), \tag{7.56b}
\]

where now the spectrum \( E_k \) is given by the expression:

\[
E_k = n B v(k) \sqrt{Q^2(Q^2 + 2)}. \tag{7.57}
\]

We now use the general expression (A.12) of \( \hat{H}_k \) in terms of the operators \( \alpha_k \) and \( \alpha_k^\dagger \) derived in Appendix A, which we shall rewrite here for definiteness:

\[
\hat{H}_k = \frac{1}{2 \gamma_k^2} \left\{ [A_k(u_k^2 + v_k^2) - 2B_k] (\alpha_k^\dagger \alpha_k + \alpha_k^\dagger \alpha_{-k}) + [B_k(u_k^2 + v_k^2) - 2A_k] (\alpha_k^\dagger \alpha_{-k} + \alpha_k \alpha_{-k}) + [A_k v_k - B_k u_k v_k] (\{[\alpha_k, \alpha_k^\dagger] + [\alpha_{-k}, \alpha_{-k}^\dagger]\}) + (B_k v_k^2 - A_k u_k v_k) ([\alpha_{-k}, \alpha_k^\dagger] + [\alpha_{-k}, \alpha_k]) \right\}, \tag{7.58}
\]

where the constants \( A_k \) and \( B_k \) are given by (the constant \( \eta_k \) is defined in Appendix A):

\[
A_k = \frac{\varepsilon_k + \eta_k}{V}, \quad B_k = \frac{v(k)}{V}. \tag{7.59}
\]

Note that the coherence factors \( u_k \) and \( v_k \) in Eq. (7.58) are now given by the expressions in Eq. (7.59). With that in mind, we want to choose a value for \( \eta_k \) that will make the quantity \( [B_k(u_k^2 + v_k^2) - 2A_k u_k v_k] \) vanish. Using this constraint and Eq. (7.58), we obtain, after a few manipulations:

\[
A_k = B_k \left( \frac{\varepsilon_k + \sigma}{n B v(k) + 1} \right). \tag{7.60}
\]
Using the definitions of $A_k$ and $B_k$ given in Eq. (7.59), we can find the expression of the quantity $\eta_k$, which is now given by:

$$\eta_k = \frac{1}{N} \frac{v(k)}{\bar{v}(k)} \left(1 + \frac{\sigma}{\varepsilon_k}\right). \quad (7.61)$$

We now are in a position to calculate the excitation energy associated with Hamiltonian $\hat{H}_k$, which is the coefficient of the quadratic terms $\alpha_k^\dagger \alpha_k$ and $\alpha_{-k}^\dagger \alpha_{-k}$ in Eq. (7.58) (it can indeed be shown that the last three terms on the rhs of this last equation do not contribute to the excitation energy, see Appendix A), i.e.:

$$\Delta E_{\text{exc}}(k) = \frac{1}{2} E_k = \frac{1}{2} n_B v(k) \sqrt{Q^2(Q^2 + 2)}, \quad (7.62a)$$

$$= \frac{1}{2\gamma_k^2} \left[A_k (u_k^2 + v_k^2) - 2B_k u_k v_k\right]. \quad (7.62b)$$

Using the results (7.19) for the coefficient $c_k$ and (7.61) for the quantity $\eta_k$, along with the definitions (7.56) of the constants $u_k$ and $v_k$, we find, after a few manipulations:

$$\Delta E_{\text{exc}}(k) = \frac{1}{2} E_k = \frac{1}{2} n_B v(k) \sqrt{Q^2(Q^2 + 2)}, \quad (7.63)$$

where we remind the reader that:

$$Q^2 = \frac{\xi_k + \sigma}{n_B \bar{v}(k)}, \quad (7.64a)$$

$$= C_d^{-1} (\tilde{k}^2 + \tilde{\sigma}) \exp(4\pi n_B a \lambda^2 \tilde{k}^2). \quad (7.64b)$$

We again would like to emphasize that $\Delta E_{\text{exc}}(k)$ is the excitation energy associated with the Hamiltonian $\hat{H}_k$. The full Hamiltonian $\hat{H} = \sum_{k \neq 0} \hat{H}_k$ contains an identical contribution $\hat{H}_{-k}$, so that the total energy cost $\Delta E_{\text{exc}}^{\text{tot}}(k)$ to bring the system from its ground state $|\Psi(N)\rangle$ to the excited state $\alpha_k^\dagger |\Psi(N)\rangle$ is given by:

$$\Delta E_{\text{exc}}^{\text{tot}}(k) = \Delta E_{\text{exc}}(k) + \Delta E_{\text{exc}}(-k), \quad (7.65a)$$

$$= n_B v(k) \sqrt{Q^2(Q^2 + 2)}. \quad (7.65b)$$

The above expression of the excitation energy, after a few manipulations, can be written in the form:

$$\frac{\Delta E_{\text{exc}}^{\text{tot}}(k)}{n_B g} = \frac{1}{C_d} \sqrt{(\tilde{k}^2 + \tilde{\sigma})(\tilde{k}^2 + \tilde{\sigma} + 2C_d e^{-4\pi n_B a \lambda^2 \tilde{k}^2})}. \quad (7.66)$$

Again, given the dilute Bose gas parameters we have considered, the exponential $\exp(-k^2 \lambda^2/2)$ is close to unity for the most interesting values of $k$ such that $k \ll \lambda^{-1}$, and hence we can write:

$$\frac{\Delta E_{\text{exc}}^{\text{tot}}(k)}{n_B g} = \frac{1}{C_d} \sqrt{(\tilde{k}^2 + \tilde{\sigma})(\tilde{k}^2 + \tilde{\sigma} + 2C_d)}. \quad (7.67)$$

Notice that the above expression reduces to the usual Bogoliubov spectrum for the single-mode theory in the limit $\tilde{\sigma} = 0$ and $C_d = 1$. In the case where $\tilde{\sigma} \neq 0$, however,
a major feature of the spectrum (7.67) is that it displays a finite gap as $k \to 0$, which is given by:

$$\Delta E_{tot}^{exc}(k=0) = \sqrt{\frac{\sigma}{\sigma + 2 C_d^2}}.$$  (7.68)

For $\sigma = 0.39$, the numerical value of the gap is given by:

$$\Delta E_{tot}^{exc}(k=0) \simeq 0.98 n_B g.$$  (7.69)

This value is comparable to the gap predicted by Hartree-Fock theory, which is given by $\Delta E_{HF}^{exc}(k=0) = n_B g$, and to the gap predicted by Girardeau and Arnowitt a long time ago using a method that is different from the one we employed in the present study.

At this point, we would like to caution the reader that the above result does not by any means imply that the actual excitation spectrum of bosons in a real (experimental) system has to be gapped. It actually only implies that the truncated Hamiltonian of Bogoliubov’s theory has a finite gap in the $k \to 0$ limit when this theory is formulated within a number-conserving framework where an accurate count of the number of bosons in the condensate is kept throughout the calculation. This author would like to make it clear that he is not by any means advocating a gapped excitation spectrum for bosons, but merely presenting what Bogoliubov’s theory predicts for this spectrum when the calculation is performed in a tightly number-conserving fashion. Going back to the Girardeau-Arnowitt number-conserving theory mentioned above, which also predicts the existence of a finite gap in the excitation spectrum, an interesting aspect of this theory is a demonstration that nonpairing “triplet” contributions to the Hamiltonian are of the right order of magnitude to cancel the excitation energy gap. Takano subsequently showed that such cancellation does indeed occur, and it may well be possible that a similar scenario takes place for the variational model studied in this paper if additional terms are included in the Bogoliubov Hamiltonian. While such a scenario cannot, a priori, be ruled
out, our results are still important on their own, because they show that, as far as Bogoliubov’s Hamiltonian is concerned, the conventional excitation spectrum of Bogoliubov’s theory becomes gapped when the calculation is performed in a number-conserving fashion. More work is needed in order to ascertain under what conditions the excitation spectrum of “real” bosons described by the full Hamiltonian of Eq. (2.2) is indeed gapped or not in the $k \to 0$ limit.

§8. Discussion

Having explored the results one obtains for the main physical observables when the full Hamiltonian $\hat{H} = \sum_{k \neq 0} \hat{H}_k$ is diagonalized taking the conservation of boson number into account, we now want to present a brief summary of our results, and discuss the implications of these results on the formulation of Bogoliubov’s theory of an interacting Bose gas.

8.1. Summary of our results

A major goal of this paper has been to clarify the nature and meaning of the standard formulation of Bogoliubov’s theory. Our investigation has shown that this theory seeks to diagonalize each single-mode Hamiltonian $\hat{H}_k$ independently. Comparison with the results of the exact numerical diagonalization of the single-mode Hamiltonian $\hat{H}_k$ has shown that Bogoliubov’s theory gives an astonishingly accurate description of the ground state energy and excitation spectrum of $\hat{H}_k$. While it is true that in a number non-conserving framework, where the $k = 0$ state is removed from the Hilbert space used to describe the system, one can write the ground state wavefunction as a simple product of the ground state wavefunctions of the $\hat{H}_k$’s, and hence diagonalizing the single-mode Hamiltonians $\hat{H}_k$ independently from one another makes sense, in a number-conserving framework diagonalizing the $\hat{H}_k$’s independently is not very helpful, since the ground state wavefunction of $\hat{H} = \sum_{k \neq 0} \hat{H}_k$ cannot in this case be written as a simple product of the ground state wavefunctions of the $\hat{H}_k$’s (the reason this is so is because the Hilbert spaces spanned by these single-mode Hamiltonians have the $k = 0$ state in common). The above observation calls for a more careful diagonalization method where the total Hamiltonian $\hat{H}$ is diagonalized directly. This is what we have attempted to do in this paper by using the fully number-conserving trial wavefunction of Eq. (7.11), and finding the variational coefficients $c_k$ in exactly the same way as in Ref. [34]. It is actually quite on purpose that we have presented the calculation of the ground state energy with such a level of detail, both for the single-mode Hamiltonian $\hat{H}_k$ thereby reproducing all the results of the conventional Bogoliubov theory, and for the total Hamiltonian $\hat{H}$. Comparing the two methods underscores the stark differences between a theory that does enforce the conservation of the total number of bosons $N$ and theories which do not, and shows explicitly that the results of Bogoliubov’s method cannot be obtained when $N$ is conserved between all the momentum modes, but only in a single-mode approach where $N$ is conserved for a single momentum mode. In the following, we shall summarize a few salient results of our variational treatment, and try to discuss how this treatment improves on the standard formulation of Bogoliubov’s method.
1. Divergence of the depletion $\langle a_k^\dagger a_k \rangle$ and of the anomalous average $\langle a_k a_k \rangle$ in the $k \to 0$ limit — As we have seen in Sec. 5.4, imposing the commutation relation $[\alpha_k, \alpha_k^\dagger] = 1$ in the standard, number non-conserving version of Bogoliubov’s theory, both the depletion $\langle a_k^\dagger a_k \rangle$ and the anomalous average $\langle a_k a_k \rangle$ diverge in the $k \to 0$ limit. The use of a number-conserving approach, as we explicitly have shown in Sections 5.2 and 5.3 for the single-mode theory and in Sec. 7.3 in presence of many momentum modes, removes these unphysical divergences and yields results that are always finite for finite $N$.

2. Use of the Hamiltonian $\hat{H}$ instead of $\hat{H} - \mu \hat{N}$ to describe the energy of the system — In addition to removing the unphysical divergences from the quantities $\langle a_k^\dagger a_k \rangle$ and $\langle a_k a_k \rangle$ in the $k \to 0$ limit, the variational method has the advantage of restoring to the Hamiltonian $\hat{H}$ its usual meaning as the operator representing the total energy of the system. As we saw in Sec. 3.2, this is not the case in the conventional formulation of Bogoliubov’s theory, where the role of the energy operator is played by the combination $\hat{H} - \mu \hat{N}$, and where the use of $\hat{H}$ gives rise to nonsensical results.

3. Commutation relations of the $\alpha_k$ operators — An interesting aspect of our investigation is that we have clarified the origin of the commutation relations between the excitation operators $\alpha_k$ and $\alpha_k^\dagger$. Indeed, the number-conserving version of these operators, where $\alpha_k$ is given by:

$$\alpha_k = \gamma_k (u_k a_k a_0^\dagger + v_k a_0^\dagger a_k),$$

obeys the following commutation relations:

$$[\alpha_{-k}, \alpha_k] = [\alpha_{-k}^\dagger, \alpha_k^\dagger] = \gamma_k^2 u_k v_k [a_k^\dagger a_k - a_k^\dagger a_k].$$

$$[\alpha_k, \alpha_k^\dagger] = \gamma_k^2 [a_k^\dagger a_0 - u_k^2 a_k^\dagger a_k + v_k^2 a_k^\dagger a_{-k}].$$

As we have seen in Sec. 5.3, imposing the commutation relation $[\alpha_k, \alpha_k^\dagger] = 1$ is nothing more than a convenient way to ensure that the excited state $\langle \Psi(N) | a_k^\dagger | \Psi(N) \rangle = 1$ is normalized to unity. Given that the rhs of Eq. (8.2b) is an operator and not a c-number, it is not possible to satisfy the commutation relation $[\alpha_k, \alpha_k^\dagger] = 1$ for all possible states in the Hilbert space, and hence for weak perturbations one simply requires that this commutation relation be satisfied in an averaged sense at the ground state, i.e. $\langle \Psi(N) | [\alpha_k, \alpha_k^\dagger] | \Psi(N) \rangle = 1$. This led us to the following condition on the constant $\gamma_k$:

$$\gamma_k^2 = \frac{1}{\langle a_0^\dagger a_0 \rangle - \langle a_k^\dagger a_k \rangle},$$

with the consequence that $u_k$ and $v_k$ verify the identity $u_k^2 - v_k^2 = 1$, much like in Bogoliubov’s approach. It is to be noted that, even in the single-mode theory of Sec. 5.4, the condition (8.3) by itself is not sufficient to recover the Bogoliubov spectrum of excitations, since we also require that the depletion of the ground state into any given momentum mode $k$ be small, $\langle a_k^\dagger a_0 \rangle \gg \langle a_k a_k \rangle$, so that we may write $\gamma_k^2 \simeq 1/\langle a_0^\dagger a_0 \rangle$. Should a situation arise where the depletion of the ground state is no longer small (such as for liquid Helium at very low temperatures, where the
condensate fraction represents only about 10% of the total system, then the full expression of \( \gamma^2 \) given above, Eq. (8.3), has to be used, and there is then no guarantee that the Bogoliubov spectrum will be recovered, even in the single-mode theory of Section 5.4.

4. Single-mode theory: number-conserving variational approach for the single-mode Hamiltonian \( \hat{H}_k \) — As mentioned in the opening paragraph to this subsection, in this paper we have shown that Bogoliubov’s theory corresponds to a decoupled approach in which each single-mode Hamiltonian \( \hat{H}_k \) is diagonalized separately from the other momentum contributions \( \hat{H}_{k'}(\neq k) \). What is more, we have performed an exact numerical diagonalization of the Hamiltonian \( \hat{H}_k \). Comparison of this exact numerical diagonalization and the variational Bogoliubov treatment shows that Bogoliubov’s theory gives spectacularly accurate results for the ground state energy and the excitation spectra of each of the single-mode Hamiltonians \( \hat{H}_k \). However, the results of Bogoliubov’s method for the depletion of the condensate are less accurate, as this method, even in its number-conserving incarnation, overestimates the depletion of the condensate by about one order of magnitude for small values of the wavevector \( k \).

5. Multi-mode theory: variational approach for the full Hamiltonian \( \hat{H} \) — The most important result of this paper, though, has to do with our variational treatment of the full Hamiltonian \( \hat{H} \), instead of the decoupled kind of treatment done in Bogoliubov’s method where each momentum contribution \( \hat{H}_k \) is diagonalized separately. In our variational approach, the \( k = 0 \) state is restored to the Hilbert space used to describe the system (by contrast to Ref. [7] where \( a_0 \) is replaced by \( \sqrt{N} \)), and an accurate count is kept of the number of bosons in the \( k = 0 \) state. As a result, we have shown that the coefficients \( c_k \) which determine the ground state wavefunction of the system are no longer given by the expression (5.22) obtained within the standard Bogoliubov approach. Instead, these coefficients are now given by the alternate expression (7.19), which has the profound consequence of giving rise to a gap in the excitation spectrum of bosons as \( k \to 0 \), by contrast to the excitation spectrum in the standard Bogoliubov theory which is gapless in that limit. Note that, since the geometrical ansatz \( \tilde{C}_n = \sqrt{1 - c_k^2 (-c_k)}^n \) for the coefficients \( \tilde{C}_n \) of the normalized ground state wavefunction \( \tilde{\psi}_k = \sum_{n=0}^{N/2} \tilde{C}_n |n\rangle \) gave such accurate results for the ground state energy of the single-mode Hamiltonian \( \hat{H}_k \), we expect the same ansatz to give equally good results when the variational method is applied to the total Hamiltonian \( \hat{H} = \sum_{k \neq 0} \hat{H}_k \), as we did in this paper.

8.2. A comment on the leading correction to the Gross-Pitaevskii value of the ground state energy of an interacting Bose gas

Several comments are in order concerning the explicit value of the ground state energy of an interacting Bose gas. In the standard Bogoliubov approach, it is claimed that this quantity is given by the expression (we now include the Gross-Pitaevskii
Fig. 15. Plot of the product $k^2 \times \langle \tilde{\psi}_k | \hat{H}_k | \tilde{\psi}_k \rangle$ vs. $k$, as obtained by exact numerical diagonalization of the single-mode Hamiltonian $\hat{H}_k$ for $N = 200$ bosons. Here the wavevector $k$ takes the values $k = 0, 0.01, 0.02, \ldots, 10$. The fact that the product $k^2 \times \langle \tilde{\psi}_k | \hat{H}_k | \tilde{\psi}_k \rangle$ in dimensionless units goes to a constant $-0.25$ at large values of $k$ indicates that $\langle \tilde{\psi}_k | \hat{H}_k | \tilde{\psi}_k \rangle$ goes to zero like $-0.25/k^2$ as $k \to \infty$, hence confirming the result of the analytical Bogoliubov theory for that quantity.

Of course, we now know that the above expression can only be derived in a number non-conserving approach, and is not the correct expression of the ground state energy when the conservation of boson number is taken into account. However, for the sake of argument, let us momentarily ignore this conceptual difficulty, and review how the final expression of the ground state energy for the total Hamiltonian $\hat{H}$ is calculated from Eq. (8.4). In the case where the Fourier components of the interaction potential $v(k)$ are all given by a single constant, $v(k) = g$, corresponding to an interaction potential which is a delta function $v(r) = g\delta(r)$ in real space, the summand in the above expression has the asymptotic form $-n_B^2 g^2/(4\epsilon_k) = -mn_B^2 g^2/(2\hbar^2 k^2)$, and hence the sum diverges in three dimensions. To take care of this divergence, a procedure is devised whereby the coupling constant $g$ is shifted by the infinite (!) quantity $mg^2 \int \frac{d^3k}{(2\pi)^3} (\hbar^2 k^2)^{-1}$, and to compensate for this shift a quantity $+ \int \frac{d^3k}{(2\pi)^3} mn_B^2 g^2/(2\hbar^2 k^2)$ is added to the expression of $E_0$, with the result:

$$E_{Bog} = \frac{1}{2} V n_B^2 v(0) - \frac{1}{2} \sum_{k \neq 0} (\epsilon_k + n_B v(k) - E_k). \tag{8.4}$$

It turns out that the two terms between parentheses on the first line of the above equation represent the first two terms in the expansion of the $s$-wave scattering term $N(N-1)v(0)/2V \simeq N^2 v(0)/2V$ in our equations:

$$E_{Bog} = \frac{1}{2} V n_B^2 v(0) - \frac{1}{2} \sum_{k \neq 0} (\epsilon_k + n_B v(k) - E_k). \tag{8.4}$$

$$E_{Bog} = \frac{1}{2} V n_B^2 v(0) - \frac{1}{2} \sum_{k \neq 0} (\epsilon_k + n_B v(k) - E_k).$$
length $a$ in terms of $g$:

$$\frac{4\pi a^2 \hbar^2}{m} \simeq g - \frac{mg^2}{\hbar^2} \int \frac{d^3k}{(2\pi)^3 k^2} + \cdots. \quad (8.6)$$

As it stands, the above expression, literally speaking, predicts a negatively infinite value of the scattering length $a$ (unless, of course, an ultraviolet cut-off is imposed on the momentum integral in such a way that the second term on the rhs of Eq. (8.6) is smaller than the first, in which case $a$ remains finite and positive; note, however, that if such a cut-off is imposed, then we are no longer dealing with a delta function potential in real space $v(r) = g\delta(r)$, but with an approximate form of the latter).

The result of the above manipulations is that the integral in the second line of Eq. (8.5) is now convergent in three dimensions, and leads to the celebrated result that is quoted in all standard textbooks on many-particle systems, where the final result is expressed not in terms of the original interaction strength $g$, but in terms of the scattering length $a$:

$$E_{Bog} = \frac{2\pi a^2 n_B}{m} \left[ 1 + \frac{128}{15} \left( \frac{n_B a^3}{\pi} \right)^{\frac{1}{2}} \right]. \quad (8.7)$$

Strictly speaking, the leading correction on the rhs of the above equation does not involve the scattering length $a$ defined in Eq. (8.6), but the “bare” counterpart $a_0$ such that $4\pi a_0^2 \hbar^2/m = g$. However, in the limit of a dilute Bose gas where $n_B a \ll 1$, one casually replaces $a_0$ by $a$ (a very questionable replacement, indeed, given that the expression of $a$ contains a divergent integral, see Eq. (8.6)), leading to:

$$E_{Bog} = \frac{2\pi a^2 n_B}{m} \left[ 1 + \frac{128}{15} \left( \frac{n_B a^3}{\pi} \right)^{\frac{1}{2}} \right]. \quad (8.8)$$

At this point, we want to argue that the manipulations leading to Eq. (8.8) are mathematically untenable, for what we simply did is shift the divergence from the sum of the expectation values $\sum_{k \neq 0} \langle \hat{H}_k \rangle_k = \frac{1}{2} \sum_{k \neq 0} (E_k - \varepsilon_k - n_B g)$ to the scattering length $a$ of Eq. (8.6), making the latter a divergent quantity, but the original divergence of the ground state energy has not been actually removed. To clarify what we mean by the above statement, let us give the bare interaction strength $g$ a numerical value, say $g = 1.0 \times 10^{-22} J \cdot A^2$ (this is not a value that is experimentally relevant to any actual system, we just made it up for the sake of argument), and ask what is the numerical value, in Joules, of the ground state energy per particle. The presence of the divergent integral on the rhs of Eq. (8.6) prevents us from giving an answer to this question, and that is what we mean by the statement that the divergence of the ground state energy has not been removed by the mathematically questionable manipulations leading to Eq. (8.8).

In fact, the above manipulations would have been perfectly legitimate had the integral on the rhs of Eq. (8.6) been finite and perturbatively small compared to the bare interaction strength $g$. The fact that this is not the case, and that the integral we just mentioned is actually divergent, makes going from $a_0$ in the correction term on the rhs of Eq. (8.7) to $a$ in Eq. (8.8) very questionable. Furthermore, and
as we mentioned above, including the divergent integral in the definition of the renormalized scattering length $a$, Eq. (8.6), merely shifts the divergence to this last quantity. In terms of the bare scattering length $a_0$, or the bare interaction strength $g$, the ground state energy is still a divergent quantity (since $a$ itself is infinite according to Eq. (8.6)), and hence we see that, strictly speaking, the manipulations leading to Eq. (8.8) did not actually remove the original divergence of the ground state energy of the system from Eq. (8.4).

We now would like to pause for a moment, and plot the product $\tilde{k}^2 \langle \hat{H}_k \rangle_k$ as obtained from the exact numerical diagonalization of the Hamiltonian $\hat{H}_k$ as a function of the wavevector $k$. This plot, given in Fig. 16, shows that the above product goes to $-0.25$ at large values of $k$, implying that the exact numerical result for $\langle \hat{H}_k \rangle_k$ goes to zero like $-\frac{0.25}{k^2}$ as $k \to \infty$, in agreement with the result of Bogoliubov’s theory. Unlike divergences that appear in other physical theories (e.g. the divergence of the perturbative expansion of $\phi^4$-type models) which can be shown to be artificial divergences and therefore need to be removed, we here are in the opposite situation where the divergence of the sum $\sum_{k \neq 0} \langle \hat{H}_k \rangle_k$ when $v(r) = g\delta(r)$ is not artificial at all, but on the contrary is part and parcel of the exact diagonalization of the Hamiltonians $\hat{H}_k$. Hence, this is a divergence which should not be tampered with and cannot be removed because it corresponds to the correct behavior of the quantity $\sum_{k \neq 0} \langle \hat{H}_k \rangle_k$ when a delta function interaction between bosons is assumed.

With that said, the whole discussion above is somewhat irrelevant, because the correct ground state energy of an interacting Bose gas, when the full Hamiltonian $H$ is diagonalized properly, is not given by Eq. (8.4). Indeed, in the improved variational procedure of Sec. 7 the ground state energy does not diverge like $-n_B^2 g^2/(4\varepsilon_k) = -0.25n_B^2 g^2/\varepsilon_k$, but rather like $-0.25C_3^2 n_B^2 g^2/\varepsilon_k$ (see Fig.
Re-examining Bogoliubov’s theory of an interacting Bose gas

which makes the whole procedure described above (consisting of adding and substracting the quantity \(-n_B g^2/(4\varepsilon_k)\)) of no great help. The root cause of the divergence of the ground state energy being the delta function form of the interaction potential, one should really only consider more realistic interactions whose Fourier transform falls off at high momentum, hence making the integral giving the ground state energy convergent. In this case, the correction to the Gross-Pitaevskii energy \(v(0)N(N-1)/2V\), expressed in terms of bare coupling constants, will be negative, as it should, and not confusingly positive as in Eq. (8.8).

8.3. Do the operators \(\alpha_k^\dagger\) really create collective sound waves?

We now turn our attention to the \(\alpha_k^\dagger\) operators, and discuss the validity of interpreting these operators as creation operators for collective phonon modes in view of the fact that the spectrum of these excitations, when the Hamiltonian is properly diagonalized in a number-conserving framework, is no longer gapless as is the case in the standard formulation of Bogoliubov’s method. To gain a little more perspective, let us remind ourselves of how phonon modes are defined in the case of a periodic monoatomic crystal. If we denote by \(\hat{d}(x)\) the second-quantized operator describing the displacement of atoms from their equilibrium locations, then we can write:

\[
\hat{d}(x) \propto \sum_k \left( \frac{\hbar}{2\omega_k V} \right)^{\frac{1}{2}} \frac{k}{k} [\beta_k e^{ik \cdot x} - \beta_k^\dagger e^{-ik \cdot x}],
\]

where \(\omega_k = ck\) (c being the speed of sound in the crystal), and where \(\beta_k^\dagger\) and \(\beta_k\) create and annihilate a phonon mode of wavevector \(k\), respectively. We thus see that the \(\beta_k\)'s are related to the displacement field of the atoms, and it would be rather awkward to try to relate these operators to the operators which describe adding or removing one atom from the system. Yet, this is exactly how the \(\alpha_k\)'s are defined in Bogoliubov’s theory, where these operators are usually interpreted in terms of phonon modes, even though they are not related to an actual displacement field, i.e. to a density fluctuation, but merely describe adding or removing a boson from the system. In the two paragraphs that follow, we want to argue that, whether it be from the perspective of the standard, number non-conserving formulation of Bogoliubov’s theory, or from the perspective of a number-conserving approach, the \(\alpha_k\)'s do not represent collective density oscillations involving all momentum modes, i.e. phonons, but correspond to single momentum mode excitations instead.

8.3.1. Nature of the \(\alpha_k\)'s in the standard, number non-conserving Bogoliubov approach

Let us discuss the nature of the excited modes \(\alpha_k\) and \(\alpha_k^\dagger\) that are defined in the standard, number non-conserving formulation of Bogoliubov’s theory. For definiteness, let us rewrite the expressions of these operators in terms of the boson creation and annihilation operators:

\[
\alpha_k = u_k a_k + v_k a_{-k}^\dagger, \quad \alpha_k^\dagger = u_k a_k^\dagger + v_k a_{-k}.
\]
From the above equations, we see that $\alpha_k^\dagger$ annihilates a single boson of momentum $-k$ with probability $v_k$, and creates a single boson of momentum $k$ with probability $u_k$. As we already mentioned above, given that $\alpha_k^\dagger$ does not act on the condensed bosons, nor does it act on the depleted bosons with momentum $k' \neq k$, it is very surprising that the state $\alpha_k^\dagger\ket{\Psi_B}$ has come to be interpreted as a phonon, the latter being a macroscopic excitation involving all the bosons in the system. As the expression of $\alpha_k$ and $\alpha_k^\dagger$ clearly shows, these operators represent physical processes involving at most two bosons, and can therefore hardly be described as “collective excitations”, or “phonons”. Another way to see this is to consider the following excited wavefunctions:

$$|\Phi_k^{(n)}\rangle = \left(\alpha_k^\dagger\right)^n\sqrt{n!}\ket{\Psi_B}, \quad (8.11a)$$
$$|\Psi_k^{(n)}\rangle = C_k^{(n)}\left(u_k\alpha_k^\dagger - v_k\alpha_{-k}\right)^n\ket{\Psi_B}. \quad (8.11b)$$

Conventional wisdom teaches us that these are two very different states: $|\Phi_k^{(n)}\rangle$ being a state with $n$ “collective phonon modes”, while the state $|\Psi_k^{(n)}\rangle$ of Eq. (8.11b) represents a state where $n$ bosons have been added to the Bogoliubov ground state. A closer look, however, reveals that these two states are actually identical, and correspond to the same quantum state obtained by adding $n$ bosons of momentum $k$ to the Bogoliubov ground state. Indeed, using the fact that $a_{-k}^\dagger = u_k\alpha_k^\dagger - v_k\alpha_{-k}$, and the fact that the operators $\alpha_k^\dagger$ and $\alpha_{-k}$ commute, we can write:

$$|\Psi_k^{(n)}\rangle = C_k^{(n)}\left[u_k\alpha_k^\dagger - v_k\alpha_{-k}\right]^n\ket{\Psi_B}, \quad (8.12a)$$
$$= C_k^{(n)}\sum_{m=0}^{n} \frac{n!}{m!(n-m)!}(u_k\alpha_k^\dagger)^m(-v_k\alpha_{-k})^{n-m}\ket{\Psi_B}. \quad (8.12b)$$

Now, given that $\alpha_k\ket{\Psi_B} = 0$ for all values of the wavevector $k$, we see that all terms in the above summation vanish, except for the term $m = n$, which gives:

$$|\Psi_k^{(n)}\rangle = C_k^{(n)}(u_k\alpha_k^\dagger)^n\ket{\Psi_B}. \quad (8.13)$$

Requiring that $|\Psi_k^{(n)}\rangle$ be normalized to unity results in the following value of the constant $C_k^{(n)}$:

$$C_k^{(n)} = \frac{1}{u_k^n\sqrt{n!}}. \quad (8.14)$$

upon which Eq. (8.13) becomes:

$$|\Psi_k^{(n)}\rangle = \frac{(\alpha_k^\dagger)^n}{\sqrt{n!}}\ket{\Psi_B} = |\Phi_k^{(n)}\rangle. \quad (8.15)$$

This proves our earlier claim that the states $|\Psi_k^{(n)}\rangle$ and $|\Phi_k^{(n)}\rangle$ correspond to the same quantum state. Eq. (8.15) is an important result, which shows that a state of the form $|\Phi_k^{(1)}\rangle = \alpha_k^\dagger\ket{\Psi_B} = \frac{u_k}{u_k}\alpha_k^\dagger\ket{\Psi_B}$ does not represent a collective phonon mode at all, and represents merely a state with one extra boson of momentum $k$ added to the Bogoliubov ground state.
8.3.2. Nature of the $\alpha_k$’s in the variational, number-conserving Bogoliubov formulation

We now want to discuss the nature of the $\alpha_k$ excitations from the point of view of the variational formulation of Bogoliubov’s theory discussed in Section 7.2. In this formulation, $\alpha_k$ is defined by Eq. (7.48), and we therefore have for $\alpha_k^\dagger$ the following expression:

$$\alpha_k^\dagger = \tilde{u}_k a_k^\dagger a_0 + \tilde{v}_k a_{-k} a_0^\dagger. \tag{8.16}$$

As we already discussed in Sec. 5.4, the two terms on the rhs of the above equation represent the two different ways the system can be excited from the ground state $|\Psi(N)\rangle$, which is an eigenstate of the total momentum operator $\hat{P}$ with eigenvalue 0, to a state with momentum $+k$. Again here, we can express $a_k^\dagger a_0$ in terms of the $\alpha_k$’s, with the result (see Eq. (A.6) of the Appendix):

$$a_k^\dagger a_0 = \frac{1}{\gamma_k} [u_k \alpha_k^\dagger - v_k \alpha_{-k}]. \tag{8.17}$$

Let us apply the operator on the lhs of the above equation to the ground state $|\Psi(N)\rangle$ of the operator $\hat{H}$. We have:

$$a_k^\dagger a_0 |\Psi(N)\rangle = \frac{1}{\gamma_k} [u_k \alpha_k^\dagger - v_k \alpha_{-k}] |\Psi(N)\rangle,$n

$$= \frac{v_k}{\gamma_k} \alpha_k^\dagger |\Psi(N)\rangle, \tag{8.18}$$

where, in going from the first to the second line, we used the fact that $\alpha_{-k} |\Psi(N)\rangle = 0$. As it can be seen from this last equation, the quantum state $\alpha_k^\dagger |\Psi(N)\rangle$ is identical to the state $a_k^\dagger a_0 |\Psi(N)\rangle$. Since the latter represents a state where one boson has been removed from the condensate and a boson has been added to the single-particle state with momentum $k$, we conclude here again that the operator $\alpha_k^\dagger$, when applied to the ground state $|\Psi(N)\rangle$, does not create a collective sound wave (of the kind that would be created by shaking the walls of the container, or varying the parameters of the confining potential in a trapped system — that is after all how a sound wave would be created experimentally — in which case all modes of the system would be excited in a collective way, not just one momentum mode as is the case here), and merely promotes a single boson from the condensate with single-particle momentum $k = 0$ to the state with single-particle momentum $+k$.

To summarize this subsection, we conclude that the gapless phonon-like spectrum of the $\alpha_k^\dagger$ operator in the standard Bogoliubov method, which in effect creates excited states for the single-mode Hamiltonian $\hat{H}_k$, has no particular physical meaning in terms of travelling sound waves. Successive application of the operator $\alpha_k^\dagger$ to the ground state $|\psi_k\rangle$ of the Hamiltonian $\hat{H}_k$ merely adds bosons to the single-particle state $e^{ikx}/\sqrt{V}$ with momentum $+k$, and hence the corresponding excitations are in no way collective, and cannot be identified as sound waves, as they routinely are in the literature. This conclusion is corroborated by the results we obtained in Sec. 7.5 where we have shown that, when the $k = 0$ state is restored into the Hilbert
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space used to describe the system and the conservation of the number of bosons is properly taken into account, the spectrum of the \( \alpha_k \) operators has a gap in the long wavelength limit \( k \to 0 \) and cannot therefore be interpreted as a propagating density disturbance corresponding to a collective sound wave. (Incidentally, it is quite instructive to recall that in the BCS theory of superconductivity, the elementary excitation operators are defined in a way that is very similar to how the \( \alpha_k \)'s are defined in Bogoliubov’s method. Yet, in BCS theory, the \( \alpha_k \) are not described as phonons, but are instead correctly identified as single-particle excitations.)

8.3.3. Proper description of phonon modes in interacting Bose systems

Having argued that the \( \alpha_k \)'s do not represent collective phonons, one may wonder how to properly describe density fluctuations in the Bose gas. It turns out that the operator generating a density excitation of wavevector \( q \) is nothing but the \( q \)-mode fluctuation of the density \( \rho(r) \):

\[
\hat{\rho}_q = \frac{1}{\sqrt{V}} \int dr e^{i q \cdot r} \rho(r).
\]

(8.19a)

\[
= \frac{1}{\sqrt{V}} \sum_k a_{q+k}^\dagger a_k.
\]

(8.19b)

Hence, the correct phonon mode of the system at wavevector \( q \) is the one given by the following wavefunction:

\[
|\Psi_q(N)\rangle = \hat{\rho}_q |\Psi(N)\rangle,
\]

(8-20)

where \( |\Psi(N)\rangle \) is the ground state wavefunction of the system. Now, it is a well-known result that the expectation value of the Hamiltonian in the above state is given by

\[
E^{(1)}_q = E_0 + \frac{\langle \Psi_q | H | \Psi_q \rangle}{\langle \Psi_q | \Psi_q \rangle} = E_0 + \frac{\hbar^2 q^2}{2mS_q},
\]

(8.21)

where \( E_0 \) is the ground state energy and \( S_q \) is the static structure factor of the system:

\[
S_q = \frac{1}{n_B} \langle \Psi(N) | \hat{\rho}_q^\dagger \hat{\rho}_q | \Psi(N) \rangle.
\]

(8.22)

For a system of bosons, it has been established long ago by Feynman on quite general grounds that the structure factor \( S_q \) varies linearly with \( q \), \( S_q \sim q \), as \( q \to 0 \), which in turns allows us to conclude that the excitation energy \( \Delta E_q = E^{(1)}_q - E_0 \) of the state \( |\Psi_q\rangle \) also varies linearly with \( q \) in the \( q \to 0 \) limit:

\[
\Delta E_q \sim q \quad \text{as} \quad q \to 0.
\]

(8-23)

We therefore conclude that the gapless phonon modes are those given by the wavefunction in Eq. (8-20). Given the expression (8.19b) of the \( q \)-mode density fluctuation \( \hat{\rho}_q \), we see that a gapless mode is obtained from the ground state \( |\Psi(N)\rangle \) by using a linear combination of creation and annihilation operators \( \sim \sum_k a_{q+k}^\dagger a_k \).
where the sum extends over all wavevectors $k$, and not simply a truncated sum over a single wavevector $q$ as is the case in the definition of the operators $\alpha_k$. This is consistent with our previous conclusion that the $\alpha_k$’s represent single momentum mode excitations whose spectrum can have a gap as $q \to 0$, much like the analogous operators in BCS theory, while the more general modes $\hat{\rho}(q)|\Psi(N)\rangle$ are collective density excitations involving all momentum modes in the system, with a gapless excitation spectrum in the $q \to 0$ limit.\(^{11,17}\)

It is interesting at this point to examine whether the standard formulation of Bogoliubov’s theory is in agreement with Feynman’s approach reviewed above. To this end, let us calculate the excitation spectrum of Eq. (8.21) and see if we indeed obtain a linear spectrum in the $q \to 0$ limit. By using the expression of $a_k$ in terms of the $\alpha_k$’s, Eq. (2.6), to express the local density operator $\hat{\rho}(q)$ in terms of the $\alpha_k$’s, and using the quadratic expression (2.11) of the Bogoliubov Hamiltonian in terms of these same operators, one easily obtains, after a straightforward calculation:

$$E^{(1)}_q = \frac{\langle \Psi(N)|\hat{\rho}_q^\dagger \hat{H} \hat{\rho}_q |\Psi(N)\rangle}{\langle \Psi(N)|\hat{\rho}_q^\dagger \hat{\rho}_q |\Psi(N)\rangle} \sum_{k \neq 0} (u_k^2 + u_{k+q}^2 + u_k u_{k+q} v_k v_{k+q}) \sum_{k \neq 0} (u_k^2 + u_{k+q}^2 + u_k u_{k+q} v_k v_{k+q}). \quad \text{(8.24a)}$$

We thus obtain that the excitation spectrum $\Delta E_q = E^{(1)}_q - \hat{E}_2$ of the state $|\Psi_q\rangle$ in Bogoliubov’s theory has a nonzero limiting value as $q \to 0$, given by:

$$\Delta E_{q \to 0} = 2 \sum_{k \neq 0} \frac{E_k u_k^2 v_k^2}{\sum_{k \neq 0} u_k^2 v_k^2} + o(q^2). \quad \text{(8.25)}$$

We therefore see that Bogoliubov’s theory does not reproduce the phonon spectrum, in the sense that the spectrum of the correct phonon mode $|\Psi_q\rangle$ has a finite gap in the $q \to 0$ limit, a result which may be attributed\(^{23}\) to the fact that Bogoliubov’s Hamiltonian is a truncated approximation to the full many-body Hamiltonian for which Feynman’s argument, Eq. (8.21), holds. Hence, for that reason we expect our number-conserving formulation of Bogoliubov’s theory to give a result that is similar to the one in Eq. (8.25), which is not necessarily gapless as $q \to 0$.

8.4. **Comment on the apparent violation of the Hugenholtz-Pines and Goldstone theorems**

We now want to address the criticism that will inevitably be made about the fact that the variational theory presented in this paper predicts an excitation spectrum which seems to violate the celebrated Hugenholtz-Pines\(^{8}\) and Goldstone\(^{42,43}\) theorems. As it has been observed in Ref.\(^{23}\), a finite gap, which appears almost inevitably in number-conserving descriptions of interacting bosons, does not in any way indicate an internal inconsistency in such theories. In the previous section we have argued that it is not correct to identify the $\alpha_k$’s as the collective phonon modes of the system, and in the present section we shall argue that the presence of a finite gap in the spectrum of the $\alpha_k$ excitations does not in any way imply the violation of...
the Goldstone theorem in our approach. But, before that, we shall start by briefly

discussing the apparent violation of the Hugenholtz-Pines theorem.

8.4.1. Apparent violation of the Hugenholtz-Pines theorem

In its simplest expression, the HPT states that the zero wavevector and zero

frequency limit of the diagonal and off-diagonal self-energies, \( \Sigma_{11}(k, \omega) \) and \( \Sigma_{12}(k, \omega) \)

respectively, are related to the chemical potential \( \mu \) through the equation:

\[
\hbar \Sigma_{11}(0, 0) - \hbar \Sigma_{12}(0, 0) = \mu. \tag{8.26}
\]

In the standard field-theoretic formulation of Bogoliubov’s theory an immediate con-

sequence of this theorem is the emergence of an excitation spectrum which does not

have a gap as \( k \to 0 \). In the formalism presented in this paper, however, a finite gap

is found, which can be seen as an indication that our variational theory violates the

HPT.

As an answer to this potential criticism, we shall note that the HPT has only been

established in the number non-conserving field-theoretic formulation of Bogoliubov’s

theory. Whether this theorem holds in number-conserving situations is far from

obvious, and is not, by any means, guaranteed. It is in fact perfectly conceivable

that a number-conserving field-theoretic formulation of the theory of interacting

bosons may not satisfy the same Hugenholtz-Pines theorem satisfied by the number

non-conserving version, in such a way that the excitation spectrum resulting from

the modified Hugenholtz-Pines theorem for the number-conserving theory is not

inconsistent with the excitation spectrum derived in the present study. To construct

a number-conserving field theory for interacting bosons is, however, a nontrivial

exercise. What is more, to obtain an equivalent to the Hugenholtz-Pines theorem

in such a theory may not even be possible in the first place, given that a number-

conserving theory would most likely not require the introduction of the off-diagonal

self energy \( \Sigma_{12}(k, \omega) \) which appears in the HPT. Making any further speculation

about this issue is far beyond the scope of this paper, and we shall therefore content

ourselves with the observation made at the beginning of this paragraph about the

fact that the HPT was established within a number non-conserving framework. As

a result, any claim about our variational theory being in violation of the HPT would

be totally unfounded, since this theory is a number-conserving one, and we simply

have no idea how one can write down an appropriate generalization of the HPT that

would be valid in number-conserving situations.

8.4.2. Apparent violation of the Goldstone theorem

Before we proceed to discuss the apparent violation of the Goldstone theorem

in our approach, we first want to digress on the applicability of this theorem to the

standard formulation of Bogoliubov’s theory. Using the expression of the operator

\( a_k \) in terms of the field operator \( \Psi(r) \):

\[
a_k = \int d r \Psi(r) \frac{e^{-ik \cdot r}}{\sqrt{V}}, \tag{8.27}
\]
the (truncated) Bogoliubov Hamiltonian \( \hat{H} = H_0 + \hat{H}_2 \) of Eq. 23:

\[
\hat{H} = \frac{1}{2} V n_0^2 v(0) + \sum_{k \neq 0} \left\{ \xi_k a_k^\dagger a_k + \frac{1}{2} n_0 v(k) \left[ a_k^\dagger a_{-k}^\dagger + a_k a_{-k} \right] \right\}
\]

(8-28)

can be rewritten in the form (note that \( v(0) \) still denotes the value of \( v(k) \) at \( k = 0 \)):

\[
\hat{H} = \frac{1}{2} V n_0^2 v(0) + \int d\mathbf{r} d\mathbf{r}' \Psi^\dagger(\mathbf{r}) \left[ \left( -\frac{\hbar^2 \nabla^2}{2m} + n_0 v(0) \right) \delta(\mathbf{r} - \mathbf{r}') + v(\mathbf{r} - \mathbf{r}') \right] \Psi(\mathbf{r}')
\]
\[
+ \frac{1}{2} n_0 \int d\mathbf{r} d\mathbf{r}' \left[ \Psi^\dagger(\mathbf{r}) v(\mathbf{r} - \mathbf{r}') \Psi^\dagger(\mathbf{r}') + \Psi(\mathbf{r}) v(\mathbf{r} - \mathbf{r}') \Psi(\mathbf{r}') \right]
\]
\[
- \frac{1}{2} n_0 v(0) \int d\mathbf{r} d\mathbf{r}' \left[ \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}') + \Psi(\mathbf{r}) \Psi(\mathbf{r}') + 4 \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}') \right].
\]

(8-29)

From this last equation, we see that the two terms on the second line and the first two terms on the third line are not invariant under the transformation \( \Psi(\mathbf{r}) \to \Psi(\mathbf{r}) e^{i\theta} \). Hence, the central premise of Goldstone’s theorem as applied to Bose systems, requiring that the Hamiltonian be invariant under global gauge transformations, is not satisfied in the standard Bogoliubov model (this is of course a direct consequence of Bogoliubov’s prescription of replacing \( a_0 \) by an “inert” c-number). One is therefore led to wonder whether Goldstone’s theorem is even applicable to the standard Bogoliubov model in the first place, and whether it is legitimate at all to interpret the gapless nature of the spectrum of the \( a_0 \) excitations as having anything to do with the alleged breakdown of the global \( U(1) \) gauge symmetry in this system.

We now turn our attention to the applicability of Goldstone’s theorem to our variational model. Here, because \( a_0 \) and \( a_0^\dagger \) are not replaced by a c-number, one can easily verify that the Bogoliubov Hamiltonian of Eq. (17) is actually invariant under the transformation \( \Psi(\mathbf{r}) \to \Psi(\mathbf{r}) e^{i\theta} \). The question now is to know whether the second premise of Goldstone’s theorem is satisfied, namely, whether our variational ground state breaks the gauge invariance of the Hamiltonian. Indeed, unless the ground state of the system breaks a continuous invariance of the Hamiltonian, a gapless mode does not necessarily exist. A case in point is provided by the Hartree-Fock Hamiltonian:

\[
\hat{H}_{HF} = \frac{v(0)}{2V} N (N - 1) + \sum_{k \neq 0} \varepsilon_k a_k^\dagger a_k + \frac{1}{2V} \sum_k \sum_{k' \neq k} v(k - k') a_k^\dagger a_k a_{k'}^\dagger a_{k'}.
\]

(8-30)

It is easy to verify that the kets given by (note that we here no longer explicitly distinguish between \( k \) and \( -k \)):

\[
|\Psi_{HF}(\{n_i\})\rangle = |N - \sum_{i=1}^\infty n_i; n_1; \ldots; n_\infty\rangle,
\]

\[
= \frac{(a_0^\dagger)^{N-\sum_i n_i} \prod_{i=1}^\infty (a_k^\dagger)^{n_i}}{\sqrt{(N-\sum_i n_i)! \prod n_i!}} |0\rangle,
\]

(8-31)
are exact eigenfunctions of the Hamiltonian $H_{HF}$ with the exact eigenvalues:

$$E_{HF}(\{n_i\}) = \frac{v(0)}{2V}N(N-1) + \sum_{i=1}^{\infty} n_i \epsilon_{k_i} + \frac{1}{2V} \sum_{i=1}^{\infty} \sum_{j \neq i} v(k_i - k_j)n_in_j.$$  \hspace{1cm} (8.32)

Assuming for simplicity that the Fourier transform $v(k)$ is positive for all values of the wavevector $k$, one can easily show that the ground state of $\hat{H}_{HF}$ is given by the state where all the bosons are condensed in the $k = 0$ single-particle state:

$$|\Psi_{HF}(N)\rangle = |N; 0, 0, \ldots\rangle.$$ \hspace{1cm} (8.33)

This state does not break the $U(1)$ gauge symmetry of the original Hamiltonian, in the sense that the action of the generator $\hat{U}(\theta) = \exp(i\theta\hat{N})$ on $|\Psi_{HF}(N)\rangle$ does not create a distinct degenerate ground state, but merely multiplies $|\Psi_{HF}(N)\rangle$ by the trivial overall constant $\exp(i\theta N)$. We therefore find ourselves in a situation where a Goldstone mode does not necessarily exist, and it is indeed found that there is a finite energy gap to any single-particle excitation of the system outside of its ground state. The variational ground state studied in this paper presents us with a very analogous situation, since it too does not break the $U(1)$ gauge symmetry (in the sense explained above), and hence is not bound to verify Goldstone’s theorem.

Having noted the above, we also note that Goldstone bosons do not always emerge in the excitation spectra of many-body systems even when a continuous symmetry is spontaneously broken. A prominent example with a strong analogy to our system is provided by the BCS theory of neutral (atomic) Fermi superfluids, where a continuous (gauge) symmetry is spontaneously broken, and yet the spectrum of the Hamiltonian has a finite gap $\Delta \neq 0$ in the $k \to 0$ limit. In this particular system, a sharp distinction is made between the spectrum obtained by diagonalizing the Hamiltonian, which is identified as one describing single-particle excitations, and the gapless Bogoliubov-Anderson density oscillations, which are identified as the correct Goldstone modes of the system. A similar line of thought has been pursued for interacting bosons in Ref. 47, where it has been argued that the spectrum of interacting bosons should have two branches: a single-particle branch, obtained by diagonalizing the Hamiltonian, which may have a gap, and a collective, gapless branch corresponding to density fluctuations, which emerges as the pole of the density-density correlation function. A similar conclusion has been reached by Kita, who in a series of recent articles has examined the nature of Goldstone bosons in an interacting Bose system using a careful analysis of the field-theoretic perturbation expansions for the one- and two-particle Green’s functions. A major reason why it is generally accepted that the Bogoliubov spectrum describes the collective Goldstone mode of an interacting Bose system is that this spectrum determines the poles of both one- and two-particle Green’s functions, as was claimed by Gavoret and Nozières, and reproduced by the dielectric formalism. Kita has argued that, since these theories were based on separate perturbative expansions for the one- and two-particle Green’s functions, they may suffer from ambiguities in how to define self-energies and vertices in presence of interactions having only a single quasiparticle
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channel, as is the case with the single-component Bose gas. To address this difficulty, Kita has reinvestigated the perturbative treatment\textsuperscript{48, 49} of both Green’s functions within a unified framework, whereby the two-particle Green’s function can be obtained from its one-particle counterpart by functional differentiation with respect to an additional potential. The result that emerged from these investigations was that single-particle excitations as described by the pole of the one-particle Green’s function are subject to severe damping effects, while the Goldstone mode exists as an isolated pole of the two-particle Green’s function\textsuperscript{50}. This conclusion, along with the conclusion of Ref. 47, suggests that one may have to look for gapless modes in collective density perturbations, just as is the case in BCS theory of neutral superfluids, and not necessarily in the poles of the single-particle Green’s function.

We conclude this subsection by noting that although the phonon modes associated with density perturbations as described by Feynman’s wavefunction and the poles of the two-particle Green’s functions of the interacting Bose system are supposed to describe the same physical phenomenon of propagating phonon waves, the deep connection between the two formalisms still needs to be elucidated. Such an elucidation would undoubtedly help us understand why and under what conditions gapped modes can exist, and how gapless modes can be meaningfully incorporated in theoretical descriptions of condensed Bose systems.

8.5. Consequence on field-theoretic formulations of Bogoliubov’s theory

We now would like to make a brief comment on the field-theoretic formulations of Bogoliubov’s method, both at $T = 0$ and at finite temperatures. It is important to realize that the field-theoretic formulations currently in use in the literature (see for example Ref. 20 and references therein) are based on the Bogoliubov ground state, which is a simple product of the individual ground states of the single-mode Hamiltonians $\hat{H}_k$, as in Eq. (7·4). Needless to say, the Green’s and spectral density functions will have a completely different structure when the field theory is formulated using the ground state discussed in this paper as a starting point. As a result, various other quantities, such as density-density correlation functions\textsuperscript{17} and the damping of quasiparticle excitations\textsuperscript{20} may end up having expressions that are qualitatively very different from those derived within the standard, number non-conserving Bogoliubov approximation.

With that said, it would also be interesting to probe whether our variational ground state can be reproduced using path integration methods. Path integrals have emerged as an elegant and powerful tool to study many-body systems, and a successful formulation in terms of path integrals which is able to describe the ground state studied in this paper may help put the Green’s function formalism of interacting bosons at finite temperatures on a firmer ground.\textsuperscript{51} However, such a path-integral formulation may technically prove to be difficult to achieve, since it would most likely require going beyond standard Gaussian integration.
8.6. Recent literature on number-conserving formulations of Bogoliubov’s theory

Before we conclude, we want to briefly discuss recent attempts to overcome the difficulties that arise due to the non-conservation of particle number in Bogoliubov’s theory, as our paper would be rather incomplete without such a discussion. One notable such attempt is the interesting work of Castin and Dum, Ref. [28], where the ground state of the interacting Bose system is found by writing the field operator $\hat{\psi}(r)$ as a sum of a condensate contribution $\phi_0(r)a_0$ and a contribution $\delta\hat{\psi}(r)$ from the $k \neq 0$ states:

$$\hat{\psi}(r) = \phi_0(r)a_0 + \delta\hat{\psi}(r),$$  \hspace{1cm} (8.34)

where $\phi_0(r)$ denotes the wavefunction of the condensed bosons. Then, the quantity $\delta\hat{\psi}(r)$ is treated as a perturbation with respect to the condensate part $\phi_0(r)a_0$, an approximation which is expected to be valid for a dilute Bose gas. Imposing a condition of the form:

$$\alpha_k |\Psi\rangle = 0,$$

where $|\Psi\rangle$ is the ground state wavefunction of the system and $\alpha_k$ is a parameter, and performing a systematic expansion in the small parameter $\varepsilon = \sqrt{N_d/N_0}$ (with $N_d$ being the total number of depleted bosons) allows one to recover the results of Bogoliubov’s theory for the depletion of the condensate and the excitation spectrum of the system. Overall, the approach presented in this work is quite thoughtful, and has the advantage of providing a clean derivation of the standard Bogoliubov results that overcomes the need to break the U(1) symmetry, hence showing that this universally accepted paradigm is not by any means required to describe condensed Bose systems. By trying to keep the conservation of the total number of bosons intact, it avoids many pitfalls of the conventional Bogoliubov method. There is a reason, however, why this approach yields Bogoliubov-type results instead of the results found in the present study. This reason has to do with a number of approximations that are made at a few key steps of the calculation, and more specifically the approximation which consists in replacing the combination $a_0^\dagger a_0$ by the total number of bosons $N$. This approximation being, to a certain extent, equivalent to Bogoliubov’s prescription, it is not at all surprising that Bogoliubov’s results are recovered. By contrast, in our variational approach, no such approximation is used, and great care is exercised in order to keep track of the exact number of bosons ($N - 2 \sum_{i} n_i$) in the condensate (see Appendix B). The sharp distinction between using the approximation $a_0^\dagger a_0 \simeq N$ on one hand, and using $a_0^\dagger a_0 = (N - 2 \sum_{i} n_i)$ on the other hand, is what leads to the differing results between the two methods.[22]

We now want to comment on the variational approach used by Leggett in Ref. [34], an approach which has been a major inspiration for the present study. In this approach, the ground state wavefunction of the system is given by (see Eq. (8.9) of Ref. [34]):

$$\Psi_N = N^{-1/2} \left( a_0^\dagger a_0^\dagger - \sum_{k>0} c_k a_k^\dagger a_{-k}^\dagger \right)^{N/2} |0\rangle.$$  \hspace{1cm} (8.35)

Although the way this wavefunction is written is different from the way we wrote the wavefunction in Eq. (7.11), a closer look reveals that these two wavefunctions are in
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Fact similar to each other in that both represent an expansion in terms of the basis states $|N - 2 \sum_i n_i; n_1, n_1; \ldots; n_i, n_i; \ldots \rangle$. In the course of the calculation, however, and in order to find the expectation value of the single-mode Hamiltonian $\hat{H}_k$ in the Bogoliubov ground state, Leggett only retains the following part of $\Psi_N$ (see Eq. (8.15) of Ref. [34]):

$$\Psi_k = N!^{-1/2}(1 - c_k^2)^{1/2} \left( a_0^\dagger a_0 - c_k a_k^\dagger a_{-k}^\dagger \right)^{N/2} |0\rangle.$$  

(8.37)

This is exactly the ground state wavefunction (5.1) of the single-mode Hamiltonian $\hat{H}_k$, which we call $|\tilde{\psi}_k\rangle$ in our manuscript. By contrast to the wavefunction given in Eq. (8.36) above, the variational wavefunction in Eq. (8.37) does not take into account the fact that the number of bosons in the condensate is given by $(N - 2 \sum_i n_i)$. Hence, this variational calculation uses the same kind of approximation we discuss in Sec. 5, in which the variational constants $c_k$ correspond to minimizing the energy of each single-mode Hamiltonian $\hat{H}_k$ independently from one another. Again, since the $k = 0$ state is shared by all the wavefunctions $|\tilde{\psi}_k\rangle$, the above procedure to find the $c_k$’s is mathematically inaccurate, even for a dilute Bose gas. This is corroborated by the fact that, when the variational calculation is done in a more careful way, where the number $(N - 2 \sum_i n_i)$ of bosons in the $k = 0$ is kept throughout the calculation, the results obtained for the ground state energy and the excitation spectrum are quite different from those of the standard Bogoliubov method, as we have explicitly shown in Sec. 7 of the present paper.

Another attempt at formulating a number-conserving theory for the ground state of interacting bosons was given by Gardiner in Ref. [26]. We will not discuss this study here, but rather point to a comment by Girardeau, Ref. [27], where Gardiner’s theory is discussed in great detail, and is shown to be a special case of the theory developed by Girardeau and Arnowitt in 1959, Ref. [25].

§9. Conclusions

To summarize, in this paper, we have given a detailed and rather thorough discussion of Bogoliubov’s theory of an interacting Bose gas. Our main point was to reassert a result which in principle should be quite well-known but is often overlooked in the literature, having to do with the fact that Bogoliubov’s theory is a theory in which each of the single-momentum contributions $\hat{H}_k$ to the total Hamiltonian $\hat{H} = \sum_{k \neq 0} \hat{H}_k$ is diagonalized independently from the other contributions $\hat{H}_k(\neq k)$, and the ground state wavefunction of the total Hamiltonian $\hat{H}$ is written as a simple product of the ground state wavefunctions of the $\hat{H}_k$’s. As a way to illustrate this point, we have discussed a variational, number conserving formulation of Bogoliubov’s method, where the ground state of each single-mode Hamiltonian $\hat{H}_k$ is found independently from the ground states of the other Hamiltonians $\hat{H}_{k'}(\neq k)$, and we have derived most of the results of Bogoliubov’s standard, number non-conserving formulation within this variational method, including the gapless excitation spectrum predicted by Bogoliubov’s theory. Arguing that the above decoupled way of
finding the ground state of the total Hamiltonian $\hat{H}$ may not be accurate, we generalized the above mentioned variational method to the total Hamiltonian $\hat{H}$, making sure to keep an accurate count of the number of bosons in the $k = 0$ state, which led us to a new ground state which has a lower overall energy and a much smaller depletion than the standard Bogoliubov ground state. It also led to an excitation spectrum of bosons which has a finite gap as $k \to 0$, by contrast to Bogoliubov’s method where this gap vanishes. This last feature has allowed us to shed more light on the $\alpha_k$ excitations of the standard Bogoliubov theory, which we argued do not represent phonon modes and correspond to single-particle excitations instead. We have argued that the existence of a gap in our number-conserving approach does not imply a violation of Goldstone’s theorem, given that our ground state does not break the $U(1)$ symmetry of the Hamiltonian, which implies that the Goldstone theorem does not apply in this case. Our results seem to support the conclusions of recent work by Bobrov\textsuperscript{47} and Kita,\textsuperscript{50} which have argued that the correct Goldstone modes of condensed Bose systems should be sought in the pole of the two-particle Green’s function, although more work still needs to be done in order to understand the connection between these approaches and the approach developed in the present paper.

Given the above, the author hopes he has made a compelling case that the standard formulation of Bogoliubov’s theory, where not much importance is attached to the conservation of boson number, is far from accurate and hence highly unsatisfactory, to say the least, and is in need of a major revision. It is the author’s hope that the discussion presented in this work will help bring about such a revision, leading to a conceptually more satisfying description of dilute Bose systems, both at $T = 0$ and at finite temperatures.

Appendix A

Diagonalization of the single mode Hamiltonian $\hat{H}_k$

In this Appendix, we show how one can diagonalize the Hamiltonian $\hat{H}_k$ in the number-conserving Bogoliubov approach. We shall here mostly focus on the case of the single-mode theory of Sec. 5. The general case being very similar, apart from a few minor differences discussed at the end of this Appendix.

A.1. Derivation of the diagonal form of $\hat{H}_k$ in terms of the $\alpha_k$ operators

Let us rewrite the expression of $\hat{H}_k$:

$$\hat{H}_k = \frac{1}{2} \varepsilon_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + \frac{\nu(k)}{2V} (a_0^\dagger a_0 a_k + a_k^\dagger a_k a_0 + a_0^\dagger a_k a_{-k}).$$

(A.1)

We now introduce the operator $b_k$ such that:

$$b_k = a_k a_0^\dagger.$$

(A.2)
It then follows that the operator $\alpha_k = \tilde{u}_k a_k a_0^\dagger + \tilde{v}_k a_{-k}^\dagger a_0$ can be written in the form:

$$\alpha_k = \tilde{u}_k b_k + \tilde{v}_k b_{-k}.$$  \hspace{1cm} (A.3)

Taking the adjoint of the above equation, we obtain:

$$\alpha_k^\dagger = \tilde{u}_k b_k^\dagger + \tilde{v}_k b_{-k}.$$  \hspace{1cm} (A.4)

These last two expressions of $\alpha_k$ and $\alpha_k^\dagger$ in terms of the $b_k$’s can easily be inverted to give the expressions of $b_k$ in terms of the $\alpha_k$’s, with the result:

$$b_k = \frac{1}{\gamma_k} \left[ u_k \alpha_k - v_k \alpha_k^\dagger \right].$$  \hspace{1cm} (A.5)

where we remind the reader that $\gamma_k^2 = \tilde{u}_k^2 - \tilde{v}_k^2$. Using the fact that $\tilde{u}_k = \gamma_k u_k$ and $\tilde{v}_k = \gamma_k v_k$, we finally can write:

$$b_k = \frac{1}{\gamma_k} \left[ u_k \alpha_k - v_k \alpha_k^\dagger \right].$$  \hspace{1cm} (A.6)

Now, it is not difficult to see that the pairing terms can be easily written in terms of the $b_k$’s:

$$a_k^\dagger a_{-k} a_0 a_0 = a_k^\dagger a_0 a_{-k}^\dagger a_0 = b_k b_{-k}^\dagger,$$  \hspace{1cm} (A.7a)

$$a_0^\dagger a_0 a_{-k} = a_k^\dagger a_0 a_{-k}^\dagger = b_k b_{-k}.$$  \hspace{1cm} (A.7b)

On the other hand, we can write for the Fock term:

$$a_k^\dagger a_k a_0^\dagger a_0 = a_k^\dagger a_k a_0 a_0^\dagger - 1,$$

$$= a_k^\dagger a_0 a_k a_0^\dagger - a_k a_k,$$

$$= b_k^\dagger b_k = a_k^\dagger a_k.$$  \hspace{1cm} (A.8)

Hence, we can rewrite for $\hat{H}_k$ the following expression:

$$\hat{H}_k = \frac{1}{2} \left( \epsilon_k - \frac{v(k)}{V} \right) (a_k^\dagger a_k + a_{-k}^\dagger a_{-k})$$

$$+ \frac{v(k)}{2V} (b_k^\dagger b_k + b_{-k}^\dagger b_{-k} + b_k b_{-k}).$$  \hspace{1cm} (A.9)

To the above Hamiltonian, we add and subtract the quantity $\frac{1}{2} \gamma_k \epsilon_k (b_k^\dagger b_k + b_{-k}^\dagger b_{-k})$, and rewrite the result in the form:

$$\hat{H}_k = \hat{H}_{1k} + \frac{1}{2} \left( \epsilon_k \eta_k + \frac{v(k)}{V} \right) (b_k^\dagger b_k + b_{-k}^\dagger b_{-k}) + \frac{v(k)}{2V} (b_k^\dagger b_{-k} + b_k b_{-k}),$$  \hspace{1cm} (A.10)

where the excess Hamiltonian $\hat{H}_{1k}$ is given by:

$$\hat{H}_{1k} = \frac{1}{2} \epsilon_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k})$$

$$- \frac{1}{2} \epsilon_k \eta_k (b_k^\dagger b_k + b_{-k}^\dagger b_{-k})$$

$$- \frac{v(k)}{2V} (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}).$$  \hspace{1cm} (A.11)
For weak perturbation, this Hamiltonian will have a very small expectation value, owing to the fact that the two terms on the first and second lines cancel each other (we remind the reader that \( b_k \equiv a_k a_k^\dagger \), and hence \( b_k^\dagger b_k = a_k^\dagger a_k a_k a_k^\dagger \); on the other hand we will see below that \( \eta_k = \gamma_k^2 \), and since \( \gamma_k^2 \sim 1/N_0 \), we see that \( \gamma_k^2 b_k^\dagger b_k = a_k^\dagger a_k \), and will henceforth be neglected altogether. (Note that, because it only involves a single momentum mode, the term on the last line on Eq. \( \text{(A.11)} \) can be neglected in the thermodynamic limit \( V \to \infty \).

We now want to fix the value of the constant \( \eta_k \). A somewhat tedious but straightforward calculation gives:

\[
\hat{H}_k = \frac{1}{2\gamma_k^2} \left\{ [A_k(u_k^2 + v_k^2) - 2B_k] (\alpha_k^\dagger \alpha_k + \alpha_k \alpha_k^\dagger - \alpha_{-k} \alpha_{-k}^\dagger) \right.
\]

\[
\left. + [B_k(u_k^2 + v_k^2) - 2A_k] (\alpha_{-k} \alpha_k^\dagger + \alpha_k \alpha_{-k}^\dagger) \right.
\]

\[
\left. + [A_k v_k^2 - B_k u_k v_k] ([\alpha_k, \alpha_k^\dagger] + [\alpha_{-k}, \alpha_{-k}^\dagger]) \right.
\]

\[
\left. + (B_k v_k^2 - A_k u_k v_k) ([\alpha_{-k}^\dagger, \alpha_k^\dagger] + [\alpha_{-k}, \alpha_k]) \right\}. \tag{A.12}
\]

where we defined the constants \( A_k \) and \( B_k \) such that:

\[
A_k = \varepsilon_k \eta_k + \frac{v(k)}{V}, \quad B_k = \frac{v(k)}{V}. \tag{A.13}
\]

We now want to fix the value of the constant \( \eta_k \) in such a way as to make the coefficient of the term \( (\alpha_k^\dagger \alpha_{-k}^\dagger + \alpha_k \alpha_{-k}) \) vanish, i.e. by imposing the condition:

\[
[B_k(u_k^2 + v_k^2) - 2A_k] = 0. \tag{A.14}
\]

Using Eqs. \( \text{(A.13)} \) and the expressions \( \text{(5.63)}-\text{(5.64)} \) of the coherence factors \( \tilde{u}_k \) and \( \tilde{v}_k \), we obtain, after a few steps:

\[
\eta_k = \gamma_k^2 \tag{A.15}
\]

Using the definition of \( \alpha_k \) in terms of the \( a_k \) operators, one can easily evaluate the commutator \( [\alpha_{-k}, \alpha_k] \), with the result:

\[
[\alpha_{-k}, \alpha_k] = [\alpha_k^\dagger, \alpha_k^\dagger] = \gamma_k^2 u_k v_k [a_k^\dagger a_k - a_{-k}^\dagger a_{-k}]. \tag{A.16}
\]

For all practical purposes, the last term on the \( \text{rhs} \) of the above equation can be neglected, since for weak perturbation \( \gamma_k^2 \sim 1/N_0 \sim 1/N \) and the expectation values of \( a_k^\dagger a_k \) and \( a_{-k}^\dagger a_{-k} \) should be almost equal, hence canceling each other. We therefore can approximate:

\[
[\alpha_{-k}, \alpha_k] = [\alpha_{-k}^\dagger, \alpha_k^\dagger] \simeq 0. \tag{A.17}
\]

On the other hand, we have already established in Eq. \( \text{(5.59)} \) of the text that the commutator \( [\alpha_k, \alpha_k^\dagger] \) is given by:

\[
[\alpha_k, \alpha_k^\dagger] \simeq \gamma_k^2 a_k^\dagger a_k - \tilde{u}_k^2 a_k^\dagger a_k + \tilde{v}_k^2 a_{-k}^\dagger a_{-k}. \tag{A.18}
\]
Given that $\tilde{u}_k = \gamma_k u_k = u_k/\sqrt{N_0}$, and $\tilde{v}_k = \gamma_k v_k = v_k/\sqrt{N_0}$, assuming weak depletion the second and last terms on the rhs of the above equation can be neglected. This implies, since $\gamma_k^2 \sim 1/N_0$ that we can approximate:

$$[\alpha_k, \alpha_k^\dagger] \approx \gamma_k^2 a_0^\dagger a_0 \sim 1.$$  \hfill (A-19)

Under these circumstances, if we use the approximation $\gamma_k^2 \approx 1/N_0 \approx 1/N$, so that $V \gamma_k \approx 1/n_B$, and then use the expressions of $u_k$ and $v_k$ in terms of $c_k$, Eqs. (5.63), one can show that:

$$n_B v(k) (u_k^2 + v_k^2) = 2(\varepsilon_k + n_B v(k)) u_k v_k,$$

then the expression of $\hat{H}_k$ reduces to:

$$\hat{H}_k = \left\{ [\varepsilon_k + n_B v(k)] v_k^2 - n_B v(k) u_k v_k \right\}$$

$$+ \frac{1}{2} \left\{ [\varepsilon_k + n_B v(k)] (u_k^2 + v_k^2) - 2n_B v(k) u_k v_k \right\} (\alpha_k^\dagger \alpha_k + \alpha_{-k}^\dagger \alpha_{-k}).$$  \hfill (A-20)

If we again use the expression of $u_k$ and $v_k$ in terms of $\varepsilon_k$, $n_B$ and $v(k)$, Eqs. (5.64) to evaluate the terms between curly braces, then we obtain after a few manipulations:

$$\hat{H}_k \approx -\frac{1}{2} [\varepsilon_k + n_B v(k) - E_k] + \frac{1}{2} E_k (\alpha_k^\dagger \alpha_k + \alpha_{-k}^\dagger \alpha_{-k}),$$  \hfill (A-21)

which is nothing but Eq. (5.67) of the text.

A.2. Proof that the excess Hamiltonian $\hat{H}_{1k}$ gives a negligible contribution to the excitation energy

In this Subsection, we want to make sure that the excess Hamiltonian $\hat{H}_{1k}$ does not contribute to the excitation spectrum. We are interested in evaluating the following quantity:

$$\Delta \hat{H}_{1k} = \langle \Psi(N) | \alpha_k \hat{H}_{1k} \alpha_k^\dagger | \Psi(N) \rangle - \langle \Psi(N) | \hat{H}_{1k} | \Psi(N) \rangle,$$

$$= \langle \Psi(N) | [\alpha_k, \hat{H}_{1k}] | \alpha_k^\dagger | \Psi(N) \rangle,$$

where, in going from the first to the second line, use has been made of the commutation relation $[\alpha_k, \alpha_k^\dagger] \approx 1$. In what follows, we shall find it convenient to decompose $\hat{H}_{1k}$ into the following sum:

$$\hat{H}_{1k} = \hat{h}_{1k} + \hat{h}_{2k},$$  \hfill (A-22)

with:

$$\hat{h}_{1k} = \frac{1}{2} (\varepsilon_k - \frac{v(k)}{V}) (a_k^\dagger a_{-k} + a_{-k}^\dagger a_{-k}),$$

$$\hat{h}_{2k} = -\frac{1}{2} \varepsilon_k n_k (b_k^\dagger b_k + b_{-k}^\dagger b_{-k}).$$  \hfill (A-23)

Calculating the commutator $[\alpha_k, \hat{h}_{1k}]$, we find:

$$[\alpha_k, \hat{h}_{1k}] = \frac{1}{2 \gamma_k^2} (\varepsilon_k - \frac{v(k)}{V}) \left[ (\tilde{u}_k^2 + \tilde{v}_k^2) \alpha_k - 2 \tilde{u}_k \tilde{v}_k \alpha_{-k} \right].$$  \hfill (A-24)
We therefore can write:

\[ \langle \Psi(N) | [\alpha_k, \hat{H}_1^k] | \alpha_k^\dagger \Psi(N) \rangle = \frac{1}{2\gamma_k^2} \left( \varepsilon_k - \frac{v(k)}{V} \right) \]

\times \langle \Psi(N) | (\tilde{u}_k^2 + \tilde{v}_k^2) \alpha_k \alpha_k^\dagger | \Psi(N) \rangle,

(A.27a)

\[ = \frac{\tilde{u}_k^2 + \tilde{v}_k^2}{2\gamma_k^2} \left( \varepsilon_k - \frac{v(k)}{V} \right) \]

(A.27b)

Similarly, calculating the commutator \([\alpha_k, \hat{H}_2^k]\), we find:

\[ [\alpha_k, \hat{H}_2^k] = -\frac{1}{2\gamma_k^2} \varepsilon_k \eta_k \left( (\tilde{u}_k^2 + \tilde{v}_k^2) \alpha_k - 2\tilde{u}_k \tilde{v}_k \alpha_{-k}^\dagger \right), \]

(A.28)

and hence:

\[ \langle \Psi(N) | [\alpha_k, \hat{H}_2^k] | \alpha_k^\dagger \Psi(N) \rangle = -\varepsilon_k \eta_k \frac{\tilde{u}_k^2 + \tilde{v}_k^2}{\gamma_k^2}. \]

(A.29)

Adding the two contributions from Eqs. (A.27) and (A.29) together, we find:

\[ \langle \Psi(N) | [\alpha_k, \hat{H}_1^k] | \alpha_k^\dagger \Psi(N) \rangle = \tilde{u}_k^2 + \tilde{v}_k^2 \]

\[ \times \left[ \varepsilon_k \left( 1 - \frac{\eta_k}{\gamma_k^2} \right) - \frac{v(k)}{V} \right]. \]

(A.30)

Given that \( \eta_k = \gamma_k^2 \), and using the fact that \( \tilde{u}_k = \gamma_k u_k \) and \( \tilde{v}_k = \gamma_k v_k \), we finally obtain:

\[ \langle \Psi(N) | [\alpha_k, \hat{H}_1^k] | \alpha_k^\dagger \Psi(N) \rangle = \frac{v(k)}{2V} (u_k^2 + v_k^2), \]

(A.31)

which indeed gives a negligible contribution to the excitation energy in the thermodynamic limit \( V \to \infty \).

At the end of this Appendix, we briefly discuss the diagonalization of \( \hat{H}_k \) when a multi-mode model governed by the full Hamiltonian \( \hat{H} = \sum_{k \neq 0} \hat{H}_k \) is considered. In this case, the coherence factors are given by Eq. (7.56), and hence the requirement (A.14) above gives a different result for \( \eta_k \) than Eq. (A.15), namely Eq. (7.61). This, in turn, leads to the boson excitation spectrum given in Eq. (7.65) of the text.

**Appendix B**

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**Expectation value of the Hamiltonian when we keep an accurate tally of the number of condensed bosons**

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In this Appendix, we give the salient features of how we calculate the expectation value of the Hamiltonian

\[ \hat{H}_{kj} = \frac{1}{2} \varepsilon_{kj} (a_{kj}^\dagger a_{kj} + a_{-kj}^\dagger a_{-kj}) + \frac{v(k)}{2V} (a_{kj}^\dagger a_{0} a_{kj}^\dagger a_{kj} + a_{0} a_{kj}^\dagger a_{-kj} + a_{-kj}^\dagger a_{0} a_{kj} a_{-kj}) \]

(B.1)
in the variational ground state $|\Psi(N)\rangle$ of Eq. (7.11), namely:

$$|\Psi(N)\rangle = Z \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} C_{n_1} \cdots C_{n_M} |N - 2 \sum_{i=1}^{M} n_i; n_1, n_1; \ldots; n_M, n_M\rangle. \tag{B.2}$$

We have:

$$a_{k_j}^\dagger a_{k_j} |\Psi(N)\rangle = Z \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} C_{n_1} \cdots C_{n_M} n_j |N - 2 \sum_{i=1}^{M} n_i; n_1, n_1; \ldots; n_M, n_M\rangle, \tag{B.3}$$

and hence:

$$\langle \Psi(N) | a_{k_j}^\dagger a_{k_j} | \Psi(N) \rangle = \frac{\sum_{n_j=0}^{\infty} n_j C_{n_j}^2}{\sum_{n_j=0}^{\infty} C_{n_j}^2}, \tag{B.4a}$$

$$= \frac{C_{n_j}^2}{1 - C_{n_j}}, \tag{B.4b}$$

where, in going from the first to the second line, we made use of the fact that $C_{n_j} = (-c_{k_j})^{n_j}$, and of the summation formulae (valid for $|x| < 1$):

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1 - x}, \tag{B.5a}$$

$$\sum_{n=0}^{\infty} nx^n = \frac{x}{1 - x}. \tag{B.5b}$$

An identical result is obtained for the expectation value of the operator $a_{-k_j}^\dagger a_{-k_j}$.

Let us now turn our attention to the Fock terms. We have:

$$a_{k_j}^\dagger a_{0} a_{0}^\dagger a_{k_j} | \Psi(N) \rangle = Z \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} C_{n_1} \cdots C_{n_M}$$

$$\times n_j \left( N - 2 \sum_{i=1}^{M} n_i \right) |N - 2 \sum_{i=1}^{M} n_i; n_1, n_1; \ldots; n_M, n_M\rangle. \tag{B.6}$$

We shall rewrite the above result in the form:

$$a_{0}^\dagger a_{0} a_{k_j}^\dagger a_{k_j} | \Psi(N) \rangle = Z \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} C_{n_1} \cdots C_{n_M} n_j (N - 2n_j)$$

$$\times |N - 2 \sum_{i=1}^{M} n_i; n_1, n_1; \ldots; n_M, n_M\rangle$$

$$- 2Z \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} C_{n_1} \cdots C_{n_M} n_j \left( \sum_{i=1(\neq j)}^{M} n_i \right)$$
we obtain, after a few manipulations:

\[ \times |N - 2 \sum_{i=1}^{M} n_i; n_1, n_1; \ldots; n_M, n_M \rangle. \]  

Hence:

\[
\langle \Psi(N) | a_{0j}^\dagger a_{0k_j}^\dagger a_{k_j} a_{0j} | \Psi(N) \rangle = Z^2 \sum_{n_1=0}^{\infty} C_{n_1}^2 \cdots \sum_{n_j=0}^{\infty} C_{n_j}^2 n_j (N - 2n_j) \cdots \sum_{n_M=0}^{\infty} C_{n_M}^2  
\]

\[
-2Z^2 \sum_{i=1}^{\infty} \left( \sum_{n_1=0}^{\infty} C_{n_1}^2 \cdots \sum_{n_i=0}^{\infty} n_i C_{n_i}^2 \cdots \sum_{n_j=0}^{\infty} n_j C_{n_j}^2 \cdots \sum_{n_M=0}^{\infty} C_{n_M}^2 \right),  
\]

\[
= \sum_{n_j=0}^{\infty} C_{n_j}^2 (N - 2n_j) - 2 \sum_{i=1}^{\infty} C_{n_i}^2 n_i \sum_{n_j=0}^{\infty} n_j C_{n_j}^2.  
\]

Using the summation formulae of Eqs. (B.5), and the additional formula:

\[
\sum_{n=0}^{\infty} n^2 x^n = \frac{x}{(1-x)^2} + \frac{2x^2}{(1-x)^3},  
\]

we obtain, after a few manipulations:

\[
\langle \Psi(N) | a_{0j}^\dagger a_{0k_j}^\dagger a_{k_j} a_{0j} | \Psi(N) \rangle \simeq N \frac{c_{k_j}^2}{1 - c_{k_j}^2} \left[ 1 - \frac{2}{N} \sum_{i=1}^{\infty} \frac{c_{k_i}^2}{1 - c_{k_i}^2} \right].  
\]

Note that, in arriving to this result, a term of the form \(-2 \left[ \frac{c_{k_j}^4}{1 - c_{k_j}^2} + \frac{2c_{k_j}^4}{(1 - c_{k_j}^2)^2} \right] \) has been neglected (this is legitimate given the fact that the terms kept have an overall factor of \(N\) at the front, which makes the term neglected very small by comparison in the thermodynamic \(N \to \infty\) limit). Note also that an identical result is obtained for the expectation value of the other Fock term, \(a_{0j}^\dagger a_{00}^\dagger a_{-k_j} a_{-k_j} \).

We now want to find the expectation value of the pairing term \(a_{0j}^\dagger a_{0k_j}^\dagger a_{-k_j}^\dagger a_{-k_j} \). We have:

\[
a_{0j}^\dagger a_{0k_j}^\dagger a_{-k_j}^\dagger a_{-k_j} | \Psi(N) \rangle = Z \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} C_{n_1} \cdots C_{n_M} \sqrt{(n_j + 1)^2}  
\]

\[
\times \sqrt{(N - 2 \sum_{i=1}^{M} n_i)(N - 1 - 2 \sum_{i=1}^{M} n_i)} \times |N - 2 - 2 \sum_{i=1}^{M} n_i; n_1, n_1; \ldots; n_j + 1, n_j + 1; \ldots; n_M, n_M \rangle,  
\]

\[
(B.11a)  
\]
If we now change the index of summation for the momentum \( \mathbf{k}_j \) from \( n_j \) to \( m_j = n_j + 1 \), we can write:

\[
\langle a_0 a_0 | a_{\mathbf{k}_j} a_{-\mathbf{k}_j} | \Psi(N) \rangle = Z \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} C_{n_1} \cdots C_{n_M} \left( N - 2m_j - \frac{3}{2} \right) \\
\times |N - 2m_j - 2 - 2 \sum_{i=1}^{M} n_i| n_1, n_1; \ldots; m_j, m_j; \ldots; n_M, n_M \rangle \\
- 2Z \sum_{i=1(\neq j)}^{M} \left( \sum_{n_1=0}^{\infty} \cdots \sum_{n_{i-1}=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} C_{n_1} C_{n_2} \cdots C_{n_{i-1}} \cdots C_{n_M} m_j n_i \right) \\
\times |N - 2m_j - 2 - 2 \sum_{i=1(\neq j)}^{M} n_i| n_1, n_1; \ldots; m_j, m_j; \ldots; n_M, n_M \rangle.
\]

Hence, we obtain for the expectation value:

\[
\langle \Psi(N) | a_0 a_0 | a_{\mathbf{k}_j} a_{-\mathbf{k}_j} | \Psi(N) \rangle = \sum_{m_j=1}^{\infty} m_j C_{m_j} C_{m_j-1} \left[ N - 2m_j + \frac{3}{2} \right] \\
- 2 \sum_{i=1(\neq j)}^{M} \left( \sum_{m_j=0}^{\infty} C_{m_j} \sum_{n_i=0}^{\infty} n_i C_{n_i} \sum_{n_j=0}^{\infty} C_{n_j} \right) .
\]

It can be verified that the only term that one has to keep in the first summation is the term proportional to \( N \) (note that this is also how the calculation is conducted in the single-mode variational theory of Sec. 5). Then, if we use the summation formulas \([13,25]\), we obtain, after a few manipulations:

\[
\langle \Psi(N) | a_0 a_0 | a_{\mathbf{k}_j} a_{-\mathbf{k}_j} | \Psi(N) \rangle = -N \frac{c_{\mathbf{k}_j}}{1 - c_{\mathbf{k}_j}^2} \left[ 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{c_{\mathbf{k}_i}^2}{1 - c_{\mathbf{k}_i}^2} \right].
\]
A similar contribution is also obtained for the expectation value of the operator \( a_0 a_k^\dagger a_k^\dagger \).

Collecting all terms, Eqs. (B.4b), (B.10) and (B.15), we obtain:

\[
\langle \Psi | H | \Psi \rangle = \varepsilon_{kj} \frac{\chi_k^2}{1 - \chi_k^2} + n_{BV}(k_j) \frac{\chi_k^2}{1 - \chi_k^2} \left[ 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{\chi_i^2}{1 - c_i^2} \right]
\]

\[
- n_{BV}(k_j) \frac{c_{kj}}{1 - c_{kj}^2} \left[ 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{c_{ki}^2}{1 - c_i^2} \right].
\]

(B.16)

For the total Hamiltonian \( \hat{H} = \sum_{j=1}^{M} \hat{H}_{kj} \), we obtain:

\[
\langle \Psi | \hat{H} | \Psi \rangle = \sum_{j=1}^{M} \left\{ \varepsilon_{kj} + n_{BV}(k_j) \left[ 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{\chi_i^2}{1 - c_i^2} \right] \frac{\chi_k^2}{1 - \chi_k^2} \right\}
\]

\[
- n_{BV}(k_j) \left[ 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{\chi_i^2}{1 - c_i^2} \right] \frac{c_{kj}}{1 - c_{kj}^2},
\]

(B.17)

which is nothing but Eq. (7.16) of the text.

**Appendix C**

**Minimization of the expectation value of the total Hamiltonian**

In this Appendix, we show how we minimize the expectation value of the Hamiltonian given in Eq. (7.16) over the coefficients \( c_{kj} \). To this end, we shall rewrite this expectation value in the form:

\[
\langle \Psi | \hat{H} | \Psi \rangle = \left[ \varepsilon_{kj} + n_{BV}(k_j) \left( 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{\chi_i^2}{1 - c_i^2} \right) \right] \frac{c_{kj}^2}{1 - c_{kj}^2}
\]

\[
- n_{BV}(k_j) \left( 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{\chi_i^2}{1 - c_i^2} \right) \frac{c_{kj}}{1 - c_{kj}^2}
\]

\[
+ \sum_{\ell=1(\neq)}^{M} \left\{ \varepsilon_{k\ell} + n_{BV}(k_\ell) \left( 1 - \frac{2}{N} \sum_{i=1(\neq \ell)}^{M} \frac{\chi_i^2}{1 - c_i^2} \right) \right\} \frac{c_{k\ell}^2}{1 - c_{k\ell}^2}
\]

\[
- n_{BV}(k_\ell) \left( 1 - \frac{2}{N} \sum_{i=1(\neq \ell)}^{M} \frac{\chi_i^2}{1 - c_i^2} \right) \frac{c_{k\ell}}{1 - c_{k\ell}^2}
\]

(C.1)

Taking the partial derivative with respect to \( c_{kj} \), we obtain:

\[
\frac{\partial (\hat{H})}{\partial c_{kj}} = \left[ \varepsilon_{kj} + n_{BV}(k_j) \left( 1 - \frac{2}{N} \sum_{i=1(\neq j)}^{M} \frac{\chi_i^2}{1 - c_i^2} \right) \right] \frac{2c_{kj}}{1 - c_{kj}^2}
\]
\[ -n_B v(k_j) \left( 1 - \frac{2}{N} \sum_{i=1 \neq j}^{M} \frac{c_{k_i}^2}{1 - c_{k_i}^2} \right) \frac{1 + c_{k_j}^2}{(1 - c_{k_j}^2)^2} \]
\[ + \sum_{\ell=1 \neq j}^{M} \left\{ n_B v(k_\ell) \left( - \frac{2c_{k_\ell}}{N (1 - c_{k_\ell}^2)} \frac{c_{k_\ell}}{1 - c_{k_\ell}^2} \right) - n_B v(k_\ell) \left( - \frac{2c_{k_\ell}}{N (1 - c_{k_\ell}^2)} \frac{c_{k_\ell}}{1 - c_{k_\ell}^2} \right) \right\}. \quad (C.2) \]

Rearranging the terms on the rhs of the above equation, and using the notation

\[ \bar{v}(k_j) = v(k_j) \left( 1 - \frac{2}{N} \sum_{i=1 \neq j}^{M} \frac{c_{k_i}^2}{1 - c_{k_i}^2} \right), \quad (C.3) \]

we can write:

\[ \frac{\partial \langle \hat{H} \rangle}{\partial c_{k_j}} = \left[ \varepsilon_{k_j} + n_B \bar{v}(k_j) - \frac{2}{N} \sum_{\ell=1 \neq j}^{M} n_B v(k_\ell) \frac{c_{k_\ell}(c_{k_\ell} - 1)}{1 - c_{k_\ell}^2} \right] \frac{2c_{k_j}}{(1 - c_{k_j}^2)^2} \]
\[ - n_B \bar{v}(k_j) \frac{1 + c_{k_j}^2}{(1 - c_{k_j}^2)^2} \quad (C.4) \]

We hence see that the equation \( \left( \frac{\partial \langle \hat{H} \rangle}{\partial c_{k_j}} \right) = 0 \) can be written in the form:

\[ \frac{1}{(1 - c_{k_j}^2)^2} \left[ 2\tilde{\varepsilon}_{k_j} c_{k_j} - n_B \bar{v}(k_j) (1 + c_{k_j}^2) \right] = 0, \quad (C.5) \]

with

\[ \tilde{\varepsilon}_{k_j} = \varepsilon_{k_j} + n_B \bar{v}(k_j) + \frac{2}{N} \sum_{\ell=1 \neq j}^{M} n_B v(k_\ell) \frac{c_{k_\ell}}{1 + c_{k_\ell}}. \quad (C.6) \]

Equation \( (C.5) \) can in turn be rewritten in the form:

\[ c_{k_j}^2 - 2 \left( \frac{\tilde{\varepsilon}_{k_j}}{n_B \bar{v}(k_j)} \right) c_{k_j} + 1 = 0, \quad (C.7) \]

which is nothing but Eq. (7.17) of the text.

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This is actually equivalent to writing for the average energy of a given system at temperature $T$ in the grand-canonical ensemble an expression of the form $E = \text{Tr}[(\hat{H} - \mu \hat{N})e^{-\beta (\hat{H} - \mu \hat{N})}] / Z_{gr}$ (with $\beta = (k_B T)^{-1}$ and $Z_{gr}$ the grand-canonical partition function), which does not of course make much sense. In the grand-canonical ensemble, the energy is always given by the thermal average of the Hamiltonian $\hat{H}$ itself, $E = \text{Tr}[\hat{H} e^{-\beta (\hat{H} - \mu \hat{N})}] / Z_{gr}$. Likewise, in the standard formulation of Bogoliubov’s method, the ground state energy should be given by the quantum average $\langle \Psi | \hat{H} | \Psi \rangle$, and not by the quantity $\langle \Psi | \hat{H} - \mu \hat{N} | \Psi \rangle$, which represents the grand potential of the system at $T = 0$. It should be mentioned here that Eq. (5) plays a crucial role in the field-theoretic formulation of Bogoliubov’s theory, since it ensures that the action of any normal-ordered product of the excitation operators $\alpha_\alpha^{\dagger}$ and $\alpha_\alpha$ on the Bogoliubov ground state is automatically zero. Indeed, the fact that the first order correction to the ground state energy in Eq. (5) is positive is quite opposite of what we expect, namely that the more involved Bogoliubov ground state has lower energy than the Gross-Pitaevskii ground state $\langle \Psi_{GP}(N) | \hat{H} | \Psi_{GP}(N) \rangle = \langle [N, 0, \ldots] \rangle$, the energy of which is generally written in the form $E_{GP} = 2\pi \hbar^2 n_B^2 / m$. For a discussion of this “paradox”, see A.J. Leggett, New J. Phys. 5, 103 (2003).
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51) Note, however, that in order to be able to describe the statistical mechanics of the interacting Bose gas all the way to the transition temperature into the normal state $T_c$, one has to take into account the Fock interactions between depleted bosons, i.e. the terms we neglected in going from Eq. (4.14a) to Eq. (4.16a). Note also that, taking these neglected Fock terms into account in the variational approach for the Bogoliubov Hamiltonian at $T = 0$ may modify the ground state energy and the total depletion of the interacting gas with respect to the results of Sec. 7.3.
52) It is worth mentioning at this point that it is not even clear whether the perturbative approach of Ref. 28 can be reformulated to produce a finite result for the number $N_k$ of depleted bosons in the state of wavevector $k$ in the $k \to 0$ limit, by analogy with the variational result (5.30) obtained within the single-mode approach. The approach developed in Refs. 7 and 34 and in the present paper has the advantage of allowing us to obtain such a finite result for $N_k$, both in the single-mode theory of Sec. 5.2 and in the multi-mode approach of Sec. 7.3.