

Gapless Hartree-Fock-Bogoliubov approximation for Bose gases

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(Received 7 December 2005; published 12 June 2006)

A dilute Bose system with Bose-Einstein condensate is considered. It is shown that the Hartree-Fock-Bogoliubov approximation can be made both conserving as well as gapless. This is achieved by taking into account all physical normalization conditions, that is, the normalization condition for the condensed particles and that for the total number of particles. Two Lagrange multipliers, introduced for preserving these normalization conditions, make the consideration completely self-consistent.

DOI: 10.1103/PhysRevA.73.063612

PACS number(s): 03.75.Hh, 05.30.Jp, 05.30.Ch

I. INTRODUCTION

The physical properties of Bose gases exhibiting Bose-Einstein condensation are now a topic of intensive research, both experimental and theoretical [1–5]. The physics of dilute weakly interacting Bose gas has been studied especially well using Bogoliubov's model and operator techniques [6–9]. Despite the apparent simplicity of the system, some principal problems in its theoretical description have not yet been well understood. Most notorious is the so-called dilemma of conserving versus gapless approximations, for which we shall offer a possible solution in this paper.

The above dilemma arises, when one attempts to describe the weakly interacting Bose gas at finite (not asymptotically small) diluteness parameter. It is absent in the original Bogoliubov approximation [6–9], which is valid only at very low temperatures $T \rightarrow 0$ and asymptotically weak interaction. The first natural extension to finite temperatures and diluteness parameters is a bosonic version of the Hartree-Fock-Bogoliubov (HFB) approximation. This is a self-consistent approximation which is guaranteed to respect all conservation laws that follow from the underlying symmetries of the Hamiltonian. However, this approximation turns out to render a gap in the spectrum of collective excitations in the condensed phase in which the global U(1) gauge symmetry of the theory is broken. Also, the Girardeau-Arnoult approximation [10] displays this gap, since it is equivalent to the HFB approximation. This contradicts the fundamental theorems of Hugenholtz and Pines [11], Goldstone [12], and Bogoliubov [9], according to which the spectrum of collective excitations in the symmetry-broken phase has to be gapless. It is well known [13–15] that the HFB approximation can be formulated as a variational approximation. There exist several other variational approximations, the so-called Φ -derivable approximations or higher effective actions [16–20], which also respect the conservation laws but lead to a gap in the spectrum. When trying to remove the gap, one usually violates the conservation laws and runs into other thermodynamic inconsistencies. The various approximations that have been studied are typically classified as either conserving or gapless. This classification and the related dilemma were first emphasized by Hohenberg and Martin [21], and later discussed in many publications, for instance, by Baym and Grinstein [19]. A very detailed discussion of this

problem, with many citations, has recently been done by Andersen [4].

In order to remove the gap in the HFB approximation, one often invokes a trick of neglecting the anomalous averages, calling this the “Popov approximation.” However, a glance at the original works by Popov [22–25] shows that he has never suggested this trick. What he actually considered was a narrow region of temperatures T in the vicinity of the condensation temperature T_c . When $T \rightarrow T_c$, then the condensate density tends to zero. The anomalous averages, being proportional to the condensate density, tend to zero together with the latter, when $T \rightarrow T_c$. As a result, their contribution becomes automatically small, without any special assumptions. Far below T_c , however, the anomalous averages can be very large, and Popov has never proposed to neglect them there. It is straightforward to demonstrate by direct calculations that at low temperatures $T \ll T_c$, the anomalous averages become of the same order as the normal averages. They can even be much larger than the latter [26], so that Popov would certainly not have been keen on proposing the so-called Popov approximation.

Moreover, preserving the anomalous averages for the phase with broken U(1) gauge symmetry is principally important, since their negligence makes the system unstable [26,27].

There have been several attempts to make the HFB approximation gapless by adding to this approximation some higher-order terms involving the Bethe-Salpeter or T -matrix approximations. The idea to modify in this way the mean-field HFB approximation goes back to Kirzhnits and Linde [28] and Baym and Grinstein [19]. Several such modifications of the HFB approximation have been considered, in which additional terms are either motivated by higher-order approximations [29,30] or just added phenomenologically [31,32]. This type of modification [28–32] possesses a number of deficiencies, which do not permit one to accept this approach as a solution to the problem. A good analysis of these deficiencies has already been done by Baym and Grinstein [19], and recently by Andersen [4].

First of all, the method of adding to the theory some additional terms in order to cancel the spectrum gap is ambiguous, not following from a general physical law. As a result, the additional terms are not uniquely defined. There are no general grounds to decide which of the variants is better.

Second, the way of mixing different approximations is not self-consistent. This is what Bogoliubov [9] called the “mis-

match of approximations.” Although such a mismatch can make the gap disappear, it is usually inconsistent with some thermodynamic equations. For instance, the chemical potential defined by the Hugenholtz-Pines theorem to yield a gapless spectrum, does not coincide with the chemical potential found from the minimization of the thermodynamic potential with respect to the condensate density. This discrepancy is a general feature of all nonself-consistent approximations, due to which they cannot properly be called gapless [4].

Moreover, if the price of making the spectrum gapless is that the thermodynamic potential cannot be minimized, this implies that the system becomes thermodynamically unstable. Thus, one has the unpleasant alternative: Either the system is gapless but unstable or seemingly stable but with a gap. This is a particular case of the general problem of thermodynamic self-consistency [33,34].

Problems with the thermodynamics of the model have the unpleasant consequences of modifying the order of the phase transition [33,34]. This happens for all approaches with mismatched approximations. Baym and Grinstein [19] emphasized that attempts to modify the HFB approximation in a nonself-consistent way lead to a first-order condensation transition, instead of the observed second-order one. Further works [4,31,32] confirmed that it is a common feature of all nonself-consistent mean-field approximations.

In the present paper, we show that the HFB approximation can be made both conserving *and* gapless, while avoiding the mismatch of approximations, thus being completely self-consistent. The solution of the problem is possible by taking into account two existing normalization conditions instead of one in all previous approximations. This makes the HFB approximation self-consistent and gapless, without any tricks or additional terms. As a consequence, condensation transition becomes second order, as it should be.

Throughout the paper, the system of units is employed with Planck and Boltzmann constants equal to unity, $\hbar \equiv 1$, $k_B \equiv 1$.

II. GRAND-CANONICAL HAMILTONIAN

We consider a dilute Bose gas, whose particle interactions are modeled by the contact potential

$$V(\mathbf{x}) = g\delta(\mathbf{x}), \quad (1)$$

with the interaction intensity

$$g \equiv 4\pi \frac{a_s}{m} \quad (2)$$

expressed through the *s*-wave scattering length a_s and particle mass m . The energy operator reads

$$\hat{H} = \int d^3x \psi^\dagger(\mathbf{x}) \left(-\frac{\nabla^2}{2m} + \frac{g}{2} \int d^3x \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \psi(\mathbf{x}) \right), \quad (3)$$

with the field operators $\psi(\mathbf{x})$ satisfying the Bose commutation relations. The operator counting the total number of particles is

$$\hat{N} = \int d^3x \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}). \quad (4)$$

In what follows, we treat a uniform system in thermodynamic equilibrium, since this is the simplest situation where the above-discussed problems reveal themselves.

If the temperature in a Bose system falls below the condensation temperature T_c , the U(1) gauge symmetry becomes broken. The symmetry breaking is taken into account by the Bogoliubov shift [8,9] of the field operator

$$\psi(\mathbf{x}) \rightarrow \Psi + \psi_1(\mathbf{x}), \quad (5)$$

where Ψ is the condensate *order parameter*, which in uniform systems is independent of \mathbf{x} , and $\psi_1(\mathbf{x})$ is the field operator of the uncondensed particles, satisfying the same Bose commutation relations as $\psi(\mathbf{x})$. Another method of first separating the zero-momentum components of the field and then replacing them by classical numbers [6,7] is completely equivalent to the shift (5), as has been rigorously proved by Ginibre [35]. The field $\psi_1(\mathbf{x})$ has no zero-momentum component so that

$$\langle \psi_1(\mathbf{x}) \rangle = 0 \quad (6)$$

and Ψ and $\psi_1(\mathbf{x})$ are orthogonal to each other:

$$\int \Psi^* \psi_1(\mathbf{x}) d^3x = 0. \quad (7)$$

The condensate order parameter Ψ defines the density of condensed particles

$$\rho_0 = |\Psi|^2. \quad (8)$$

Above T_c where Ψ vanishes, there is no condensate. Below T_c , one has $\Psi \neq 0$ and thus a finite condensate density ρ_0 .

The free energy of the system is

$$F = -T \ln \text{Tr } e^{-\beta \hat{H}}, \quad (9)$$

with $\beta \equiv 1/T$. After substituting shift (5) into \hat{H} , the model contains two field variables, the condensate order parameter Ψ and the space-dependent field $\psi_1(\mathbf{x})$. They give rise to *two* normalization conditions. One is related to the definition of the total number of particles

$$N = \langle \hat{N} \rangle. \quad (10)$$

A second normalization condition fixes the number of condensed particles

$$N_0 = \rho_0 V = |\Psi|^2 V. \quad (11)$$

In stable equilibrium, the free energy gains a minimum under the normalization conditions (10) and (11). This conditional minimization is equivalent to the unconditional minimum of the grand-canonical potential

$$\Omega = -T \ln \text{Tr } e^{-\beta H}, \quad (12)$$

with the grand-canonical Hamiltonian

$$H = \hat{H} - \mu_0 N_0 - \mu \hat{N}, \quad (13)$$

in which μ_0 and μ are the Lagrange multipliers enforcing the normalization conditions (10) and (11). The minimum of the grand-canonical potential (12) is determined by the equations

$$\frac{\partial \Omega}{\partial N_0} = 0, \quad \frac{\partial^2 \Omega}{\partial N_0^2} > 0. \quad (14)$$

The first derivative is given by the expectation value

$$\frac{\partial \Omega}{\partial N_0} = \left\langle \frac{\partial H}{\partial N_0} \right\rangle. \quad (15)$$

The second derivative is calculated from

$$\frac{\partial^2 \Omega}{\partial N_0^2} = \left\langle \frac{\partial^2 H}{\partial N_0^2} \right\rangle + \beta \Delta^2 \left(\frac{\partial H}{\partial N_0} \right), \quad (16)$$

with the notation

$$\Delta^2(\hat{O}) \equiv \langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2$$

for the dispersion of an operator \hat{O} .

For a uniform system, the field operator of the uncondensed particles is expandable in plane waves as

$$\psi_1(\mathbf{x}) = \sum_{\mathbf{k} \neq 0} a_{\mathbf{k}} \frac{e^{i\mathbf{k} \cdot \mathbf{x}}}{\sqrt{V}}. \quad (17)$$

Performing the Bogoliubov shift (5), together with the expansion (17), we obtain for the grand-canonical Hamiltonian (13) the sum of five terms

$$H = \sum_{n=0}^4 H^{(n)}, \quad (18)$$

depending on the power of the operators $\psi_1(\mathbf{x})$. The zero-order term

$$H^{(0)} = \left(\frac{1}{2} \rho_0 g - \varepsilon \right) N_0, \quad (19)$$

with

$$\varepsilon \equiv \mu_0 + \mu, \quad (20)$$

is free of $\psi_1(\mathbf{x})$. The first-order term in Eq. (19) vanishes, since decomposition (17) contains only nonzero momenta. The second-order term is

$$H^{(2)} = \sum_{\mathbf{k} \neq 0} \left(\frac{k^2}{2m} + 2\rho_0 g - \mu \right) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{\rho_0 g}{2} \sum_{\mathbf{k} \neq 0} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}} a_{\mathbf{k}}). \quad (21)$$

In the third-order term,

$$H^{(3)} = \sqrt{\frac{\rho_0}{V}} g \sum_{\mathbf{p}, \mathbf{q}}' (a_{\mathbf{q}}^\dagger a_{\mathbf{p}+\mathbf{q}} a_{-\mathbf{p}} + a_{-\mathbf{p}}^\dagger a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{q}}), \quad (22)$$

the prime on the summation symbol implies that $\mathbf{p} \neq 0$, $\mathbf{q} \neq 0$, and $\mathbf{p} + \mathbf{q} \neq 0$. In the fourth-order term

$$H^{(4)} = \frac{g}{2V} \sum_{\mathbf{k}} \sum_{\mathbf{p}, \mathbf{q}}' a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{p}+\mathbf{k}} a_{\mathbf{q}-\mathbf{k}}, \quad (23)$$

the summation does not include any zero-momentum operators, so that the prime means that $\mathbf{p} \neq 0$, $\mathbf{q} \neq 0$, $\mathbf{k} + \mathbf{p} \neq 0$, and $\mathbf{k} - \mathbf{q} \neq 0$.

The field operators in momentum space $a_{\mathbf{k}}$ satisfy the following conditions. From Eq. (7), we have

$$\langle a_{\mathbf{k}} \rangle = 0 \quad (\mathbf{k} \neq 0), \quad (24)$$

and owing to the uniformity of the system:

$$\langle a_{\mathbf{k}}^\dagger a_{\mathbf{p}} \rangle = \delta_{\mathbf{k}, \mathbf{p}} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle, \quad \langle a_{\mathbf{k}} a_{\mathbf{p}} \rangle = \delta_{-\mathbf{k}, \mathbf{p}} \langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle. \quad (25)$$

Note that μ in Eq. (21) is the chemical potential enforcing the normalization condition (10). In a system without Bose-Einstein condensate, there is no need to introduce another Lagrange multiplier. However, as soon as the gauge symmetry is broken and a Bose-Einstein condensate appears, the theory acquires the new variable Ψ , the order parameter of the condensate, which satisfies the normalization condition (11). For the self-consistency of the theory, it is then necessary to take account of this additional normalization condition, which requires the second Lagrange multiplier μ_0 . Without the latter, the theory cannot be made self-consistent, and the normalization condition for the condensed particles cannot be guaranteed.

It is worth emphasizing that μ is the chemical potential existing for the system in both the gauge-symmetric and the broken-symmetry phase. At T_c , the chemical potential is continuous, $\mu(T_c - 0) = \mu(T_c + 0)$. One should not confuse μ with μ_0 which is just a Lagrange multiplier guaranteeing the validity of the normalization condition (11), and keeping the theory self-consistent and the system stable.

III. HARTREE-FOCK-BOGOLIUBOV APPROXIMATION

We are now prepared to treat the Hamiltonian (18) with our modified HFB approximation. For this, we introduce some notations. The momentum distribution of particles

$$n_{\mathbf{k}} \equiv \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle \quad (26)$$

will be referred to as the *normal average*, contrary to the *anomalous average*

$$\sigma_{\mathbf{k}} \equiv \langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle. \quad (27)$$

Summing these averages over momenta, one gets the density of uncondensed particles

$$\rho_1 \equiv \frac{1}{V} \sum_{\mathbf{k} \neq 0} n_{\mathbf{k}} \quad (28)$$

and the anomalous density

$$\sigma_1 \equiv \frac{1}{V} \sum_{\mathbf{k} \neq 0} \sigma_{\mathbf{k}}. \quad (29)$$

In the HFB approximation, the third-order term (22) is zero,

$$H^{(3)} = 0, \quad (30)$$

because of Eq. (24). The fourth-order term (23), finally, becomes

$$\begin{aligned} H^{(4)} = & \sum_{\mathbf{k} \neq 0} \rho_1 g \left(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} - \frac{1}{2} n_{\mathbf{k}} \right) + \frac{1}{V} \sum_{\mathbf{k}, \mathbf{p} \neq 0} g \left[n_{\mathbf{k}+\mathbf{p}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \right. \\ & \left. + \frac{1}{2} (\sigma_{\mathbf{k}+\mathbf{p}} a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + \sigma_{\mathbf{k}+\mathbf{p}}^* a_{-\mathbf{p}} a_{\mathbf{p}}) - \frac{1}{2} (n_{\mathbf{k}+\mathbf{p}} n_{\mathbf{p}} + \sigma_{\mathbf{k}+\mathbf{p}} \sigma_{\mathbf{p}}^*) \right]. \end{aligned} \quad (31)$$

Let us define the shifted particle energies

$$\xi_{\mathbf{k}} \equiv \frac{k^2}{2m} + 2\rho g - \mu, \quad (32)$$

where

$$\rho \equiv \rho_0 + \rho_1 \quad (33)$$

is the total particle density. We also introduce the notation

$$\Delta \equiv (\rho_0 + \sigma_1)g. \quad (34)$$

Then, Hamiltonian (18) can be written in the HFB approximation as

$$H_{\text{HFB}} = E_{\text{HFB}} + \sum_{\mathbf{k} \neq 0} \xi_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k} \neq 0} \Delta (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}} a_{\mathbf{k}}), \quad (35)$$

where

$$E_{\text{HFB}} \equiv H^{(0)} - \frac{1}{2} (2\rho_1^2 + \sigma_1^2) g V. \quad (36)$$

Using this Hamiltonian in the grand-canonical potential (12), we have

$$\frac{\partial \Omega}{\partial N_0} = (\rho + \rho_1 + \sigma_1)g - \varepsilon, \quad (37)$$

and the second derivative is given by

$$\frac{\partial^2 \Omega}{\partial N_0^2} = \frac{g}{V}. \quad (38)$$

Minimizing the grand-canonical potential according to conditions (14), we obtain

$$\varepsilon = (\rho + \rho_1 + \sigma_1)g, \quad (39)$$

with the stability condition $g > 0$.

The Hamiltonian (35) is quadratic and can be diagonalized by means of the Bogoliubov's canonical transformation

$$a_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}} + v_{-\mathbf{k}}^* b_{-\mathbf{k}}^\dagger. \quad (40)$$

This brings the Hamiltonian (35) to the Bogoliubov form

$$H_B = E_B + \sum_{\mathbf{k} \neq 0} \varepsilon_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, \quad (41)$$

with the nonoperator energy term

$$E_B \equiv E_{\text{HFB}} + \frac{1}{2} \sum_{\mathbf{k} \neq 0} (\varepsilon_{\mathbf{k}} - \xi_{\mathbf{k}}) \quad (42)$$

and the Bogoliubov spectrum

$$\varepsilon_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 - \Delta^2}. \quad (43)$$

By the Hugenholtz-Pines theorem [11–13], the spectrum must be gapless:

$$\lim_{k \rightarrow 0} \varepsilon_{\mathbf{k}} = 0, \quad \varepsilon_{\mathbf{k}} \geq 0. \quad (44)$$

Inserting Eqs. (32) and (34) into Eq. (43), we obtain for the chemical potential the equation

$$\mu = (\rho + \rho_1 - \sigma_1)g. \quad (45)$$

It is easy to check that the same chemical potential (45) follows from the Hugenholtz-Pines form $\mu = \Sigma_{11}(0, 0) - \Sigma_{12}(0)$ by employing Green function techniques. Both real-time or thermal Green functions can be used, since they are just analytical continuations of each other [36]. Expression (45) is the standard form of the chemical potential in the HFB approximation (see details in the review article [4]).

Comparing Eqs. (20), (39), and (45), we find that the chemical potential of the condensate must satisfy

$$\mu_0 = \varepsilon - \mu = 2\sigma_1 g. \quad (46)$$

In the broken-symmetry phase, where the anomalous average $\sigma_1 \neq 0$, one has $\mu_0 \neq 0$. The value μ_0 can be zero only for an ideal gas, when $g \rightarrow 0$, or in the Bogoliubov approximation [6,7], where the third- and fourth-order Hamiltonian terms (22) and (23) are neglected. But in general, the Lagrange multiplier μ_0 is nonzero, thus making the theory self-consistent.

Using the chemical potential (45) in Eq. (32), we have

$$\xi_{\mathbf{k}} = \frac{\mathbf{k}^2}{2m} + \Delta, \quad (47)$$

and the spectrum (43) takes the form

$$\varepsilon_{\mathbf{k}} = \sqrt{(c\mathbf{k})^2 + \left(\frac{\mathbf{k}^2}{2m}\right)^2}, \quad (48)$$

with the sound velocity

$$c \equiv \sqrt{\frac{\Delta}{m}}. \quad (49)$$

In the long-wave limit $k \rightarrow 0$, the quasiparticle energy $\varepsilon_{\mathbf{k}}$ behaves like ck , thus being gapless, as it should.

For the normal average (26), we find

$$n_{\mathbf{k}} = (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) f_{\mathbf{k}}^b + v_{\mathbf{k}}^2, \quad (50)$$

while for the anomalous average (27), we get

$$\sigma_{\mathbf{k}} = (1 + 2f_{\mathbf{k}}^b) u_{\mathbf{k}} v_{\mathbf{k}}, \quad (51)$$

where the momentum distribution of bosonic quasiparticle excitations

$$f_k^b \equiv \langle b_k^\dagger b_k \rangle = \frac{1}{e^{\beta \varepsilon_k} - 1} \quad (52)$$

can be written in the form

$$f_k^b = \frac{1}{2} \left(\coth \frac{\varepsilon_k}{2T} - 1 \right). \quad (53)$$

The coefficient functions of the Bogoliubov transformation (40) satisfy

$$u_k^2 - v_k^2 = 1, \quad u_k v_k = -\frac{\Delta}{2\varepsilon_k}, \quad (54)$$

and

$$u_k^2 + v_k^2 = \frac{\sqrt{\varepsilon_k^2 + \Delta^2}}{\varepsilon_k} = \frac{\xi_k}{\varepsilon_k}, \quad (55)$$

and read explicitly

$$u_k^2 = \frac{\sqrt{\varepsilon_k^2 + \Delta^2} + \varepsilon_k}{2\varepsilon_k} = \frac{\xi_k + \varepsilon_k}{2\varepsilon_k}, \quad (56)$$

and

$$v_k^2 = \frac{\sqrt{\varepsilon_k^2 + \Delta^2} - \varepsilon_k}{2\varepsilon_k} = \frac{\xi_k - \varepsilon_k}{2\varepsilon_k}. \quad (57)$$

In this way, for the normal average (26), we obtain

$$n_k = \frac{\sqrt{\varepsilon_k^2 + \Delta^2}}{2\varepsilon_k} \coth \frac{\beta \varepsilon_k}{2} - \frac{1}{2}, \quad (58)$$

while the anomalous average (27) becomes

$$\sigma_k = -\frac{\Delta}{2\varepsilon_k} \coth \frac{\beta \varepsilon_k}{2}. \quad (59)$$

The anomalous average (59) is important as compared to the normal average (58). For this purpose, consider these averages as functions of ε_k in the range

$$0 \leq \varepsilon_k. \quad (60)$$

At low momenta or energies, such that $\varepsilon_k \ll \Delta$ and $\varepsilon_k \ll T$, the asymptotic behavior of the normal average (58) is

$$n_k \approx \frac{T\Delta}{\varepsilon_k^2} + \frac{\Delta}{12T} + \frac{T}{2\Delta} - \frac{1}{2}, \quad (61)$$

whereas the anomalous average (59) is

$$\sigma_k \approx -\frac{T\Delta}{\varepsilon_k^2} - \frac{\Delta}{12T} + \frac{\varepsilon_k^2 \Delta}{720T^3}. \quad (62)$$

From here, it is evident that in the long-wave limit the anomalous average is of the same order of magnitude as the normal one, $n_k \approx |\sigma_k|$, only their signs are opposite.

In the short-wave limit, when $\varepsilon_k \gg \Delta$ and $\varepsilon_k \gg T$, the asymptotic behavior of the normal average is

$$n_k \approx \left(\frac{\Delta}{2\varepsilon_k} \right)^2 - \left(\frac{\Delta}{2\varepsilon_k} \right)^4 + e^{-\beta \varepsilon_k}, \quad (63)$$

whereas that of the anomalous average is

$$\sigma_k \approx -\frac{\Delta}{2\varepsilon_k} (1 + 2e^{-\beta \varepsilon_k}). \quad (64)$$

In this limit, the magnitude of the anomalous average becomes much larger than the normal one.

Summarizing, we conclude that, in the above two limits, we have

$$|\sigma_k| \approx n_k \quad (k \rightarrow 0), \quad |\sigma_k| \gg n_k \quad (k \rightarrow \infty). \quad (65)$$

Consequently, the anomalous average is always important.

In the large-volume limit, the sums (28) and (29) can be calculated as momentum integrals, leading to the density of uncondensed particles (28):

$$\rho_1 = \frac{1}{2} \int \frac{d^3 k}{(2\pi)^3} \left[\frac{\sqrt{\varepsilon_k^2 + \Delta^2}}{\varepsilon_k} \coth \frac{\beta \varepsilon_k}{2} - 1 \right], \quad (66)$$

while the anomalous density (29) becomes

$$\sigma_1 = - \int \frac{d^3 k}{(2\pi)^3} \frac{\Delta}{2\varepsilon_k} \coth \frac{\beta \varepsilon_k}{2}. \quad (67)$$

Taking into account relation (34) and using the notation

$$\alpha \equiv \int \frac{d^3 k}{(2\pi)^3} \frac{g}{2\varepsilon_k} \coth \frac{\beta \varepsilon_k}{2}, \quad (68)$$

we obtain

$$\Delta = \frac{\rho_0 g}{1 + \alpha}, \quad (69)$$

so that the anomalous density (67) can be represented in the form

$$\sigma_1 = -\frac{\rho_0 \alpha}{1 + \alpha}. \quad (70)$$

The quantity (68) is ultraviolet divergent. This divergence is caused by the modeling of the short-range interaction in the dilute-gas approximation by a δ -function potential (1). There are two ways of removing this divergence. One may either use a more realistic interaction potential $V(\mathbf{x})$, whose Fourier transform $V_{\mathbf{k}}$ goes to zero for $k \rightarrow \infty$, for instance Gaussian-type potentials [37–39]. More efficiently, with the same physical consequences in the dilute limit, one renormalizes the δ -function potential, replacing it by the scattering matrix obtained from the Lippmann-Schwinger equation. This simply renormalizes the coupling constant g to the renormalized g_R defined by

$$\frac{1}{g_R} \equiv \frac{1}{g} + \int \frac{d^3 k}{(2\pi)^3} \frac{1}{\mathbf{k}^2/2m - i0}. \quad (71)$$

Indeed, the relation to the scattering length in Eq. (2) is really only valid for the renormalized coupling constant g_R , which is usually not mentioned for brevity, until the ultraviolet divergences appear. This procedure is standard for eliminating divergences in calculating the ground-state energy [2–4] as well as the anomalous averages [40–42]. Keeping in mind such a correction, we may consider the quantity (68) as finite.

It is easy to check that condensation proceeds in a second-order phase transition. When $\rho_0 \rightarrow 0$, $\rho_1 \rightarrow \rho$, we see that $\Delta \rightarrow 0$ and $\varepsilon_{\mathbf{k}} \rightarrow k^2/2m$. From Eq. (66), we find the condensation temperature

$$T_c = \frac{2\pi}{m} \left[\frac{\rho}{\zeta(3/2)} \right]^{2/3}, \quad (72)$$

which coincides with that of the ideal gas, as it should be for a dilute gas in mean-field approximation.

IV. ZERO TEMPERATURE

The above equations can be calculated explicitly in the zero-temperature limit, where the density (66) becomes

$$\rho_1 = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \left(\frac{\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta^2}}{\varepsilon_{\mathbf{k}}} - 1 \right). \quad (73)$$

This can also be represented as

$$\rho_1 = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \left(\frac{\xi_{\mathbf{k}}}{\varepsilon_{\mathbf{k}}} - 1 \right). \quad (74)$$

Substituting Eqs. (47) and (48), we find

$$\rho_1 = \frac{(mc)^3}{3\pi^2}. \quad (75)$$

For the fraction of condensed particles

$$n_0 \equiv \frac{\rho_0}{\rho} = 1 - n_1 = 1 - \frac{\rho_1}{\rho}, \quad (76)$$

we obtain

$$n_0 = 1 - \frac{(mc)^3}{3\pi^2} \quad (\rho a^3 = 1), \quad (77)$$

where a is the mean interparticle distance.

The integral (68) becomes, after the renormalization of g according to Eq. (71),

$$\alpha = \frac{g}{2} \int \left(\frac{1}{\varepsilon_{\mathbf{k}}} - \frac{2m}{k^2} \right) \frac{d^3k}{(2\pi)^3}, \quad (78)$$

where g_R is sloppily replaced by g , as usual in such calculations. The value of α is

$$\alpha = -\frac{1}{\pi^2} m^2 c g, \quad (79)$$

so that the anomalous average (70) becomes

$$\sigma_1 = \frac{\rho_0 m^2 c g}{\pi^2 - m^2 c g}. \quad (80)$$

This way of removing the ultraviolet divergences is quantitatively exact for calculating quantities depending only on the scattering length a_s in one-loop approximations [4]. For strong interactions, the shape of the interaction potential becomes important [4,37–39]. In what follows, we shall consider the anomalous average (80) for arbitrary g , but keep in mind that at large g , this expression for σ_1 can be only qualitatively correct. Being proportional to ρ_0 , the anomalous density σ_1 tends to zero for $\rho_0 \rightarrow 0$. However, in a dilute gas at low temperature, ρ_0 is close to ρ as follows from Eq. (77).

In further calculations, it is convenient to introduce the *diluteness parameter*

$$\delta \equiv \rho^{1/3} a_s = \frac{a_s}{a} \quad (81)$$

and to introduce the reduced dimensionless sound velocity

$$\hat{c} \equiv c a m. \quad (82)$$

With this notation, the fraction of condensed particles is given by

$$n_0 = 1 - \frac{\hat{c}^3}{3\pi^2}, \quad (83)$$

and the fraction of uncondensed particles by

$$n_1 = \frac{\hat{c}^3}{3\pi^2}. \quad (84)$$

Combining Eq. (79) with relation (2) for the renormalized g , we obtain

$$\alpha = -\frac{4}{\pi} \hat{c} \delta. \quad (85)$$

The anomalous average (80) is then

$$\sigma_1 = \frac{4\rho\hat{c}\delta}{\pi - 4\hat{c}\delta} n_0. \quad (86)$$

To define the above quantities (83)–(86) as functions of the diluteness parameter (81), we have to know the dependence on δ of the reduced sound velocity (82). For this purpose, we use Eq. (69) in the form

$$\Delta = \frac{4\pi^2\delta}{\pi - 4\hat{c}\delta} \left(\frac{n_0}{ma^2} \right), \quad (87)$$

and recall that $\Delta = mc^2$ according to Eq. (49). Thus, Eq. (87) becomes

$$8\hat{c}^3 - 3\pi\hat{c}^2 + 12\pi^2\delta = 0, \quad (88)$$

which fixes the reduced sound velocity as a function $\hat{c}(\delta)$ of the diluteness parameter. There exists a positive solution of Eq. (88) for \hat{c} in the δ -interval $0 \leq \delta \leq \delta_c$, limited by the critical value

$$\delta_c \equiv \frac{1}{4} \left(\frac{\pi}{3} \right)^{1/3} = 0.253873. \quad (89)$$

Remarkably, there exists an interesting relation between the anomalous average (86) and the density of uncondensed particles ρ_1 . We take the identity following from $\Delta = mc^2$:

$$\Delta ma^2 = (mac)^2 = \hat{c}^2, \quad (90)$$

and substitute on the left-hand side Δ from Eq. (87) to obtain

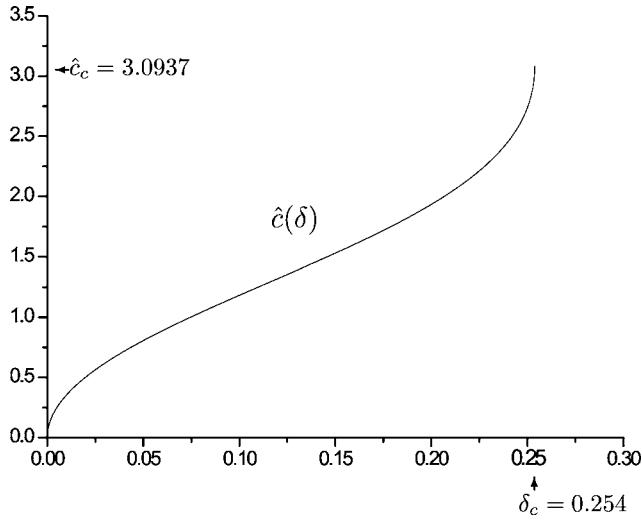


FIG. 1. The reduced sound velocity $\hat{c}=\hat{c}(\delta)$ as a function of the diluteness parameter δ , which is given by the solution of Eq. (88).

$$\hat{c}^2 = \frac{4\pi^2 \delta n_0}{\pi - 4\hat{c}\delta}. \quad (91)$$

Inverting this with respect to δ yields

$$\delta = \frac{\pi \hat{c}^2}{4(\pi^2 n_0 + \hat{c}^3)}. \quad (92)$$

Substituting Eq. (92) into Eq. (86), we obtain

$$\sigma_1 = 3\rho_1. \quad (93)$$

That is, the anomalous average is three times larger than the normal one. This emphasizes once more that at low temperatures the anomalous averages are important.

At the asymptotically small diluteness parameter $\delta \ll 1$, the reduced sound velocity (82) in Eq. (88) behaves as

$$\hat{c} \simeq 2\sqrt{\pi}\delta^{1/2} + \frac{16}{3}\delta^2 + \frac{320}{9\sqrt{\pi}}\delta^{7/2} \quad (\delta \ll 1), \quad (94)$$

while the condensate fraction (83) has the expansion

$$n_0 \simeq 1 - \frac{8}{3\sqrt{\pi}}\delta^{3/2} - \frac{64}{3\pi}\delta^3. \quad (95)$$

Keeping only the first term in the expansion (94), we obtain the Bogoliubov sound velocity $c_B = \sqrt{4\pi\rho a_s/m}$. Retaining on the right-hand side of Eq. (95) the first two terms, we obtain the Bogoliubov depletion formula [6–9]. In the Sec. V, we show that the ground-state energy in the limit $\delta \rightarrow 0$ also gives the known Bogoliubov expression. Thus, in the limit of the small diluteness parameter δ , our equations have the correct asymptotic behavior, reproducing the results of the Bogoliubov approximation.

When the diluteness parameter approaches the critical value (89), the sound velocity $c=\hat{c}/am$ has the expansion

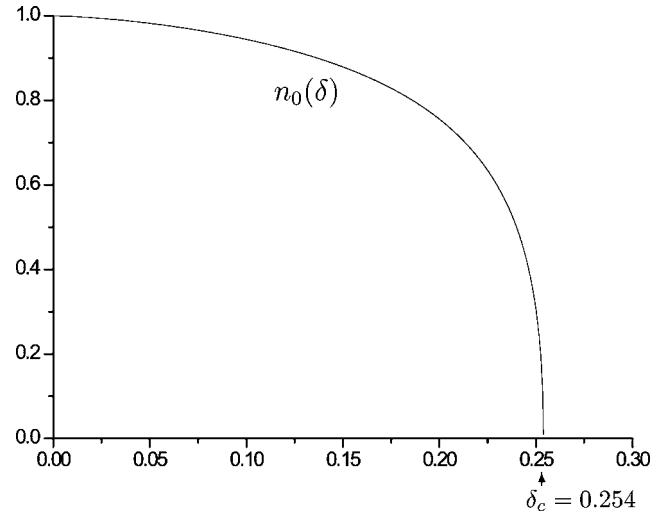


FIG. 2. The condensate fraction $n_0=n_0(\delta)$ as a function of δ , obtained from Eq. (83).

$$\hat{c} \simeq \hat{c}_c - 2\sqrt{3\pi}(\delta_c - \delta)^{1/2} + 8\left(\frac{\pi}{3}\right)^{1/3}(\delta_c - \delta) \quad (\delta \rightarrow \delta_c - 0), \quad (96)$$

with

$$\hat{c}_c \equiv (3\pi^2)^{1/3} = 3.093668. \quad (97)$$

And the condensate fraction is given by

$$n_0 \simeq 6\left(\frac{3}{\pi}\right)^{1/6}(\delta_c - \delta)^{1/2} - 20\left(\frac{3}{\pi}\right)^{1/3}(\delta_c - \delta) \quad (\delta \rightarrow \delta_c - 0). \quad (98)$$

At the critical depletion (89), we have

$$c = \frac{(3\pi^2)^{1/3}}{am}, \quad n_0 = 0 \quad (\delta = \delta_c). \quad (99)$$

The disappearance of the condensate fraction for $\delta \geq \delta_c$ at zero temperature is a signal for a *quantum phase transition*. Here, this transition occurs as a function of the diluteness parameter δ . To display the critical behavior of physical properties, it is convenient to introduce the relative distance variable from the quantum critical point

$$\tau \equiv \frac{\delta - \delta_c}{\delta_c}. \quad (100)$$

Then, the reduced sound velocity behaves in the vicinity of the critical point as

$$\frac{\hat{c} - \hat{c}_c}{\hat{c}_c} \simeq -\tau^{1/2} + \frac{2}{3}\tau \quad (\tau \ll 1). \quad (101)$$

For the condensate fraction, we obtain

$$n_0 \simeq 3\tau^{1/2} - 5\tau \quad (\tau \ll 1), \quad (102)$$

implying that the critical exponent β for the order parameter Ψ is $1/4$.

The overall behavior of the reduced sound velocity $\hat{c} = \hat{c}(\delta)$ and of the condensate fraction $n_0 = n_0(\delta)$ as functions of the diluteness parameter δ are shown in Figs. 1 and 2, respectively. The function $\hat{c}(\delta)$ in Fig. 1 is calculated from Eq. (88). Substituting this $\hat{c}(\delta)$ into Eq. (83), we get the condensate fraction $n_0(\delta)$ plotted in Fig. 2.

V. THERMODYNAMIC CONSISTENCY

As a final important point, we convince ourselves that our self-consistent bosonic HFB approximation involving the new Lagrange multiplier μ_0 is consistent with the thermodynamic formalism, in contrast to previous attempts to generalize the HFB approximation to condensed Bose systems. For the discussion of the inconsistencies, we mention once more the work of Hohenberg and Martin [21] and the subsequent papers [17–19,30–32,43]. The most recent and very clear analysis of the problem was given in the review article by Andersen [4].

The grand-canonical potential Ω in Eq. (12) and the associated Hamiltonian H in Eq. (13) make it possible to find all thermodynamic properties of the system. The free energy (9) is connected with the grand potential (12) through the relation

$$\Omega = F - \mu_0 N_0 - \mu N. \quad (103)$$

The Lagrange multipliers μ_0 and μ should not be confused with the standard chemical potential defined for the system without condensate. In the presence of a condensate, its role is played by what we may call *effective system chemical potential*, denoting it by $\tilde{\mu}$. In the condensed phase, it is given by

$$\tilde{\mu} \equiv \mu_0 n_0 + \mu, \quad (104)$$

where $n_0 \equiv N_0/N$. With this definition, the grand-canonical potential (103) satisfies the usual thermodynamic relation

$$\Omega = F - \tilde{\mu} N. \quad (105)$$

Its differential satisfies

$$d\Omega = -SdT - PdV - Nd\tilde{\mu}, \quad (106)$$

where S is entropy and P pressure. For the free energy F , this implies

$$dF = -SdT - PdV + \tilde{\mu}dN. \quad (107)$$

Thus, the system chemical potential $\tilde{\mu}$ is given by the derivative

$$\tilde{\mu} = \left(\frac{\partial F}{\partial N} \right)_{TV}. \quad (108)$$

From these expressions, we may calculate all thermodynamic properties of the condensed Bose gas. Thus, our self-consistent HFB approximation obeys the standard thermodynamic formalism.

As an illustration, let us verify the consistency of the above two definitions (104) and (108) for the system chemical potential. To be explicit, consider a dilute Bose gas at

zero temperature, representing the universal terms [4], which are asymptotically exact for all short-range interaction potentials with scattering length a_s .

At zero temperature, the free energy coincides with the internal ground-state energy, $F=E$. Then, Eq. (108) reduces to

$$\tilde{\mu} = \left(\frac{\partial E}{\partial N} \right)_V \quad (T=0). \quad (109)$$

The internal energy is, by definition,

$$E = \langle H \rangle + \tilde{\mu}N, \quad (110)$$

where H is the grand-canonical Hamiltonian (13). The average $\langle H \rangle$ is given in the HFB approximation by

$$\langle H \rangle = E_B = E_{\text{HFB}} + V \int \frac{d^3 k}{(2\pi)^3} (\varepsilon_{\mathbf{k}} - \xi_{\mathbf{k}}), \quad (111)$$

where, according to Eqs. (42) and (19),

$$\begin{aligned} E_{\text{HFB}} &= H^{(0)} - \frac{gV}{2}(2\rho_1^2 + \sigma_1^2) = N_0 \left(\frac{1}{2}\rho_0 g - \mu_0 - \mu \right) \\ &\quad - \frac{gV}{2}(2\rho_1^2 + \sigma_1^2). \end{aligned} \quad (112)$$

For the explicit calculation of the integral in (111) in the dilute gas, we perform the usual subtraction implied by the renormalization of g in Eq. (71). The subtracted integral becomes

$$\frac{1}{2} \int \frac{d^3 k}{(2\pi)^3} \left[\varepsilon_{\mathbf{k}} - \xi_{\mathbf{k}} + \frac{m^3 c^4}{k^2} \right] = \frac{8m^4 c^5}{15\pi^2}. \quad (113)$$

Employing the results of Sec. IV, we find for the internal energy, which at $T=0$ is the ground-state energy,

$$E \approx \frac{gN^2}{2V} \left(1 + \frac{128}{15\sqrt{\pi}} \delta^{3/2} \right). \quad (114)$$

This is the expression derived by Lee *et al.* [44,45] for a hard-sphere potential. It is universal in the sense that it applies to any short-range potential with scattering length a_s [4]. Differentiating Eq. (114) with respect to N we obtain, according to Eq. (109) and using the fact that $F=E$ at $T=0$, the effective chemical potential

$$\tilde{\mu} \approx \rho g \left(1 + \frac{32}{3\sqrt{\pi}} \delta^{3/2} \right), \quad (115)$$

where we have inserted the derivative $\partial\delta/\partial N = \delta/3N$. The same result is obtained from Eq. (104), showing the self-consistency of our HFB approximation.

It is important to emphasize that the self-consistency in our approach has been achieved by accurately taking into account all normalization conditions, which required the introduction of the additional Lagrange multiplier μ_0 . It is due to the latter that our HFB approximation is completely self-consistent and displays no gap in the spectrum. Without μ_0 , we would plunge back to the known problem of the standard HFB approximation, which is not self-consistent and pos-

sesses an unphysical gap in the spectrum [17–19,30–32,43].

In conclusion, we have presented a new bosonic self-consistent HFB approximation. It is derived from a variational principle and preserves all symmetries of the Hamiltonian. At the same time, it is gapless in the condensed phase, thus solving an old outstanding problem of Bose systems. We did not invoke any unjustified tricks as in previous attempts with the same goal, such as omitting anomalous averages, and avoided any mismatch of approximations by adding additional phenomenological terms to remove the gap. This became possible by accurately taking into account

two normalization conditions. Thus our HFB approximation is conserving, gapless, and self-consistent.

ACKNOWLEDGMENTS

We thank E. P. Yukalova for numerical calculations and useful advice. One of the authors (V.I.Y.) is grateful for financial support of the German Research Foundation and to the Physics Department of the Freie Universität Berlin for its hospitality.

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