Bose-Einstein-condensed systems of hard spheres at high density

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The properties of Bose-Einstein-condensed systems of hard spheres at high density are studied by taking into account higher-order corrections beyond the Hartree-Fock-Bogoliubov approximation. Based on a diagrammatic technique of the perturbation expansion starting from the Bogoliubov approximation, we show that the effective interactions separate into two distinct parts: the screened and condensate-mediated interactions. The latter is described by the exchange of virtual quasiparticles between noncondensate bosons via the Bose-Einstein condensate and is attractive for small energy transfer. We calculate the condensation temperature, excitation spectrum, and condensate density in the whole region of the gas parameter. It is shown that the condensate temperature decreases compared to that of an ideal Bose gas due to hard-sphere interactions. We find that the condensate-mediated attraction between noncondensate bosons leads to an enhancement of the anomalous self-energy and, as a consequence, to the emergence of a roton minimum in the excitation spectrum and to the strong suppression of the condensate fraction in the region of high density.

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I. INTRODUCTION

The physical properties of Bose-Einstein-condensed systems are currently a topic of intensive research. The most thorough studies have been accomplished for weakly interacting Bose gases [1–7], where the Bogoliubov theory [8] is applicable and the interparticle interactions can be modeled by a contact potential. Extension of the Bogoliubov theory to Bose systems with strong interactions and high density, such as superfluid ^{4}He, is of long-standing interest. Present-day Feshbach-resonance techniques do allow for the variation of the interaction strength in a very wide range for trapped alkali gases [9–11].

A natural extension of the Bogoliubov theory is a self-consistent theory within the Hartree-Fock-Bogoliubov (HFB) approximation. The self-consistent HFB approximation, however, has well-known problems [1], such as the violation of various conservation laws and the presence of an energy gap in the excitation spectrum. Proukakis *et al.* [12] have argued that these problems arise because the actual interaction potential is simply replaced with a contact potential, which is equivalent to a t matrix, approximated to first order in the s-wave scattering length. As a matter of fact, the use of the first-order approximation for the t matrix in the HFB approximation is not really consistent since it involves an overcounting of diagrams that contribute to the anomalous self-energy [1,13].

There have been several attempts to make the HFB approximation self-consistent by neglecting the anomalous self-energy diagrams [14,15], by adding to this approximation some higher-order terms [16–19], or by introducing an additional normalization condition [3]. Recently we [20] have developed a self-consistent t matrix theory of the HFB approximation for Bose systems of hard spheres by replacing the actual potential by a t matrix obtained from the Lippmann-Schwinger equation. The self-consistent HFB spectrum has the Brueckner-Sawada form [21] with modified coefficients, being gapless and linear for small wave vectors. As wave vectors become large, however, this spectrum changes from linear to quadratic monotonously without a roton minimum. The phonon-roton spectrum of superfluid ^{4}He has been deduced by Landau [22] in the course of analyzing thermodynamic properties and has been confirmed by many experiments.

In this paper, we investigate the effects of higher-order self-energy diagrams beyond the HFB approximation for Bose systems of hard spheres at high density. Based on a diagrammatic technique of perturbation theory starting from the Bogoliubov approximation, we show that the effective interactions between noncondensate bosons separate two distinct parts: one is the screened interaction, which can be represented as the sum of repeated polarization functions, and another part is the sum of the remaining diagrams, which cannot be represented as the form of a screened interaction. The latter is a quasiparticle-exchange interaction between noncondensate bosons via the Bose-Einstein condensate, which becomes attractive for small energy transfer. For Bose systems of hard spheres, the screened interaction and vertex corrections can be neglected and the leading higher-order corrections to the HFB approximation come from the self-energy diagrams involving the condensate-mediated attraction at low temperature. Using the condensate-mediated attraction calculated in the HFB approximation, we calculate the excitation spectrum, condensate density, and condensation temperature as a function of the gas parameter. We use the system of units with $\hbar \equiv 1$ and $k_B \equiv 1$.

II. SELF-ENERGY AND EFFECTIVE INTERACTIONS

The system we are concerned with consists of N bosons with zero spin, enclosed in a box of volume V and interacting through the two-body potential $v(\mathbf{r})$. In the presence of a Bose-Einstein condensate, the U(1) symmetry of the system is spontaneously broken and the field operator is separated by means of the Bogoliubov prescription [8] into two parts:

$$\psi(r) = n_0^{1/2} + \varphi(r), \tag{1}$$

where $n_0 = N_0/V$ is the condensate density, and the field operator

$$\varphi(\mathbf{r}) = V^{-1/2} \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{2}$$

describes noncondensate bosons.

With this Bogoliubov prescription, we obtain for the grand-canonical Hamiltonian of Bose-Einstein-condensed systems the sum of five terms,

$$H = H^{(0)} + H^{(1)} + H^{(2)} + H^{(3)} + H^{(4)}, \tag{3}$$

depending on the power of $\varphi(\mathbf{r})$. The zero-order term is free of $\varphi(\mathbf{r})$, which is given by a c-number,

$$H^{(0)} = \left[\tfrac{1}{2} n_0 v(0) - \mu\right] N_0. \tag{4}$$

The first-order term vanishes, that is, $H^{(1)} = 0$, because this would violate momentum conservation. The second-, third-, and fourth-order terms are given by

$$H^{(2)} = \frac{1}{V} \sum_{\mathbf{k}\neq 0} \Big\{ [(\varepsilon_k - \mu) + N_0 v(0) + N_0 v(\mathbf{k})] a_{\mathbf{k}}^{+} a_{\mathbf{k}} + \frac{N_0}{2} v(\mathbf{k}) [a_{\mathbf{k}}^{+} a_{-\mathbf{k}}^{+} + a_{\mathbf{k}} a_{-\mathbf{k}}] \Big\}, \tag{5}$$

$$H^{(3)} = \left(\frac{n_0}{V}\right)^{1/2} {\sum_{\mathbf{k},\mathbf{q}}}' v(\mathbf{q}) [a_{\mathbf{k}}^{+} a_{\mathbf{q}}^{+} a_{\mathbf{k}+\mathbf{q}} + a_{\mathbf{k}+\mathbf{q}}^{+} a_{\mathbf{k}} a_{\mathbf{q}}], \tag{6}$$

$$H^{(4)} = \frac{1}{2V} {\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}}' v(\mathbf{q}) a_{\mathbf{k}+\mathbf{q}}^{+} a_{\mathbf{k}'-\mathbf{q}}^{+} a_{\mathbf{k}'} a_{\mathbf{k}}, \tag{7}$$

respectively. Here, $v(\mathbf{q})$ is the Fourier transform of the interparticle potential $v(\mathbf{r})$, μ is the chemical potential, and $\varepsilon_{\mathbf{k}} = \mathbf{k}^2/2m$. The primes on the summation symbols imply that the summation does not include any zero-momentum operators.

In order to evaluate the thermodynamical properties of the system, we can use the single-particle Green's function for noncondensate bosons, which is defined as

$$G_{11}(\mathbf{k},\tau) = -\langle T_\tau a_{\mathbf{k}}(\tau) a_{\mathbf{k}}^{+}(0)\rangle, \tag{8}$$

with the modified $\tau-$dependent Heisenberg picture

$$a_{\mathbf{k}}(\tau) = e^{H\tau} a_{\mathbf{k}} e^{-H\tau}, \quad a_{\mathbf{k}}^{+}(\tau) = e^{H\tau} a_{\mathbf{k}}^{+} e^{-H\tau}. \tag{9}$$

Here, the brackets $\langle\cdots\rangle$ denote the grand canonical ensemble average. In the above Bogoliubov broken-symmetry prescription, the condensate acts like a classical particle reservoir, which noncondensate bosons can enter and leave via scattering, and the number of bosons in the system described by noncondensate operators $a_{\mathbf{k}}^{+}$ and $a_{\mathbf{k}}$ is no longer a constant of motion. Therefore, we must also introduce two anomalous Green's functions,

$$G_{12}(\mathbf{k},\tau) = -\langle T_\tau a_{\mathbf{k}}(\tau) a_{-\mathbf{k}}(0)\rangle, \tag{10}$$

$$G_{21}(\mathbf{k},\tau) = -\langle T_\tau a_{-\mathbf{k}}^{+}(\tau) a_{\mathbf{k}}^{+}(0)\rangle, \tag{11}$$

which represent the disappearance and appearance of two noncondensate bosons. The Green's function $G_{11}(\mathbf{k},\tau)$ is usually called the normal Green's function, which represents the propagation of a single boson.

The Dyson equations for the normal and anomalous Green's functions in Bose-Einstein-condensed systems were first derived by Beliaev [23] and can be compactly written in a 2×2 matrix form as

$$G^{-1}(p) = G_0^{-1}(p) - \Sigma(p), \tag{12}$$

with

$$G(p) = \begin{pmatrix} G_{11}(p) & G_{12}(p) \\ G_{21}(p) & G_{11}(-p) \end{pmatrix}, \tag{13}$$

$$\Sigma(p) = \begin{pmatrix} \Sigma_{11}(p) & \Sigma_{12}(p) \\ \Sigma_{21}(p) & \Sigma_{11}(-p) \end{pmatrix}, \tag{14}$$

$$G_0^{-1}(p) = \begin{pmatrix} g^{-1}(p) & 0 \\ 0 & g^{-1}(-p) \end{pmatrix}, \tag{15}$$

where $g(p) = [i\omega_n - \varepsilon_{\mathbf{k}} + \mu]^{-1}$ is the free-boson Green's function. We use the letter p to represent the four-dimensional vector $(\mathbf{k}, i\omega_n)$, where $\omega_n = 2\pi n T$, with $n = 0,1,2,\ldots$, is the boson Matsubara frequency. In the self-energy matrix $\Sigma(p)$, the diagonal element, $\Sigma_{11}(p)$, is the normal self-energy, and the off-diagonal elements, $\Sigma_{21}(p)$ and $\Sigma_{12}(p)$, are the anomalous self-energies.

Since Σ is a 2×2 matrix, it can be expanded in the complete set consisting of the unit matrix $\mathbf{1}$ and the Pauli matrixes $\boldsymbol{\tau} = (\tau^1, \tau^2, \tau^3)$ as follows:

$$\Sigma(p) = i\omega_n [1 - Z(p)]\tau^3 + S(p)\mathbf{1} + \Delta(p)\tau^1, \tag{16}$$

where Z, S, and Δ are defined by

$$i\omega_n [1 - Z(p)] = \tfrac{1}{2}[\Sigma_{11}(p) - \Sigma_{11}(-p)], \tag{17}$$

$$S(p) = \tfrac{1}{2}[\Sigma_{11}(p) + \Sigma_{11}(-p)], \tag{18}$$

$$\Delta(p) = \Sigma_{21}(p) = \Sigma_{12}(p). \tag{19}$$

The Dyson equation, Eq. (12), can be solved to give

$$G(p) = \frac{1}{D(p)} \{ i\omega_n Z(p)\tau^3 + [\varepsilon(\mathbf{k}) - \mu + S(p)]\mathbf{1} + \Delta(p)\tau^1 \}, \tag{20}$$

with

$$D(p) = [i\omega_n Z(p)]^2 - [\varepsilon(\mathbf{k}) - \mu + S(p)]^2 + \Delta^2(p). \tag{21}$$

This equation expresses the Green's function in terms of the exact self-energy and is therefore entirely general. Approximate solutions are determined by our choice of self-energy.

The Green's function can be used to calculate the physical quantities of Bose-Einstein-condensed systems. The poles of the Green's function give the energy spectrum of elementary excitations. It is easy to check that, in the $\mathbf{k}\to 0$ limit, the Green's function has a pole at $i\omega_n = 0$ if

$$\mu = \Sigma_{11}(0,0) - \Sigma_{12}(0,0). \tag{22}$$

In fact, this relation can be shown to be true to all orders in perturbation theory and is known as the Hugenholtz-Pines theorem [24,25]. The density of particles in the system is given from its definition by

$$n = n_0 - T \int \frac{d^3k}{(2\pi)^3} \sum_n e^{i\omega_n 0^+} G(\mathbf{k}, i\omega_n). \tag{23}$$

This relation may be used together with Eq. (22) to find the condensate density $n_0(n,T)$. The problem is thus reduced to the evaluation of the Green's functions within an approximation for the self-energies.

The Bogoliubov approximation consists of keeping the lowest-order self-energy diagrams that contain condensate lines. The self-energy in the Bogoliubov approximation can be written as

$$\Sigma_B(p) = n_0 v(0)\mathbf{1} + n_0 v(\mathbf{k})(\mathbf{1} + \tau^1). \tag{24}$$

Using Eq. (24) in Eq. (12), we obtain

$$\begin{aligned} G_B^{-1}(p) &= G_0^{-1}(p) - \Sigma_B(p) \\ &= i\omega_n \tau^3 - [\varepsilon_{\mathbf{k}} - \mu + n_0 v(0) + n_0 v(\mathbf{k})]\mathbf{1} \\ &\quad - n_0 v(\mathbf{k})\tau^1. \end{aligned} \tag{25}$$

This is the Green's function in the Bogoliubov approximation. Note that it is the exact result obtained from a quadratic approximation to the Hamiltonian, i. e., by neglecting the third- and fourth-order terms $H^{(3)}$ and $H^{(4)}$ in Eq. (3).

The Bogoliubov approximation can be made the starting point for a systematic perturbation expansion, in which the unperturbed operator is the quadratic Bogoliubov Hamiltonian $H_0 = H^{(0)} + H^{(2)}$ and the perturbation is given by $H_I = H^{(3)} + H^{(4)}$. In this perturbation theory, the Dyson equation can be written as

$$G^{-1}(p) = G_B^{-1}(p) - \tilde{\Sigma}(p), \tag{26}$$

where $\tilde{\Sigma}(p)$ is the sum of all higher-order self-energy diagrams beyond the Bogoliubov approximation. Combining this equation with the Dyson-Beliaev equation (12), the self-energy is obtained by

$$\begin{aligned} \Sigma(p) &= \Sigma_B(p) + \tilde{\Sigma}(p) \\ &= n_0 v(0)\mathbf{1} + n_0 v(\mathbf{k})(1 + \tau^1) + \tilde{\Sigma}(p). \end{aligned} \tag{27}$$

We develop a diagrammatic technique of perturbation theory starting from the Bogoliubov approximation and calculate the higher-order corrections $\tilde{\Sigma}(p)$ to the self-energy $\Sigma(p)$. With this result for $\tilde{\Sigma}$, we show the diagrammatic representation for the self-energy $\Sigma = \Sigma_B + \tilde{\Sigma}$ in Fig. 1(a).

It is very important to emphasize that the interaction lines of $H^{(3)}$ included in the perturbation $H_I = H^{(3)} + H^{(4)}$ can have only one condensate line either coming out or going in. Therefore, the diagrams of the higher-order self-energy $\tilde{\Sigma}$ cannot involve the interaction lines with two condensate lines. From this fact, we see that the interaction diagrams can separate into two distinct parts. One is the usual screened interaction $V_s(q)$, shown in Fig. 1(b), which is represented as the sum of repeated polarization functions and can be written as

$$\begin{aligned} V_s(q) &= v(\mathbf{q}) + v(\mathbf{q})\Pi(q)v(\mathbf{q}) + v(\mathbf{q})\Pi(q)v(\mathbf{q})\Pi(q)v(\mathbf{q})\cdots \\ &= v(\mathbf{q}) + v(\mathbf{q})\Pi(q)V_s(q), \end{aligned} \tag{28}$$

where $\Pi(q)$ is the polarization function.

Another part, V_k, is the sum of the remaining diagrams, shown in Fig. 1(c), which cannot be represented as the form of the screened interaction in Eq. (28). This interaction V_k is a quasiparticle-exchange interaction between noncondensate bosons via the Bose-Einstein condensate. We shall call this

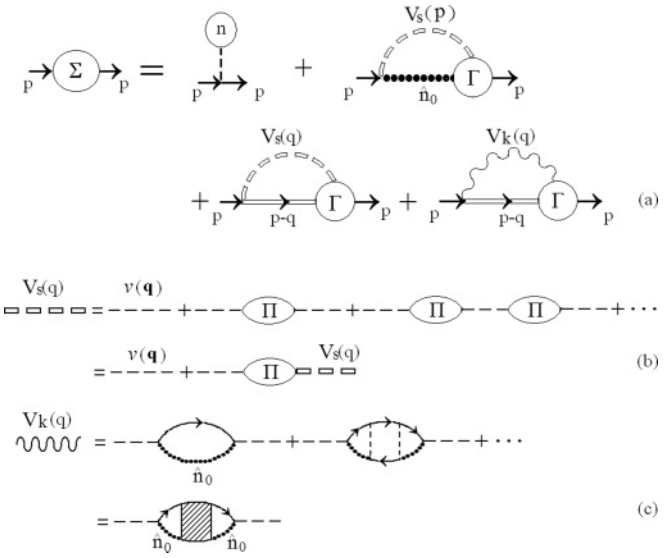

FIG. 1. Diagrammatic representation for the self-energy (a), screened interaction (b), and condensate-mediated interaction (c). A solid line with momentum p represents the Green's function matrix $G(p)$, a dotted line denotes the matrix $\hat{n}_0 = n_0(\mathbf{1} + \tau^1)$ having zero momentum, a dashed line is the bare interaction $v(\mathbf{q})$, Γ is the vertex function, and Π is the polarization function.

interaction the condensate-mediated interaction. Note that the condensate-mediated interaction exists only between noncondensate bosons, but neither between condensate bosons nor between the condensate and noncondensate bosons.

The self-energy diagrams shown in Fig. 1(a) can be written explicitly as

$$\begin{aligned} \Sigma(p) &= nv(0)\mathbf{1} + n_0 V_s(p)(\mathbf{1} + \tau^1)\Gamma(0,p;p) \\ &\quad - T\int \frac{d^3q}{(2\pi)^3} \sum_{i\omega_n} [V_s(q) + V_k(q)]G(p-q) \\ &\quad \times \Gamma(p-q,q;p), \end{aligned} \tag{29}$$

where Γ is the vertex function. In the weakly Bose-Einstein-condensed limit ($n_0/n \ll 1$), the condensate-mediated interaction V_k can be neglected and then Eq. (29) reduces to that proposed by Pashitskii *et al.* [26]. Our main aim in the present paper is to investigate the effects of the condensate-mediated interaction V_k on the properties of Bose-Einstein-condensed systems.

III. BOSE-EINSTEIN CONDENSATION TEMPERATURE

In this section, we study the properties of Bose systems of hard spheres near the Bose-Einstein condensation temperature T_c. Since the condensate density n_0 is very small near T_c, we can neglect the higher-order corrections and use the HFB approximation defined by Eq. (29) with $V_k = 0$, $V_s = v$, and $\Gamma = 1$. The self-energy $\Sigma(p)$ in the HFB approximation is written explicitly as

$$\begin{aligned} \Sigma(\mathbf{k}) &= nv(0)\mathbf{1} + n_0 v(\mathbf{k})(\mathbf{1} + \tau^1) \\ &\quad - \int \frac{d^3q}{(2\pi)^3} v(\mathbf{k}-\mathbf{q}) T \sum_{i\omega_n} G(\mathbf{q}, i\omega_n). \end{aligned} \tag{30}$$

Since $v(\mathbf{k})$ does not depend on the frequency, one sees that neither does $\Sigma(\mathbf{k})$. With the separation into the normal and anomalous components,

$$\Sigma(\mathbf{k}) = [nv(0) + \phi(\mathbf{k})]\mathbf{1} + \Delta(\mathbf{k})\tau^1, \tag{31}$$

the Dyson-Beliaev equation, Eq. (12), yields

$$G(\mathbf{k},i\omega_n) = \frac{i\omega_n\tau^3 + e(\mathbf{k})\mathbf{1} - \Delta(\mathbf{k})\tau^1}{[i\omega_n - E(\mathbf{k})][i\omega_n + E(\mathbf{k})]}, \tag{32}$$

where $E(\mathbf{k}) = \sqrt{e^2(\mathbf{k}) - \Delta^2(\mathbf{k})}$ is the excitation spectrum given by the poles of Green's functions, with the notations $e(\mathbf{k}) = \varepsilon(\mathbf{k}) - \tilde{\mu} + \phi(\mathbf{k})$ and $\tilde{\mu} = \mu - nv(0)$.

By substituting Eq. (32) into the self-energy equation (30) and performing the frequency sum, we obtain the following equations for $\phi(\mathbf{k})$ and $\Delta(\mathbf{k})$:

$$\phi(\mathbf{k}) = n_0 v(\mathbf{k}) + \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} v(\mathbf{k}-\mathbf{q}) \times \left[\frac{e(\mathbf{q})}{E(\mathbf{q})}\coth\frac{E(\mathbf{q})}{2T} - 1\right], \tag{33}$$

$$\Delta(\mathbf{k}) = n_0 v(\mathbf{k}) - \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} v(\mathbf{k}-\mathbf{q})\frac{\Delta(\mathbf{q})}{E(\mathbf{q})}\coth\frac{E(\mathbf{q})}{2T}. \tag{34}$$

By introducing the quantity $T(\mathbf{k})$ defined by $\Delta(\mathbf{k}) = n_0 T(\mathbf{k})$, Eq. (34) can be rewritten for $T(\mathbf{k})$ as follows:

$$T(\mathbf{k}) = v(\mathbf{k}) + \int \frac{d^3q}{(2\pi)^3} v(\mathbf{k}-\mathbf{q})K(\mathbf{q})T(\mathbf{q}), \tag{35}$$

with $K(\mathbf{q}) = -[2E(\mathbf{q})]^{-1}\coth E(\mathbf{q})/2T$. For free particles with $E(\mathbf{q}) = \varepsilon(\mathbf{q}) = \mathbf{k}^2/2m$ at the zero temperature $T = 0$, Eq. (35) reduces to the Lippmann-Schwinger equation for a t matrix $t(\mathbf{k}) = t(\mathbf{k},\mathbf{k}' = 0)$:

$$t(\mathbf{k}) = v(\mathbf{k}) + \int \frac{d^3q}{(2\pi)^3} v(\mathbf{k}-\mathbf{q})K_0(\mathbf{q})t(\mathbf{q}), \tag{36}$$

with $K_0(\mathbf{q}) = -[2\varepsilon(\mathbf{q})]^{-1}$. This t matrix describes a transition due to the collision between two particles in vacuum via the interparticle potential $v(\mathbf{k})$. When comparing Eq. (35) with Eq. (36), one sees that the quantity $T(\mathbf{k})$ is a t matrix describing the similar effect in a medium with the quasiparticle energy $E(\mathbf{k})$.

In a similar way in our previous work [20], we use the Lippmann-Schwinger equation, Eq. (36), to eliminate the bare interaction $v(\mathbf{k})$ in Eq. (35) for the t matrix $T(\mathbf{k})$, arriving at

$$T(\mathbf{k}) = t(\mathbf{k}) + \int \frac{d^3q}{(2\pi)^3} t(\mathbf{k}-\mathbf{q})[K(\mathbf{q}) - K_0(\mathbf{q})]T(\mathbf{q}). \tag{37}$$

This is the equation for $T(\mathbf{k})$ expressed in terms of the t matrix $t(\mathbf{k})$ instead of the bare interaction $v(\mathbf{k})$. In order to eliminate the bare interaction $v(\mathbf{k})$ in Eq. (33) for $\phi(\mathbf{k})$, we use Eq. (35) for $T(\mathbf{k})$ to obtain

$$\phi(\mathbf{k}) = n_0 T(\mathbf{k}) + \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} T(\mathbf{k}-\mathbf{q}) \times \left[\frac{e(\mathbf{q}) + \phi(\mathbf{q})}{E(\mathbf{q})}\coth\frac{E(\mathbf{q})}{2T} - 1\right]. \tag{38}$$

This equation expresses $\phi(\mathbf{k})$ in terms of the t matrix $T(\mathbf{k})$, while $T(\mathbf{k})$ in turn is expressed in terms of the vacuum t matrix $t(\mathbf{k})$ determined by Eq. (36). In other words, through the intermediate function $T(\mathbf{k})$, we can relate $\phi(\mathbf{k})$ directly to the t matrix $t(\mathbf{k})$. Thus, we have obtained a set of the self-consistent equations for the normal and anomalous self-energies $\phi(\mathbf{k})$ and $\Delta(\mathbf{k})$ in terms of a t matrix $t(\mathbf{k})$ within the HFB approximation for a finite temperature.

We are now ready to calculate the excitation spectrum by solving Eqs. (36)–(38) for a hard-sphere interaction with radius a. By solving Eq. (36), we obtain

$$t(\mathbf{k}) = \frac{4\pi a}{m}\frac{\sin ka}{ka}, \tag{39}$$

with $k = |\mathbf{k}|$. Since the t matrix $t(\mathbf{k})$ in Eq. (39) depends only on $k = |\mathbf{k}|$, we can put the solutions of Eqs. (37) and (38) in the forms

$$T(k) = zt(k), \tag{40}$$

$$\phi(k) = \delta T(k) = \delta z t(k). \tag{41}$$

Then, the chemical potential is given from Eq. (22) by

$$\tilde{\mu} = z(\delta - n_0)\frac{4\pi a}{m} \tag{42}$$

and the excitation energy $E(\mathbf{k}) = \sqrt{e^2(\mathbf{k}) - \Delta^2(\mathbf{k})}$ reduces to

$$E(k) = \frac{1}{2ma^2}\xi(ka), \tag{43}$$

with

$$\xi(x) = \left\{\left[x^2 - (\eta - \eta_0)z + \eta z\frac{\sin x}{x}\right]^2 - \left[\eta_0 z\frac{\sin x}{x}\right]^2\right\}^{1/2}. \tag{44}$$

Here the parameters $\eta = 8\pi\delta a^3$ and $\eta_0 = 8\pi n_0 a^3$ have been introduced.

The equations for parameters z and δ are obtained by substituting Eqs. (40) and (41) into Eqs. (37) and (38):

$$z = 1 - z\frac{2}{\pi}\int_0^\infty dx \sin^2 x\left[\frac{1}{\xi(x)}\coth\frac{\xi(x)}{2t} - \frac{1}{x^2}\right], \tag{45}$$

$$\eta = z\eta_0 + \frac{2}{\pi}\int_0^\infty dx x \sin x \times \left(\frac{x^2 - z(\eta-\eta_0) + 2z\eta x^{-1}\sin x}{\xi(x)}\coth\frac{\xi(x)}{2t} - 1\right), \tag{46}$$

with $t = 2\pi a^2 T$ being the dimensionless temperature. From Eq. (23) the parameter $\eta_0 = 8\pi n_0 a^3$ is given by

$$\eta_0 = 8\pi n a^3 - \frac{2}{\pi}\int_0^\infty dx x^2 \times \left(\frac{x^2 - z(\eta-\eta_0) + z\eta x^{-1}\sin x}{\xi(x)}\coth\frac{\xi(x)}{2t} - 1\right). \tag{47}$$

Given a temperature t and gas parameter na^3, Eqs. (45)–(47) enable us to determine the parameters z, η, and η_0.

We start by calculating the Bose-Einstein condensation temperature t_c. This is the temperature at which all the particles can be accommodated in the excited states and is determined

by $\eta_0(t_c) = 0$. We obtain from Eq. (47) the following equation for t_c:

$$\int_0^\infty dx x^2 \left[\coth \frac{x^2 - \Lambda_1(1 - x^{-1}\sin x)}{2t_c} - 1 \right] = 4\pi^2 n a^3, \tag{48}$$

with $\Lambda_1 = zn$. Here, the parameters z and η are determined by Eqs. (45) and (46) with $\eta_0 = 0$ and $t = t_c$. From Eq. (46) the parameter $\Lambda_1 = zn$ is given by

$$\Lambda_1 = z\frac{2}{\pi}\int_0^\infty dx x \sin x \left[\frac{x^2 - \Lambda_1(1 - 2x^{-1}\sin x)}{x^2 - \Lambda_1(1 - x^{-1}\sin x)} \times \coth \frac{x^2 - \Lambda_1(1 - x^{-1}\sin x)}{2t_c} - 1 \right]. \tag{49}$$

Equation (45) yields

$$z^{-1} = \frac{2}{\pi}\int_0^\infty dx \frac{\sin^2 x}{x^2 - \Lambda_1(1 - x^{-1}\sin x)} \times \coth \frac{x^2 - \Lambda_1(1 - x^{-1}\sin x)}{2t_c}. \tag{50}$$

Given the gas parameter na^3, Eq. (48) together with Eqs. (49) and (50) enable us to determine the condensate temperature.

First, we find an analytic expression for t_c in the low-density limit ($na^3 \ll 1$). The integrals come mainly from the range of small x, where we can use $x^{-1}\sin x \simeq 1 - x^2/6$. In this case, Eqs. (49) and (50) yield $z = 1$ and $\Lambda_1 = 8\pi na^3$, and we get from Eq. (48)

$$\frac{t_c - t_{c0}}{t_{c0}} = -\frac{2\pi}{9.93} n^{1/3} a, \tag{51}$$

where t_{c0} is the condensation temperature of the ideal Bose gas. Thus the condensation temperature T_c decreases compared to that of an ideal Bose gas and the relative shift is linear with $n^{1/3}a$ in the low-density limit. This linear relation has first been predicted by Baym *et al.* [27,28], using effective-field-theory methods, but an increase in T_c has been obtained in their calculations and other calculations (see review article [1]). We show that T_c decreases due to hard-sphere interaction in good agreement with the experiments on liquid ^{4}He.

In order to investigate the dependence of the condensation temperature T_c on the parameter $\gamma = n^{1/3}a$, we solve numerically the system of Eqs. (48)–(50). Figure 2 presents

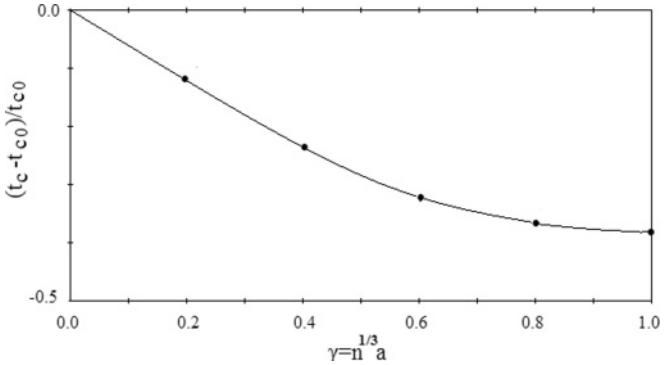

FIG. 2. Bose-Einstein condensation temperature shift $\Delta t = (t_c - t_{c0})/t_{c0}$ as a function of the gas parameter $\gamma = n^{1/3}a$.

the shift $\Delta t = (t_c - t_{c0})/t_{c0}$ calculated as a function of the gas parameter γ. At small γ, up to $\gamma = 0.2$, the shift is proportional to γ. For $\gamma = 0.61$ corresponding to liquid ^{4}He, we have $\Delta t = -0.33$, yielding $T_c = 2.11$ K, which is close to the superfluid transition temperature 2.17 K. In the region of larger $\gamma > 0.7$, the shift is almost constant as $\Delta t = -0.35$.

We now turn to the calculation of the excitation spectrum $E(k)$ and condensate density n_0 by solving Eqs. (45)–(47) self-consistently. At the condensate temperature T_c, we have $\eta_0 = 0$ and then Eq. (44) reduces to

$$\xi(x) = x^2 - \Lambda_1(1 - x^{-1}\sin x), \tag{52}$$

with $x = ka$. The parameter Λ_1 is determined by solving Eqs. (49) and (50) together with Eq. (48), which is given as a function of the gas parameter $n^{1/3}a$. In the long-wavelength limit $k \to 0, \xi(x) = (1 - \Lambda_1/6)x^2$ and the excitation spectrum $E(k)$ behaves like a free-particle spectrum $k^2/2m*$, with the effective mass $m* = m/(1 - \Lambda_1/6)$. Since the parameter Λ_1 is very small, we can neglect it in the calculation. At the low-density limit $na^3 \ll 1$, we obtain $\Lambda_1 = 8\pi na^3$, which is the order of 10^{-4} for ^{87}Rb with $na^3 = 0.39 \times 10^{-6}$. For a high-density system such as ^{4}He with $na^3 = 0.23$, we solve Eqs. (49) and (50) numerically and obtain $\Lambda_1 = 0.33 \times 10^{-3}$. In the following, we neglect the parameter Λ_1 in the calculation of the excitation spectrum, which is a good approximation.

At $T < T_c$, the above approximation corresponds to $\eta = z\eta_0$, neglecting the second term in Eq. (46). Using this approximation in Eq. (43) for the excitation spectrum $E(k)$, we obtain

$$E(k) = \left[\left(\frac{k^2}{2m} \right)^2 + 2\Lambda \left(\frac{k}{2ma} \right)^2 \frac{\sin ka}{ka} \right]^{1/2}, \tag{53}$$

with the parameter $\Lambda = z\eta_0$. The equation for Λ is obtained from Eq. (45) by

$$\eta_0 = \Lambda\frac{2}{\pi}\int_0^\infty dx \frac{\sin^2 x}{(x^4 + 2\Lambda x \sin x)^{1/2}} \times \coth \frac{(x^4 + 2\Lambda x \sin x)^{1/2}}{2t}. \tag{54}$$

This equation gives us Λ as a function of the parameter $\eta_0 = 8\pi n_0 a^3$. The equation for Λ is obtained from Eq. (47) for the condensate density n_0 as

$$\eta_0 = 8\pi na^3 - \frac{2}{\pi}\int_0^\infty dx \left[\frac{x^4 + \Lambda x \sin x}{(x^4 + 2\Lambda x \sin x)^{1/2}} \times \coth \frac{(x^4 + 2\Lambda x \sin x)^{1/2}}{2t} - x^2 \right]. \tag{55}$$

Equations (53)–(55) constitute the equations of the excitation spectrum $E(k)$ and the condensate density n_0 for Bose systems of hard spheres in the self-consistent HFB approximation.

Note that the spectrum (53) formally has the same form as the Brueckner-Sawada spectrum [21], but now Eq. (54) for the parameter Λ is different from their equation. The Brueckner-Sawada equation for Λ can be obtained by neglecting the anomalous self-energy term $(\Lambda x^{-1}\sin x)^2$ in the denominator $(x^4 + 2\Lambda x \sin x)^{1/2} = [(x^2 + \Lambda x^{-1}\sin x)^2 - (\Lambda x^{-1}\sin x)^2]^{1/2}$ in Eq. (54) for $T = 0$. Brueckner and Sawada put $n_0 = n$, thus neglecting the depletion of the condensate.

For $na^3 = 0.23$ corresponding to the experimental density of liquid ^{4}He with hard-sphere radius $a = 0.22$ nm, the Brueckner-Sawada equation then gives $\Lambda = 40$. The excitation spectrum calculated by Eq. (53) with Brueckner and Sawada's value of $\Lambda = 40$ is shown to have the essential features of the phonon-roton spectrum deduced by Landau [22] from experiments. However, the Brueckner and Sawada's result leads to serious errors in the calculation of other quantities. Using $\Lambda = 40$, Eq. (55) gives $n_0 = -1.7n$, which is a physically senseless negative value for the condensate density.

For a given temperature T and gas parameter na^3 with hard-sphere radius a, Eqs. (54) and (55) must be solved simultaneously for the parameters Λ and η_0. The excitation spectrum $E(k)$ is given by Eq. (53) and the condensate density n_0 is calculated by $n_0/n = \eta_0/8\pi na^3$. For $na^3 = 0.23$, the same values as Brueckner and Sawada's values, we obtain $\Lambda = 14$ and $n_0/n = 0.64$ at $T = 0$. When $\Lambda > 20$, as shown by Parry and ter Haar [29], the Brueckner-Sawada spectrum (53) has the essential feature of a phonon-roton spectrum of liquid ^{4}He. In the high-density limit $na^3 \to 1$, we find $\Lambda = 19$ and $n_0/n = 0.52$. Our calculations show that the HFB approximation is insufficient to explain the presence of a roton minimum in the excitation spectrum of liquid ^{4}He. In order to resolve this problem, we investigate the effects of the higher-order self-energy diagrams beyond the HFB approximation in the following section.

IV. ATTRACTIVE INTERACTION VIA THE BOSE-EINSTEIN CONDENSATE

We now turn to the investigation of the effects of higher-order self-energy diagrams beyond the HFB approximation. For the Bose system of hard spheres, it seems reasonable to neglect the screening effects and vertex corrections in Eq. (29) and keep the self-energy diagram containing the condensate-mediated interaction $V_K(q)$. With the approximations $\Pi = 0$ and $\Gamma = 1$, we obtain

$$\Sigma(p) = \Sigma_{\rm HFB}(p) + \Sigma_K(p), \tag{56}$$

with

$$\Sigma_K(p) = -T \int \frac{d^3q}{(2\pi)^3} \sum_{i\omega_n} V_k(q) G(p-q), \tag{57}$$

where $\Sigma_{\rm HFB}(p)$ is the self-energy in the HFB approximation and $V_K(q)$ is the condensate-mediated interaction represented by Fig. 1(c).

In the one-loop approximation, $V_K(q)$ can be written explicitly as

$$V_K(q) = n_0 v^2(\mathbf{q}) Tr[(\mathbf{1} + \tau^1)\mathbf{G}(q)]. \tag{58}$$

By using the Green's function in the HFB approximation and replacing the bare interaction $v(\mathbf{q})$ by the many-body t matrix $T(\mathbf{q})$ in the first-order approximation for Eq. (35), we have

$$V_K(\mathbf{q},\nu) = 2n_0 T^2(\mathbf{q}) \frac{\varepsilon(\mathbf{q}) - \Delta(\mathbf{q})}{\nu^2 - E^2(\mathbf{q}) + i0^+}, \tag{59}$$

with $E(\mathbf{q}) = [\varepsilon(\mathbf{q})^2 + 2n_0\varepsilon(\mathbf{q})T(\mathbf{q})]^{1/2}$. It is clear from Eq. (59) that $V_K(\mathbf{q},\omega)$ becomes an attractive interaction when the energy transfer ν is small, that is, $|\nu| \leqslant E(\mathbf{q})$. In the static limit $\nu \to 0$, Eq. (59) reduces to

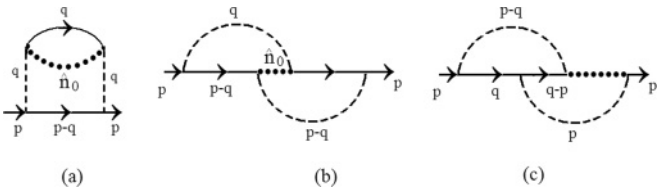

FIG. 3. Self-energy diagrams in the second-order approximation.

$$V_K(\mathbf{q},\nu = 0) = -\lambda(\mathbf{q})T(\mathbf{q}), \tag{60}$$

with

$$\lambda(\mathbf{q}) = \frac{2n_0 T(\mathbf{q})}{\mathbf{q}^2/2m + 2n_0 T(\mathbf{q})}. \tag{61}$$

Thus, the condensate-mediated interaction can be attractive when energy transfer between noncondensate bosons is small. This attraction can lead to pairing between noncondensate bosons in the states $\mathbf{k}$ and $-\mathbf{k}$ and to the enhancement of the corresponding anomalous self-energy.

We here note that $\mathbf{\Sigma}_K(p)$ is one of the second-order self-energy diagrams containing one condensate line $n_0(\mathbf{1} + \tau^1)$, as shown in Fig. 3. The self-energy $\mathbf{\Sigma}_K(p)$ represented by Fig. 3(a) involves $v^2(\mathbf{q})$, while Figs. 3(b) and 3(c) involve $v(\mathbf{q}) \cdot v(\mathbf{p} - \mathbf{q})$. Since $v(\mathbf{q}) \sim \sin ka/ka$, Figs. 3(b) and 3(c) give the negligible contributions for a finite $\mathbf{p}$. Thus, the leading contribution comes from the self-energy diagram $\mathbf{\Sigma}_K(p)$ involving the condensate-mediated interaction $V_K(q)$.

Using $\Sigma_{\rm HFB}(p)$ and $V_K(q)$ calculated in the HFB approximation, we calculate the self-energy given by Eq. (56). In Eq. (57) for $\mathbf{\Sigma}_K(p)$, the integral comes mainly from the range of small $\mathbf{q}$ and we can use the static potential $V_K(\mathbf{q},\nu = 0) = -\lambda T(\mathbf{q})$, with $\lambda = \lambda(\mathbf{q} \to 0) = 1$. With this approximation, one can then perform the frequency sum in Eq. (57) to obtain

$$\Sigma(p) = [nv(0) + \phi(\mathbf{k})]\mathbf{1} + \Delta(\mathbf{k})\tau^1, \tag{62}$$

with

$$\Delta(\mathbf{k}) = n_0 T(\mathbf{k}) + \lambda \int \frac{d^3q}{(2\pi)^3} T(\mathbf{k}-\mathbf{q}) \frac{\Delta(\mathbf{q})}{2E(\mathbf{q})} \coth \frac{E(\mathbf{q})}{2T}, \tag{63}$$

$$\phi(\mathbf{k}) = \Delta(\mathbf{k}) - \lambda \int \frac{d^3q}{(2\pi)^3} T(\mathbf{k}-\mathbf{q}) \times \left[\frac{e(\mathbf{q}) + \Delta(\mathbf{q})}{2E(\mathbf{q})} \coth \frac{E(\mathbf{q})}{2T} - \frac{1}{2} \right], \tag{64}$$

where $E(\mathbf{k}) = \sqrt{e^2(\mathbf{k}) - \Delta^2(\mathbf{k})}$ is the excitation spectrum determined by the poles of the Green's functions. Here, we use the notation $e(\mathbf{k}) = \varepsilon(\mathbf{k}) - \tilde{\mu} + \phi(\mathbf{k})$, with $\tilde{\mu} = \mu - nv(0)$.

As discussed above, the second term in Eq. (63) is very small and can be neglected, leading to $\phi(\mathbf{k}) = \Delta(\mathbf{k})$. Putting the solution of Eq. (64) in the form $\Delta(\mathbf{k}) = Dn_0 T(\mathbf{k})$, we have

$$D = 1 + \lambda \frac{2D\Lambda}{\pi\eta_0} \int_0^\infty dx \frac{\sin^2 x}{(x^4 + 2D\Lambda x \sin x)^{1/2}} \times \coth \frac{(x^4 + 2D\Lambda x \sin x)^{1/2}}{t}, \tag{65}$$

where the parameter Λ is given by Eq. (54) in the HFB approximation. The excitation spectrum can be written as

$$E(\mathbf{k}) = \left[\left(\frac{k^2}{2m}\right)^2 + 2D\Lambda\left(\frac{k}{2ma}\right)^2 \frac{\sin ka}{ka}\right]^{1/2}, \quad (66)$$

with $k = |\mathbf{k}|$. Comparing this with Eq. (53) shows that the parameter D describes the effect of pairing between noncondensate bosons due to the condensate-mediated attraction. If this attraction is neglected, namely, $\lambda = 0$, then $D = 1$ and Eq. (66) reduces to the Brueckner-Sawada spectrum. If we take into account the presence of this attraction ($\lambda = 1$), we obtain an enhancement of the anomalous self-energy in Eq. (63) and $D > 1$, which can yield the appearance of a roton minimum in the spectrum.

Equation (65) must be solved self-consistently together with the equation for $\eta_0 = 8\pi n_0 a^3$, which is given by

$$\eta_0 = 8\pi na^3 - \frac{2}{\pi}\int_0^\infty dx \left[\frac{x^4 + D\Lambda x \sin x}{(x^4 + 2D\Lambda x \sin x)^{1/2}} \times \coth\frac{(x^4 + 2D\Lambda x \sin x)^{1/2}}{t} - x^2\right]. \quad (67)$$

Given a gas parameter $\gamma = n^{1/3}a$ and temperature T, Eqs. (65) and (67) enable us to determine the parameters D and η_0, using the parameter Λ obtained in the HFB approximation. If we use the same value $a = 0.22$ nm as Brueckner and Sawada for the hard-sphere radius so that $na^3 = 0.23$ ($\gamma = 0.61$) for liquid ^{4}He at $T = 0$, we find $D\Lambda = 29$, with $\Lambda = 14$, and $n_0/n = 0.11$. Figure 4 shows the excitation spectrum calculated from Eq. (66) with $D\Lambda = 29$ and its HFB approximation (53) with $\Lambda = 14$ and $D = 1$. The calculated spectrum has the essential features of the phonon-roton spectrum deduced by Landau [22] from experiment. The excitation spectrum of Bose systems of hard spheres has the Bogoliubov form in the low-density region $\gamma < 0.54$, while it has the essential features of the phonon-roton spectrum in the high-density region $\gamma > 0.54$.

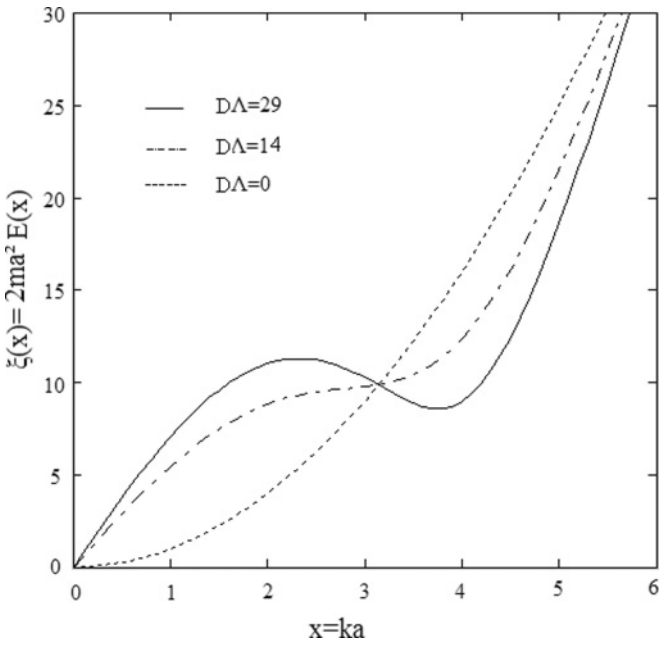

FIG. 4. Excitation spectrum for the Bose system of hard spheres at zero temperature. The solid line is the result obtained from taking into account the condensate-mediated attraction ($\lambda = 1$), while the dashed-dotted line is the HFB approximation ($\lambda = 0$). The dotted line is the spectrum of free bosons above the condensation temperature T_c.

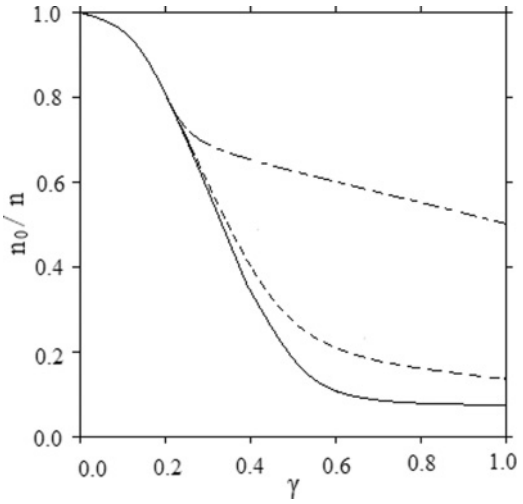

FIG. 5. Condensate density n_0 as a function of the gas parameter $\gamma = n^{1/3}a$ at $T = 0$. The dashed-dotted line corresponds to the HFB approximation and the dashed line is the result of the Yukalov-Yukalova theory [30].

For the whole region of γ, we solve numerically the system of Eqs. (65) and (67) at $T = 0$, showing the condensate density n_0 as a function of γ in Fig. 5. The dashed-dotted line is the condensate density in the self-consistent HFB approximation [20] and the dotted line is the results obtained in the Yukalov-Yukalova approximation [30]. At small γ, up to $\gamma \approx 0.3$, n_0 practically coincides with the HFB approximation, where the excitation spectrum has the Bogoliubov form without a roton minimum. For $\gamma > 0.54$, the excitation spectrum has a roton minimum and n_0 becomes smaller than the HFB approximation and approaches the nearly constant value 0.08 as $\gamma \to 1$. At $\gamma \approx 0.61$ corresponding to liquid ^{4}He, we have $n_0/n = 0.11$, which is close to the condensate fraction $n_0/n \approx 0.1$, measured in experiments (as is reviewed in Refs. [31,32]) as well as obtained by Monte Carlo simulations [33]. We see that the strong suppression of the condensate fraction at high density is related to the appearance of a roton minimum in the excitation spectrum.

V. CONCLUSIONS

The properties of Bose-Einstein-condensed systems of hard spheres at high density have been studied by taking into account higher-order corrections beyond the HFB approximation. Based on a diagrammatic technique of the perturbation expansion starting from the Bogoliubov approximation, we have shown that the effective interaction diagrams separate into two distinct parts: the screened interaction and the condensate-mediated attraction. The latter exists only between noncondensate bosons in the presence of a Bose-Einstein condensate. For Bose systems of hard spheres, the screened interaction and vertex corrections can be neglected and the leading higher-order corrections to the HFB approximation

come from the self-energy diagram involving the condensate-mediated attraction in low temperature.

Near T_c, the higher-order corrections can be neglected because the condensate density n_0 is very small and we use the self-consistent HFB approximation. We have calculated the Bose-Einstein condensation temperature T_c as a function of the gas parameter for Bose systems of hard spheres. It is shown that T_c decreases compared with that of an ideal Bose gas; the shift is proportional to the gas parameter $\gamma = n^{1/3}a$ in the low-density limit, while it is still finite, though small, in the high-density limit. For $\gamma = 0.61$ corresponding to liquid ^{4}He with hard-sphere radius $a = 0.22$ nm, we have $T_c = 2.11$ K, which is very close to the critical temperature $T_c = 2.17$ K of liquid ^{4}He.

We have calculated the excitation spectrum and condensate density as a function of the gas parameter for Bose systems of hard spheres at low temperature by taking into account the effect of the condensate-mediated attraction between noncondensate in the static approximation. The excitation spectrum of Bose systems of hard spheres has the Bogoliubov form at low-density region $\gamma < 0.54$, while it has the essential features of the phonon-roton spectrum deduced by Landau [22] in the high-density region $\gamma > 0.54$. It is shown that the condensate density in the high-density region becomes smaller than the results of the HFB approximation and the Yukalov-Yukalova theory [30] due to the appearance of a roton minimum in the spectrum.

Summarizing, we can state that the condensate-mediated attraction between noncondensate bosons leads to an enhancement of the anomalous self-energy and, as a consequence, to the emergence of a roton minimum in the excitation spectrum and to the strong suppression of the condensate fraction in the region of high density.

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