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Short-range particle correlations in a dilute Bose gas

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The thermodynamics of a homogeneous dilute Bose gas with an arbitrarily strong repulsion between particles is investigated on the basis of the exact relation connecting the pair correlation function with the in-medium pair wave functions and occupation numbers. It is shown that the effective-interaction scheme, which is reduced to the Bogoliubov model with the effective pairwise potential, is not acceptable for investigating the short-range particle correlations in a dilute strongly interacting Bose gas. In contrast to this scheme, our model is thermodynamically consistent and free of the ultraviolet divergences due to accurate treatment of the short-range boson correlations. An equation for the in-medium scattering amplitude is derived that makes it possible to find the in-medium renormalization for the pair wave functions at short boson separations. Low-density expansions for the main thermodynamic quantities are reinvestigated on the basis of this equation. In addition, the expansions are found for the interaction and kinetic energies per particle. It is demonstrated that for a many-boson system of hard spheres the interaction energy is equal to zero for any boson density. The exact relationship between the chemical potential and in-medium pair wave functions is also established.

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I. INTRODUCTION AND BASIC EQUATIONS

The well-known experiments with magnetically trapped alkali-metal atoms [1] have significantly renewed interest in the theory of Bose-Einstein condensation (see, e.g., Ref. [2]). In particular, it has recently been demonstrated by the present authors [3] that the customary way of investigating a dilute Bose gas with a purely repulsive and arbitrarily strong interaction [4] is thermodynamically inconsistent. At $n=N/V\to 0$ this method is known [5] to be reduced to the Bogoliubov model [6] with the ''bare'' pairwise potential $\Phi(r)$ replaced by an effective, ''dressed'' one. This is why below the approach of Ref. [4] is called the ''effective-interaction method.'' The dressed pairwise potential is usually derived by summing the ladder diagrams and involves, as is assumed, all the necessary information on the short-range spatial correlations of bosons [4]. In the final expressions use of the effective interaction results in substituting the exact scattering length a for its Born approximation a_0 [5]. This allows for operating with strongly singular potentials, but at the price of loss of the thermodynamic consistency. In contrast, the strong-coupling generalization of the Bogoliubov model proposed by the present authors in [3] is based on a *variational* procedure and does not invoke any mean-field arguments. Owing to this structure of the generalization we do not need to worry about the thermodynamic consistency.

The trouble mentioned above gives rise to various misrepresentations of the effective-interaction approach. For example, the condition of self-consistency leads to zero condensate depletion within the pseudopotential model [7]. Another manifestation is an irrelevant picture of the pair boson correlation at short particle separations. This important point calls for a comprehensive analysis which was not fulfilled in Ref. [3] for reasons of space. Thus, in the present paper, we continue reinvestigation of a dilute Bose gas with an arbitrarily strong repulsion between particles within the model proposed in [3], the short-range boson correlations being of special interest now. Zero temperature is under consideration below.

The formalism of the present paper is concerned with a reduced density matrix of the second order (the two-matrix) and its eigenfunctions, which we call, following Bogoliubov [8], the in-medium pair wave functions. As the two-matrix and its eigenfunctions are not often discussed in the modern scientific literature on Bose-Einstein condensation, it is worth noting some basic notation and formulas. The two-matrix for a many-body system of spinless bosons can be represented as [9]

$$\rho_2(\mathbf{r}_1',\mathbf{r}_2';\mathbf{r}_1,\mathbf{r}_2)=\frac{F_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')}{N(N-1)},$$

where the pair correlation function is given by

$$F_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')=\langle\hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}^\dagger(\mathbf{r}_2)\hat{\psi}(\mathbf{r}_2')\hat{\psi}(\mathbf{r}_1')\rangle. \tag{1}$$

Here $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$ denote the boson field operators. Use of the pair correlation function, which differs from the two-matrix only by the normalization factor, is more convenient in the thermodynamic limit ($n=N/V=\text{const},\ \ V\to\infty$) when $F_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')\propto 1$ while $\rho_2(\mathbf{r}_1',\mathbf{r}_2';\mathbf{r}_1,\mathbf{r}_2)\propto 1/V^2$. Recently it has been found [3,10,11] that for a uniform Bose system with a small depletion of the zero-momentum state the correlation function (1) can be written in the thermodynamic limit as follows:

$$\begin{aligned}F_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')=&\,n_0^2\varphi^*(r)\varphi(r')+2n_0\\&\times\int\frac{d^3q}{(2\pi)^3}n_q\varphi^*_{\mathbf{q}/2}(\mathbf{r})\varphi_{\mathbf{q}/2}(\mathbf{r}')\\&\times\exp[i\mathbf{q}\cdot(\mathbf{R}'-\mathbf{R})],\end{aligned} \tag{2}$$

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where $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$, $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_2)/2$, and similar relations hold for $\mathbf{r}'$ and $\mathbf{R}'$, respectively. In Eq. (2) $n_0=N_0/V$ is the density of particles in the zero-momentum one-boson state, $n_q=\langle \hat{a}^\dagger_{\mathbf{q}}\hat{a}_{\mathbf{q}}\rangle$ stands for the distribution of the uncondensed bosons over momenta, and $\varphi(r)$ and $\varphi_{\mathbf{q}/2}(\mathbf{r})$ are pair wave functions in medium in the center-of-mass system. That is, $\varphi(r)$ is the wave function of a pair of particles, both being condensed. In turn, $\varphi_{\mathbf{q}/2}(\mathbf{r})$ denotes the wave function of the relative motion of a pair of bosons with the total momentum $\hbar\mathbf{q}$, this pair including one condensed and one uncondensed particle. So Eq. (2) takes into account the condensate-condensate and supracondensate-condensate pair states and is related to the situation of a small depletion of the zero-momentum one-boson state. For the pair wave functions we have

$$\varphi(r)=1+\psi(r),\quad \varphi_{\mathbf{p}}(\mathbf{r})=\sqrt{2}\cos(\mathbf{p}\cdot\mathbf{r})+\psi_{\mathbf{p}}(\mathbf{r})(p\neq 0), \tag{3}$$

where the scattering waves $\psi(r)$ and $\psi_{\mathbf{p}}(\mathbf{r})$ obey the boundary conditions for $r\to\infty$

$$\psi(r)\to 0,\quad \psi_{\mathbf{p}}(\mathbf{r})\to 0, \tag{4}$$

which follow from the Bogoliubov principle of correlation weakening [8]. The Fourier transforms of the functions $\psi(r)$ and $\psi_{\mathbf{p}}(\mathbf{r})$ can explicitly be expressed in terms of the Bose operators $\hat{a}^\dagger_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}$ [10]:

$$\psi(k)=\langle \hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}\rangle/n_0,\psi_{\mathbf{p}}(\mathbf{k})=\sqrt{\frac{V}{2n_0}}\frac{\langle \hat{a}^\dagger_{2\mathbf{p}}\hat{a}_{\mathbf{p}+\mathbf{k}}\hat{a}_{\mathbf{p}-\mathbf{k}}\rangle}{n_{2p}}. \tag{5}$$

In the representation (2) the terms corresponding to the supracondensate-supracondensate ‘‘channel’’ are neglected, i.e., we omit the contribution of pairs of particles that are both uncondensed. Additionally, it is assumed that there are no bound states of pairs of bosons, which is obviously realized for a purely repulsive interaction between bosons.

The diagonal matrix element of the pair correlation function (2) is proportional to the pair distribution function

$$g(r)=F_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1,\mathbf{r}_2)/n^2 \tag{6}$$

that can be observed directly in scattering experiments. Derivation of Eqs. (2)–(5) and detailed discussion can be found in Ref. [10].

The two limiting cases $n\to 0$ and $r\to 0$ correspond to the situation when the behavior of two particles in the medium is determined by the ordinary two-body problem provided the pairwise interaction $\Phi(r)$ is repulsive and goes to infinity at short boson separations. In particular, when $n\to 0$ we have $(n-n_0)/n\to 0$ and, as has been known since the Bogoliubov original paper and follows also from Eqs. (2) and (6),

$$g(r)\to[\varphi^{(0)}(r)]^2. \tag{7}$$

Here $\varphi^{(0)}(r)$ is defined by $\varphi^{(0)}(r)=\lim_{n\to 0}\varphi(r)$ and obeys the ordinary two-body Schrödinger equation in the center-of-mass system (9) (see Ref. [6]). Similarly, $\varphi^{(0)}_{\mathbf{p}}(\mathbf{r})=\lim_{n\to 0}\varphi_{\mathbf{p}}(\mathbf{r})$ obeys the Schrödinger equation related to the eigenvalue $\hbar^2p^2/m$ that corresponds to the relative motion of two particles with momentum $\hbar\mathbf{p}$. These conditions should be satisfied in any theory that appropriately takes into account the short-range correlations of particles. Below we show that our model [3] leads to the correct picture of the spatial correlations [in contrast to the effective-interaction approach, which leads to negative values of the pair distribution function (see Sec. V)].

Having at our disposal the distribution function n_k and the set of pair wave functions $\varphi(r)$ and $\varphi_{\mathbf{p}}(\mathbf{r})$, we are able to calculate the main thermodynamic quantities of the system of interest. In particular, the mean energy per particle is expressed in terms of n_k and $g(r)$ via the well-known formula (see, e.g., Ref. [9])

$$\varepsilon=\int\frac{d^3k}{(2\pi)^3}T_k\frac{n_k}{n}+\frac{n}{2}\int d^3r g(r)\Phi(r), \tag{8}$$

where $T_k=\hbar^2k^2/2m$ is the one-particle kinetic energy, m is the ‘‘bare’’ mass of the particles, and $n=N/V$ stands for the boson density.

The organization of this paper is as follows. In Sec. II we give, for convenience, helpful information concerning the classification of pairwise potentials used in the ordinary two-body problem. In Sec. III the Bogoliubov model of a weakly interacting Bose gas is considered within a variational scheme. This scheme yields a system of two equations connecting n_k with $\varphi(r)$. As to the supracondensate-condensate pair wave functions, they are the symmetrized plane waves in the Bogoliubov model: $\psi_{\mathbf{p}}(\mathbf{r})=0$. In the next section the low-density expansions for the condensate depletion and mean energy per particle of a weak-coupling Bose gas are calculated within the Bogoliubov model. The effective-interaction approach of Ref. [4] is analyzed in Sec. V. Using the results of the previous Secs. III and IV, we show that the effective-interaction approach is thermodynamically inconsistent. This inconsistency turns out to be directly related to an irrelevant picture of the short-range spatial boson correlations. In particular, for a strongly singular potential the effective-interaction scheme yields for the pair distribution function the nonphysical result $g(r=0)=-1$ in the limit $n\to 0$. It is also demonstrated that the well-known ultraviolet divergence appearing in the effective-interaction approach as well as the thermodynamic inconsistency occur because the Bogoliubov framework is used beyond the range of its validity. The regularizing procedure, which consists in omitting the divergent integral $\int d^3k/k^2$, can be justified provided the quantities of interest depend on the pairwise potential through the mediation of the scattering length [Eq. (11) below]. Section VI concerns a correct strong-coupling generalization of the Bogoliubov model. This generalization is based on Eq. (6) taken together with Eq. (2) but not with its linearized variant Eq. (25) (below) used in the effective-interaction approach, which is the weak-coupling approximation for $g(r)$. A variational procedure similar to that of Sec. III is formulated. It provides the system of equations that should be solved to find the pair wave functions in conjunction with the momentum distribution. For a dilute Bose gas this system is reduced to a set of two equations connecting n_k and $\varphi(r)$. There is an essential difference between these equations and those of Sec. III. Now the pairwise potential

$\Phi(r)$ appears only in the combination $\varphi(r)\Phi(r)$, which allows for using the strongly singular potentials beyond the effective-interaction scheme. In what concerns the supracondensate-condensate contribution to the thermodynamic quantities, it can be calculated with the relation $\lim_{p\to 0}\varphi_{\mathbf{p}}(\mathbf{r})=\sqrt{2}\varphi(r)$ resulting from Eqs. (3) and (4). In Sec. VII we investigate the short-range renormalization for $\varphi(r)$ conditioned by the presence of surrounding bosons. Its long-range behavior is also discussed. The whole investigation of this section is based on the in-medium Lippmann-Schwinger equation coming from the equation for $\varphi(r)$ found in Sec. VI. In Sec. VIII the low-density expansions for the Bose condensate depletion, the energy per particle, and the chemical potential are found within the model presented in Sec. VI, various methods of calculation being used. For this purpose we establish the exact relationship between the chemical potential and pair wave functions in a condensed many-boson system. Here we also evaluate the kinetic and interaction energies per particle which, to our knowledge, have never been calculated before. It should be stressed that they explicitly depend on the shape of the pairwise potential even in the leading order of the low-density expansion. In the framework of our approach we are able to perform all the calculations concerning the kinetic and potential energies both directly and with the Hellmann-Feynman theorem, in contrast to the effective-interaction method. The main results and prospects are discussed in the last section.

II. CLASSIFICATION OF INTERACTION POTENTIALS

Before further consideration we recall the classification of the pairwise interactions $\Phi(r)$ that is used in the ordinary two-body problem. In this paper we deal only with short-range potentials that go to zero for $r\to\infty$ as $\Phi(r)\to 1/r^m$ $(m>3)$, or even faster. Let us consider the solution of the two-body Schrödinger equation in the center-of-mass system,

$$-\frac{\hbar^2}{m}\nabla^2\varphi^{(0)}(r)+\Phi(r)\varphi^{(0)}(r)=0, \tag{9}$$

which corresponds to the scattering state with the momentum $p=0$: $\varphi^{(0)}(r)=1+\psi^{(0)}(r)$, where the scattering part behaves as

$$\psi^{(0)}(r)\to -a/r \tag{10}$$

when $r\to\infty$. Owing to this boundary condition with the real quantity a, the solution $\varphi^{(0)}(r)$ is chosen to be real also. The scattering length a is defined by means of the scattering amplitude $U^{(0)}(0)$:

$$a=\frac{m}{4\pi\hbar^2}U^{(0)}(0), \tag{11}$$

$$U^{(0)}(0)=\int d^3r\,\varphi^{(0)}(r)\Phi(r). \tag{12}$$

As applied to Eq. (9), the perturbation technique gives the expansion for its solution

$$\psi^{(0)}(k)=\psi_1^{(0)}(k)+\psi_2^{(0)}(k)+\cdots, \tag{13}$$

$$\psi_1^{(0)}(k)=-\Phi(k)/(2T_k), \tag{14}$$

which leads to the following expansion for the scattering length (11):

$$a=a_0+a_1+a_2+\cdots, \tag{15}$$

$$a_0=\frac{m}{4\pi\hbar^2}\Phi(k=0),\quad a_1=-\frac{m}{4\pi\hbar^2}\int\frac{d^3k}{(2\pi)^3}\frac{\Phi^2(k)}{2T_k}. \tag{16}$$

Here $\psi^{(0)}(k)$ and $\Phi(k)$ stand for the Fourier transforms of $\psi^{(0)}(r)$ and $\Phi(r)$, respectively. If we restrict ourselves to the first terms in Eqs. (13) and (15) [$\psi^{(0)}(k)\simeq\psi_1^{(0)}(k)$ and $a\simeq a_0$] we arrive at the Born approximation for the wave function and the scattering length, respectively.

The interaction is called the weak-coupling one, provided the Born approximation works well, in particular,

$$\int\frac{d^3k}{(2\pi)^3}\frac{\Phi^2(k)}{2T_k}\ll\Phi(k=0). \tag{17}$$

This is valid if, first, the potential $\Phi(r)$ is integrable, and, second, it is proportional to a small parameter, the coupling constant. The latter implies that $|\psi^{(0)}(r)|\ll 1$, and so the Born approximation (14) is nothing but a linearization of Eq. (9) with respect to $\psi^{(0)}(r)$, proportional to the coupling constant:

$$\frac{\nabla^2[1+\psi^{(0)}(r)]}{[1+\psi^{(0)}(r)]}\simeq\nabla^2\psi^{(0)}(r).$$

The potential is called singular if it is integrable but the Born approximation does not work well. Finally, the potential is of strongly singular, or hard-core, type if it is not integrable [$\Phi(r)\to 1/r^m(m\geqslant 3)$ for $r\to 0$], and the terms (14) and (16) thus cannot exist. In the present paper a pairwise interaction of this type is exactly implied when we speak about the strong-coupling regime. For example, the well-known Lennard-Jones potential corresponds to this case together with the hard-sphere interaction,

$$\Phi(r)=\begin{cases}+\infty, & r<a\\ 0, & r>a.\end{cases} \tag{18}$$

In the strong-coupling regime the solution of Eq. (9) obeys the boundary condition $\varphi^{(0)}(r=0)=0$, otherwise the interaction energy $E_{int}=\int d^3r[\varphi^{(0)}(r)]^2\Phi(r)$ and the scattering length (11) would be infinitely large.

In further consideration we make use of the variational theorem for the scattering amplitude (12):

$$\delta U^{(0)}(0)=\int d^3r\left[\psi^{(0)}(r)\,\delta\!\left(-\frac{\hbar^2}{m}\nabla^2\right)\psi^{(0)}(r)+\varphi^{(0)}(r)\,\delta(\Phi(r))\varphi^{(0)}(r)\right]. \tag{19}$$

In order to prove this relation, we represent Eq. (12) in the form

$$U^{(0)}(0)=\int d^3r\left(\frac{\hbar^2}{m}|\nabla\psi^{(0)}(r)|^2+[\varphi^{(0)}(r)]^2\Phi(r)\right), \tag{20}$$

which can be found using integration by parts and taking into account the Schrödinger equation (9) and the boundary condition (10). Further, varying Eq. (20) and keeping in mind Eqs. (9) and (10), we arrive at Eq. (19). The relation (19) is analogous to the variational theorem for the energy:

$$\delta E_n=\int d^3r\,\varphi_n^{(0)}(\mathbf{r})\,\delta\left(-\frac{\hbar^2}{m}\nabla^2+\Phi(r)\right)\varphi_n^{(0)}(\mathbf{r}).$$

Here the real wave function $\varphi_n^{(0)}(\mathbf{r})$ obeys the Schrödinger equation for a bound state with energy E_n. Equation (20) can be represented in the more convenient form

$$\int d^3r[\varphi^{(0)}(r)]^2\Phi(r)=4\pi\hbar^2(a-b)/m. \tag{21}$$

Here one more characteristic length b (in addition to a) has been introduced:

$$b=\frac{1}{4\pi}\int d^3r|\nabla\psi^{(0)}(r)|^2. \tag{22}$$

It follows from Eq. (22) that b is a positive quantity. We stress that b is not expressed in terms of a and depends on a particular shape of the interaction potential $\Phi(r)$. For example, when $\Phi(r)$ is the hard-sphere potential (18), we have $b=a$, while for $\Phi(r)$ close to zero, in the weak-coupling regime, we have $b\simeq -a_1$, $a\simeq a_0$, and hence $b\ll a$.

Lastly, from the definitions (11) and (22) and the variational theorem (19) it follows that

$$\gamma\frac{\partial a}{\partial\gamma}=m\frac{\partial a}{\partial m}=a-b, \tag{23}$$

where we introduce the auxiliary parameter γ called the coupling constant [i.e., $\Phi(r)\rightarrow\gamma\Phi(r)$]. The first equality in Eq. (23) implies that $a=a(\gamma m)$, which is an obvious consequence of the definition (11) and the Schrödinger equation (9). The relations (23) demonstrate that the quantity b is expressed in terms of a and its derivative with respect to γ (or m) rather than in terms of a.

III. VARIATIONAL TREATMENT OF THE BOGOLIUBOV MODEL

Although the aim of this paper is to investigate a dilute Bose gas with strong-coupling interaction, it is instructive to start with the Bogoliubov model related to the weak-coupling regime. This regime implies a minor role of particle scattering, both in the medium and out of it, and thus is characterized by the following inequalities for the scattering waves (3):

$$|\psi(r)|\ll 1,\quad |\psi_{\mathbf{p}}(\mathbf{r})|\ll 1. \tag{24}$$

In particular, the Bogoliubov model operates with the choice [3,10,11]

$$|\psi(r)|\ll 1,\quad \psi_{\mathbf{p}}(\mathbf{r})=0.$$

As the depletion of the Bose condensate $(n-n_0)/n$ is small in a weakly interacting many-boson system, we have for the one-particle density matrix $F_1(r)=\langle\hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_2)\rangle$

$$\left|\frac{F_1(r)}{n}\right|=\left|\int\frac{d^3k}{(2\pi)^3}\frac{n_k}{n}\exp(i\mathbf{k}\cdot\mathbf{r})\right|\leqslant\frac{n-n_0}{n}\ll 1.$$

So the Bogoliubov scheme of treating a Bose gas involves two small quantities $\psi(r)$ and $F_1(r)/n$ and completely neglects scattering in the supracondensate-condensate sector of $g(r)$: $\psi_{\mathbf{p}}(\mathbf{r})=0$. This along with Eq. (2) allows for rewriting Eq. (6) in the following form:

$$g(r)=1+2\psi(r)+\frac{2}{n}\int\frac{d^3k}{(2\pi)^3}n_k\exp(i\mathbf{k}\cdot\mathbf{r}). \tag{25}$$

Here we have restricted ourselves to the terms linear in $\psi(r)$ and $F_1(r)/n$. In addition, it is implied that $\psi^*(r)=\psi(r)$, for the pair wave functions can be chosen as real quantities. Inserting Eq. (25) into Eq. (8), we are able to employ a variational procedure to derive the unknown quantities $\psi(k)$ and n_k. In so doing, we should realize that n_k and $\psi(k)$ are not independent variables. In fact, there are no spatial boson correlations in the absence of interaction [12]. Hence in this case $\psi(k)=0$, and, as we investigate the ground state, all the bosons are condensed, $n_k=0$. In the presence of interaction $\psi(k)\neq 0$, which leads to a nonzero depletion and so $n_k\neq 0$. Within the Bogoliubov model $\psi(k)$ is related to n_k by

$$n_k(n_k+1)=n_0^2\psi^2(k). \tag{26}$$

Indeed, according to the canonical Bogoliubov transformation, quasiparticle operators $\hat{\alpha}_{\mathbf{k}}^\dagger$ and $\hat{\alpha}_{\mathbf{k}}$ are connected with the operators of the primordial bosons by the expression

$$\hat{a}_{\mathbf{k}}=u_k\hat{\alpha}_{\mathbf{k}}+v_k\hat{\alpha}_{-\mathbf{k}}^\dagger,\quad \hat{a}_{\mathbf{k}}^\dagger=u_k\hat{\alpha}_{\mathbf{k}}^\dagger+v_k\hat{\alpha}_{-\mathbf{k}}, \tag{27}$$

where

$$u_k^2-v_k^2=1. \tag{28}$$

Within the Bogoliubov model the ground state of the system of interest is the Bogoliubov quasiparticle vacuum, and so at zero temperature we have

$$\langle\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}}\rangle=0. \tag{29}$$

Then, using Eqs. (5), (27), and (29), one can find

$$n_k=v_k^2,\quad \psi(k)=u_kv_k/n_0,$$

which in conjunction with Eq. (28) leads to Eq. (26). We remark that beyond the Bogoliubov scheme Eq. (26) is not valid and should be corrected [see Eq. (51) in the present paper and discussion on this question in Ref. [3]].

Now, inserting Eq. (25) into Eq. (8) and varying the resulting expression with respect to $\psi(k)$ and n_k, we derive

$$\delta\varepsilon=\int\frac{d^3k}{(2\pi)^3}\left([T_k+n\Phi(k)]\frac{\delta n_k}{n}+n\Phi(k)\,\delta\psi(k)\right). \tag{30}$$

According to Eq. (26) infinitesimal changes $\delta\psi(k)$ and δn_k are connected by

$$\delta\psi(k)=\frac{(2n_k+1)\,\delta n_k}{2n_0^2\psi(k)}+\frac{\psi(k)}{n_0}\int\frac{d^3q}{(2\pi)^3}\,\delta n_q, \tag{31}$$

where the equality

$$n=n_0+\int\frac{d^3k}{(2\pi)^3}n_k$$

is implied. Taking $\delta\varepsilon=0$ and using Eqs. (30) and (31), we find the following equation:

$$-2T_k\psi(k)=\frac{n^2}{n_0^2}\Phi(k)(1+2n_k)+2n\psi(k)\times\left(\Phi(k)+\frac{n}{n_0}\int\frac{d^3q}{(2\pi)^3}\Phi(q)\psi(q)\right). \tag{32}$$

Note that Eq. (32) is able to yield results accurate only to the leading order in $(n-n_0)/n$ because Eq. (25) is valid to the next-to-leading order [13]. So Eq. (32) should be written in the form

$$-2T_k\psi(k)=\Phi(k)(1+2n_k)+2n\psi(k)\Phi(k), \tag{33}$$

which, with the help of Eq. (25), can be represented as

$$\frac{\hbar^2}{m}\nabla^2\varphi(r)=\Phi(r)+n\int d^3y\,\Phi(y)[g(|\mathbf{r}-\mathbf{y}|)-1]. \tag{34}$$

Equation (34) is very similar to the Bethe-Goldstone equation. Necessary details concerning Eq. (34) can be found in Refs. [11,14]. We remark that the right-hand side (rhs) of Eq. (34) can be thought of as the in-medium potential of the boson-boson interaction in the Born approximation. Indeed, Eq. (34) is derived from the more general equation given by Eq. (56) below by means of linearization in $\psi(r)$ and $F_1(r)/n$. So the Bogoliubov model can be treated as the in-medium Born approximation for its generalization developed on the basis of Eqs. (2) and (6) beyond the weak-coupling regime (see Sec. VI). In accordance with this treatment, Eq. (34) at $n=0$ is nothing but the Fourier transform of Eq. (14), while Eq. (56) is reduced to the exact Schrödinger equation (9) at $n=0$. We will return to this important point in Sec. V.

The system of Eqs. (26) (here we should set $n=n_0$) and (33) can easily be solved, which leads to the familiar results [6]

$$n_k=\frac{1}{2}\left(\frac{T_k+n\Phi(k)}{\sqrt{T_k^2+2nT_k\Phi(k)}}-1\right), \tag{35}$$

$$\psi(k)=-\frac{1}{2}\frac{\Phi(k)}{\sqrt{T_k^2+2nT_k\Phi(k)}}. \tag{36}$$

IV. DENSITY EXPANSIONS IN THE BOGOLIUBOV MODEL

As we mentioned, in this paper we investigate the strong-coupling regime for a dilute Bose gas. So considering a dilute Bose gas in the weak-coupling approximation can be a good exercise providing us with useful information. Let us investigate the thermodynamics of a dilute many-boson system within the Bogoliubov model. With Eqs. (8), (25), (35), and (36) we derive

$$\varepsilon=\frac{n}{2}\Phi(0)+\frac{1}{2n}\int\frac{d^3q}{(2\pi)^3}\times\left(\sqrt{T_q^2+2nT_q\Phi(q)}-T_q-n\Phi(q)\right). \tag{37}$$

Here we describe in detail the method for obtaining the low-density expansions for expressions like Eq. (37). This equation can be represented in the following form:

$$\varepsilon=\frac{n}{2}\left(\Phi(0)-\int\frac{d^3q}{(2\pi)^3}\frac{\Phi^2(q)}{2T_q}\right)+I, \tag{38}$$

where

$$I=\tfrac{1}{2}\int\frac{d^3q}{(2\pi)^3}\left(\sqrt{\frac{T_q^2}{n^2}+2\frac{T_q}{n}\Phi(q)}-\frac{T_q}{n}-\Phi(q)+\frac{\Phi^2(q)}{2(T_q/n)}\right).$$

Now, with the ‘‘scaling’’ substitution

$$\mathbf{q}=\mathbf{q}'\sqrt{2mn}/\hbar, \tag{39}$$

we derive

$$\frac{I}{n^{3/2}}=\frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int\frac{d^3q'}{(2\pi)^3}f(q',n), \tag{40}$$

where

$$f(q',n)=\sqrt{(q')^4+2(q')^2\Phi(q'\sqrt{2mn}/\hbar)}-(q')^2-\Phi(q'\sqrt{2mn}/\hbar)+\frac{\Phi^2(q'\sqrt{2mn}/\hbar)}{2(q')^2}.$$

The advantage of the representation (38) is that the resulting integral in Eq. (40) uniformly converges for $q'\to\infty$ with respect to n for $n\to 0$, and thus we obtain

$$\lim_{n\to 0}\frac{I}{n^{3/2}}=\frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int\frac{d^3q'}{(2\pi)^3}f(q',n=0).$$

Here the integral is readily calculated, and the main asymptotics for $I(n)$ is given by

$$I \simeq \frac{8}{15\pi^2}\left(\frac{mn}{\hbar^2}\right)^{3/2}\Phi^{5/2}(0). \tag{41}$$

Further, with the help of Eqs. (16), (38), and (41), the expression (37) is rewritten as

$$\varepsilon = \frac{2\pi\hbar^2 n(a_0+a_1)}{m} + \frac{2\pi\hbar^2 n a_0}{m}\,\frac{128}{15\sqrt{\pi}}\sqrt{na_0^3} + \cdots. \tag{42}$$

Thus, we obtain the first two terms in the density expansion for the energy per particle within the Bogoliubov model.

The density expansion for the condensate depletion is inferred from Eq. (35) in the same manner employing the substitution (39):

$$\zeta = \frac{n-n_0}{n} = \int \frac{d^3q}{(2\pi)^3}\,\frac{n_q}{n} = \frac{8\sqrt{na_0^3}}{3\sqrt{\pi}} + \cdots. \tag{43}$$

Now let us discuss the range of validity of the Bogoliubov model. First, the condensate depletion (43) should be small as the representation for the pair correlation function (2) that we start from is valid only in this case. Note that, if we expand the depletion with respect to the coupling constant γ [we assume that $\Phi(r) \propto \gamma$], we also arrive at Eq. (43) since the occupation number (35) depends only on the production $n\gamma$. Thus, the condition $na_0^3 \ll 1$ should be fulfilled. Second, we exploit the weak-coupling character of the pairwise interaction $\Phi(r)$, which implies that the condition (17) should also be satisfied. Note that Bogoliubov himself realized this necessary condition since he treated the term $n\Phi(0)/2 = 2\pi\hbar^2 n a_0/m$ involved in the mean energy (37) as the major one [6]. Beyond the inequality (17) the model may be thermodynamically unstable. In particular, the opposite case

$$\Phi(0) < \int \frac{d^3k}{(2\pi)^3}\,\frac{\Phi^2(k)}{2T_k} \tag{44}$$

leads to a negative scattering length in the next-to-Born approximation $a = a_0 + a_1 < 0$, which at sufficiently low densities results in the incorrect sign for the compressibility $-\partial^2 E/\partial V^2 = \partial P/\partial V > 0$ as is seen from Eq. (42). Note that this important point is not always stressed in the literature. Moreover, Bru and Zagrebnov [15] proposed a model reduced to the Bogoliubov approach but in conjunction with the inequality (44). We have to conclude that this model hardly has physical sense.

V. SHORT-RANGE CORRELATIONS AND ULTRAVIOLET DIVERGENCE WITHIN THE EFFECTIVE-INTERACTION APPROACH

After the detailed consideration in the previous sections, we can argue that the Bogoliubov model with the ‘‘bare’’ potential $\Phi(r)$ replaced by an effective one [4] is thermodynamically inconsistent. Indeed, the basic relations of the Bogoliubov model (25) and (26) do not depend explicitly on interaction. Hence, the pairwise potential appearing in Eqs. (33)–(36) comes from Eq. (8), which is the general relation valid in both the weak- and strong-coupling regimes. Thus, a calculating procedure based on Eqs. (25) and (26) has to eventuate in Eqs. (33)–(36). Otherwise, as in the case of using the Bogoliubov model with an effective interaction, this procedure does not yield a result minimizing the mean energy. Note that we do not mean, of course, that the *t*-matrix approach or the pseudopotential method cannot be applied in quantum scattering problems. It is only stated that the usual way of combining the ladder diagrams with the random-phase approximation ones (‘‘bubbles’’) leads to a thermodynamic inconsistency.

To clarify the reason for this inconsistency, let us take a look at the picture of the spatial boson correlations derived in the framework of the effective-interaction approach. According to the paper by Hugenholtz and Pines [4] [see Eq. (5.10a) therein], the structure factor

$$S(k) = 1 + n\int d^3r\,[g(r)-1]\exp(-i\mathbf{k}\cdot\mathbf{r}) \tag{45}$$

of a strong-coupling Bose gas can be written at $n \to 0$ as follows:

$$S(k) = 1 + 2\frac{n_0}{n}\langle \hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}}\rangle + \frac{n_0}{n}\left(\langle \hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}\rangle + \langle \hat{a}^\dagger_{-\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}}\rangle\right). \tag{46}$$

Using Eq. (5), the equality $\psi(k) = \psi^*(k)$ [16], and definition (45) of the structure factor, one can readily verify that Eq. (46) is reduced to Eq. (25). This Bogoliubov relation does not depend on the interaction potential explicitly. So use of the dressed interaction can in no way disturb the form of Eq. (25), and, therefore, the effective-interaction approach deals with a pair distribution function whose structure has obvious weak-coupling character. In particular, from Eq. (46) it can be found that $g(r) \to 1 + 2\psi^{(0)}(r)$ for $n \to 0$, as opposed to the correct strong-coupling result given by Eq. (7). However, the wave function $\varphi^{(0)}(r)$ obeys Eq. (9) in the effective-interaction approach [17], while within the Bogoliubov model $\varphi^{(0)}(r)$ is the solution of Eq. (34) at $n=0$. This equation [Eq. (34) at $n=0$] comes from the Schrödinger equation (9) in the Born approximation (see the discussion in Sec. III). Thus, the effective-interaction approach is not totally reduced to the weak-coupling framework due to its features of strong-coupling character. *Exactly this combination of the peculiarities of both the strong- and weak-coupling regimes is the reason for the thermodynamic inconsistency mentioned above.*

It is also worth noting that this combination of the features of weakly and strongly interacting Bose gases leads not only to the thermodynamic inconsistency, but also to an irrelevant picture of the short-range boson correlations. Indeed, in the case of a strongly singular pair interaction for the solution of Eq. (9) we have $\varphi^{(0)}(r=0)=0$ (see Sec. II), which provides $\psi^{(0)}(r=0)=-1$. Within the effective-interaction scheme $g(r)$ obeys Eq. (25) while $\varphi^{(0)}(r)$ satisfies Eq. (9). This implies that $g(r=0) \to 1 + 2\psi^{(0)}(r=0) = -1$ in the zero-density limit when $(n-n_0)/n \to 0$. The result obtained does not agree with the physical sense of $g(r)$ (the conditional probability) and has nothing to do with the strong-coupling regime when the relation $g(r=0)=0$ has to be satisfied. The situation is even aggravated if we recall that the scattering parts of the supracondensate-condensate pair wave functions $\psi_{\mathbf{p}}(\mathbf{r})$ are equal to zero in the Bogoliubov model. So, in what concerns the pair distribution function, the ‘‘triple’’ correlations involved in Eq. (5) for $\psi_{\mathbf{p}}(\mathbf{k})$ are completely ignored within the effective-interaction scheme. However, when deriving an equation for the effective potential, these correlations are taken into consideration, for example, within the Beliaev approach (see the discussion in the review [18]). So we face one more combination of the weak- and strong-coupling features that is characteristic of the approach of Ref. [4].

Since the short-range behavior of the pair distribution function is not correct within the effective-interaction approach, one can expect some problems related to evaluation of the mean energy (8). Let us consider the effective-interaction method in its simplest variant, the so-called pseudopotential model (see the paper by Lee, Huang, and Yang of Ref. [4]). This variant implies the replacement $\Phi(r)\to\delta(\mathbf{r})4\pi\hbar^2a/m$, and hence for the Fourier transform we have

$$\Phi(k)\to4\pi\hbar^2a/m=\text{const}, \tag{47}$$

where a is the scattering length (11) obtained from the Schrödinger equation (9). So the pseudopotential model is reduced to the Bogoliubov model with the effective pairwise interaction given by Eq. (47). In a well-known textbook [5] one can find two ways of calculating the leading and next-to-leading terms of the low-density expansion of the energy of a dilute Bose gas within the pseudopotential model. One of them (see pp. 314–319) consists in dealing directly with the Hamiltonian of the system and faces the divergent integral $\int d^3k/k^2$ (the ultraviolet divergence). The second (given on pp. 218–223) allows for calculating the difference $\varepsilon-\mu/2$ and does not lead to any divergence.

In the previous section we have derived the low-density expansion (42) corresponding to the Bogoliubov model. This expansion can help us to understand the reasons for the ambiguous result of the pseudopotential model. Use of the pseudopotential (47) leads to the substitution $a\to a_0$ in Eq. (42). In addition, $a_1\to-\infty$ as it becomes proportional to $\int d^3k/k^2$ [see Eq. (16)]. This agrees with the result of the first way of calculating ε in the textbook [5]. The divergent integral is usually removed because it is assumed that ‘‘this divergence is not very basic’’ [5]. So, we arrive at the correct expression [Eq. (70) below], which is found in our model beyond any divergences. The reason for the singularity is obvious because the necessary condition (17) of the validity of the Bogoliubov model is not satisfied. However, the question remains why the pseudopotential approach results nevertheless in the correct final expression (70)? The point is that the effective-interaction scheme actually involves an additional assumption, namely, the Landau postulate (see the footnote in Ref. [6] and discussion in Ref. [4]). This postulate asserts that the properties of dilute quantum gases are ruled by the scattering length a [19]. Let us consider how the additional assumption is used when deriving the low-density expansion for the mean energy. According to the Landau argument this expansion should be of the form

$$\varepsilon=c_1(a)n+c_2(a)n^{3/2}+\cdots, \tag{48}$$

where the factors c_i can depend on various quantities but one of them, the ‘‘bare’’ potential $\Phi(r)$, is involved only through the mediation of the scattering length (11). Substituting the Born series (15) in the expressions for $c_i(a)$ in the *weak-coupling* regime, we obtain

$$c_i(a)=c_i(a_0+a_1+\cdots)\simeq c_i(a_0)+\left.\frac{\partial c_i(a)}{\partial a}\right|_{a=a_0}a_1+\cdots. \tag{49}$$

As the functional dependencies $c_i(a)$ are of the same form in both the weak- and strong-coupling regimes, one is able to restore them by keeping the Born terms $c_i(a_0)$ in the expansion (48) and omitting others (dependent on $a_1,a_2,\ldots$). It can readily be verified in this way that Eq. (42) leads to Eq. (70). Thus, the pseudopotential approach provides (after regularization) the correct result given by Eq. (70) because it is equivalent, in the first two orders of the low-density expansion, to a calculating scheme using the Bogoliubov model together with Eqs. (48) and (49) based on the Landau postulate [20]. Note that this simple scheme looks even more accurate and justified than the pseudopotential approach. At least, it allows for investigating a strongly interacting Bose gas beyond any ultraviolet divergence which appears as a result of violating the subtle balance of correlation terms coming from the boson-boson scattering. However, neither the pseudopotential approach nor the Bogoliubov model used together with Eqs. (48) and (49) can yield adequate microscopic results concerning the strong-coupling regime.

The second way of calculating $\varepsilon(n)$ within the pseudopotential model allows one to find the low-density expansion (48) starting from the difference

$$\varepsilon-\frac{\mu}{2}=\varepsilon-\frac{1}{2}\frac{\partial(\varepsilon n)}{\partial n}\simeq-\frac{2\pi\hbar^2na_0}{m}\frac{32}{15\sqrt{\pi}}\sqrt{na_0^3}, \tag{50}$$

where Eq. (42) and the well-known thermodynamic relation $\mu=\partial[n\varepsilon(n)]/\partial n$ are of use. There is no divergent integral here due to the specific property of the expansion (42): a_1 is involved only in the leading-order term that is exactly canceled in Eq. (50) [20]. The solution of the differential equation (50) (after replacing a_0 by a) is of the form $\varepsilon=c_1n+(2\pi\hbar^2na/m)(128/15\sqrt{\pi})\sqrt{na^3}$. To specify c_1, a constant of integration, one again needs to involve information additional to Eq. (50). Following Landau and *postulating* that c_1 depends on the pairwise potential only through the mediation of the scattering length a, one arrives at $c_1=2\pi\hbar^2a/m$, which eventuates in Eq. (70).

Thus, we remark one more that the effective-interaction approach *taken in conjunction with the Landau postulate* yields the correct expansion (70). Even Wu’s term [21] in the low-density expansion of the energy of a strong-coupling Bose gas is likely to be correct because it is present in the weak-coupling calculations beyond the Bogoliubov model [22]. However, the microscopic results found within the effective-interaction approach should be reexamined. So a correct strong-coupling generalization of the Bogoliubov model should be constructed. It is also of importance that the density expansions for the quantities depending on the form of $\Phi(r)$, for example, the interaction (76) and kinetic (77) energies below, cannot be derived directly within the effective-interaction scheme. We discuss this point in Sec. VIII E.

VI. STRONG-COUPLING GENERALIZATION OF THE BOGOLIUBOV MODEL

To avoid the serious problems mentioned in the previous section, we should abandon the effective-interaction method and use a way based on Eq. (2). Equations (2), (6), and (8) make it possible to express ε in terms of the pair wave functions and momentum distribution. So a variational procedure similar to that of Sec. III can be employed to determine these basic quantities. In so doing we should again keep in mind that the momentum distribution depends on the scattering waves (see Sec. III). However, now we are not able to use the Bogoliubov relation (26), which does not take into account scattering in the supracondensate-condensate sector. In [3] the following extension of Eq. (26) was proposed:

$$n_k(n_k+1)=n_0^2\psi^2(k)+2n_0\int\frac{d^3q}{(2\pi)^3}\,n_q\psi^2_{\mathbf{q}/2}(\mathbf{k}). \tag{51}$$

This expression was derived with the help of the reasonable expectation that the equation for $\psi_{\mathbf{p}}(\mathbf{k})$ should be reduced to the equation for $\psi(k)$ in the limit $p\to 0$. It is interesting to note the obvious structural parallels between Eqs. (2) and (51). Now, inserting Eqs. (2) and (6) into Eq. (8) and then perturbing $\psi(k)$ and n_k under the condition (51), we find

$$-2T_k\psi(k)=U(k)(1+2n_k)+2n\psi(k)U'(k). \tag{52}$$

Here $U(k)$ and $U'(k)$ are defined by

$$U(k)=\int d^3r\,\varphi(r)\Phi(r)\exp(-i\mathbf{k}\cdot\mathbf{r}), \tag{53}$$

$$U'(k)=\int d^3r[\varphi^2_{\mathbf{k}/2}(\mathbf{r})-\varphi^2(r)]\Phi(r) -\int\frac{d^3q}{(2\pi)^3}\,\frac{U(q)}{\psi(q)}[\psi^2_{\mathbf{k}/2}(\mathbf{q})-\psi^2(q)]. \tag{54}$$

An equation for $\psi_{\mathbf{p}}(\mathbf{k})$ can be derived in the same manner. Note that we have the following limiting relation:

$$\lim_{p\to 0}\varphi_{\mathbf{p}}(\mathbf{r})=\sqrt{2}\,\varphi(r), \tag{55}$$

where the factor $\sqrt{2}$ comes from the second expression in Eq. (3). Using the equation for $\psi_{\mathbf{p}}(\mathbf{k})$, one can be convinced that $\psi_0(k)\equiv\lim_{p\to 0}\psi_{\mathbf{p}}(\mathbf{k})=\mathrm{const}\times\psi(k)$. We should put this constant equal to $\sqrt{2}$ in order to obtain Eq. (55) [23]. So we have $\varphi(r)-\sqrt{2}\varphi_{\mathbf{p}}(\mathbf{r})\propto p^2$ (see Ref. [10] in [3]), which provides $U'(k)-U(k)\propto k^4$ for $k\to 0$. Additionally, it is easy to verify that $[U(k)-U'(k)]/T_k\to 0$ when $k\to\infty$. Therefore at small densities $n[U'(k)-U(k)]\ll T_k$ for all momenta. This is why the difference between $U'(k)$ and $U(k)$ does not play a role when calculating the first two terms of the low-density expansions for the basic thermodynamic quantities. Thus, at sufficiently small densities Eq. (52) can be rewritten in the following form:

$$\frac{\hbar^2}{m}\nabla^2\varphi(r)=\varphi(r)\Phi(r)+n \times\int d^3y\,\varphi(y)\Phi(y)[g_{tr}(|\mathbf{r}-\mathbf{y}|)-1], \tag{56}$$

where $g_{tr}(r)$ stands for the truncated pair distribution function, which is equal to the right-hand side of Eq. (25) even beyond the weak-coupling regime.

Equations (2) [and, hence, Eqs. (6) and (8)] and (51) are written with the condensate-condensate and supracondensate-condensate channels taken into account. As these relations are accurate to the next-to-leading order in $(n-n_0)/n$, Eq. (52) can be accurate only to the leading order in $(n-n_0)/n$. So it would be wrong to solve Eq. (52) together with Eq. (51). One should investigate Eq. (52) in conjunction with the shortened version of Eq. (51) given by Eq. (26), where the equality $n=n_0$ is implied. The system of Eqs. (26) and (52) has the following solution:

$$n_k=\frac{1}{2}\left(\frac{\tilde{T}_k+nU(k)}{\sqrt{\tilde{T}_k^2+2n\tilde{T}_kU(k)}}-1\right), \tag{57}$$

$$\psi(k)=-\frac{1}{2}\,\frac{U(k)}{\sqrt{\tilde{T}_k^2+2n\tilde{T}_kU(k)}} \tag{58}$$

with $\tilde{T}_k=T_k+n[U'(k)-U(k)]$. As to the supracondensate-condensate states, the goal of this paper makes it possible not to go into details concerning $\varphi_{\mathbf{p}}(\mathbf{r})$. It is sufficient only to use Eq. (55). In the zero-density limit $n=0$ Eq. (58) is reduced to the equation $\psi(k)=\psi^{(0)}(k)=-U^{(0)}(k)/(2T_k)$, which can be rewritten in the form of Eq. (9). So at small densities all thermodynamic quantities can be expressed in terms of the vacuum (out-medium) scattering amplitude $U^{(0)}(k)$ given by

$$U^{(0)}(k)=\int d^3r\,\varphi^{(0)}(r)\Phi(r)\exp(-i\mathbf{k}\cdot\mathbf{r}). \tag{59}$$

Below it is shown that this feature of Eqs. (57) and (58) results directly in Eqs. (65), (69), and (70). So the low-density energy expansion given by Eq. (70) is determined in our model beyond any additional assumptions like the Landau postulate in the pseudopotential approach. Equations (57) and (58) yield $n_k\propto 1/k$ and $\psi(k)\propto 1/k$ at small boson momenta. This is totally consistent with the well-known ‘‘$1/k^2$’’ Bogoliubov theorem [8]. It is interesting that the correct low-momentum behavior of n_k and $\psi(k)$ comes from the relation $U'(k)-U(k)\propto k^4$ which follows from Eq. (54) taken in conjunction with Eq. (55), a result of the principle of correlation weakening. Note that Eqs. (35) and (36) derived within the Bogoliubov model can be obtained from Eqs. (57) and (58) by replacing $\tilde{T}_k$ and $U(k)$ with T_k and $\Phi(k)$, respectively. So in what concerns Eqs. (57) and (58), the situation in our strong-coupling generalization of the Bogoliubov model does look as if we operated with a weakly interacting Bose gas of the quasiparticles with the renormalized kinetic energy $\tilde{T}_k$ and the effective interaction $U(r)=\varphi(r)\Phi(r)$. This is close to the expectations following from the effective-interaction approach [4]. Due to the boundary condition $U(k)-U'(k)\propto k^4$ at small k the mass of the quasiparticles coincides with that of the primordial bosons. However, as was mentioned in Ref. [3], Eq. (51) is the simplest of the possible approximations, which are fixed by the necessary condition that the Bethe-Goldstone equation for $\psi_{\mathbf{p}}(\mathbf{k})$ is reduced to the equation for $\psi(k)$ in the limit $p\to 0$. These approximations lead to the same low-density expansions for thermodynamic quantities (the energy, the chemical potential, the condensate depletion) in the leading and next-to-leading terms. However, the difference in the thermodynamics has to appear at small but finite densities as well as in the higher-order terms in the density expansions. The same goes for the microscopic picture given by Eqs. (57) and (58). Here the different approximations of the relationship between the momentum distribution and pair wave functions can lead to some different details. In particular, we cannot *a priori* exclude the possibility that there is a more relevant variant of Eq. (51) which leads to $U'(k)-U(k)\propto k^2 (k\to 0)$. In this situation the quasiparticle mass would be $m^*=m/(1+\beta n)$, where $\beta=\lim_{k\to 0}[U'(k)-U(k)]/T_k$.

VII. SHORT-RANGE BOSON SPATIAL CORRELATIONS

Now, to elaborate on the picture of the short-range boson correlations, let us investigate how the correlation hole stipulated by the repulsion between bosons at small separations changes due to the influence of the surrounding bosons. At $n\to 0$ this hole is completely specified by the condensate-condensate pair wave function $\varphi(r)$. Exploring how $U(k)$ is expressed in terms of $U^{(0)}(k)$ makes it possible to know how $\varphi(r)$ differs from $\varphi^{(0)}(r)$ at small boson separations. Note that the relation connecting $U(k)$ with $U^{(0)}(k)$ has been published in our previous paper [3] without supporting calculations for reasons of space. Let us give these important calculations here. Using the definition of $U(k)$ and Eq. (58), for the scattering amplitude one can find

$$U(k)=\Phi(k)-\tfrac{1}{2}\int\frac{d^3q}{(2\pi)^3}\frac{\Phi(|\mathbf{k}-\mathbf{q}|)U(q)}{\sqrt{\tilde{T}_q^2+2n\tilde{T}_qU(q)}},\qquad(60)$$

which can be called the in-medium Lippmann-Schwinger equation. Let us rewrite Eq. (60) in the form

$$U(k)=\Phi(k)-\tfrac{1}{2}\int\frac{d^3q}{(2\pi)^3}\frac{\Phi(|\mathbf{k}-\mathbf{q}|)U(q)}{T_q}-I,$$

where for I we have

$$I=\tfrac{1}{2}\int\frac{d^3q}{(2\pi)^3}\left(\frac{\Phi(|\mathbf{k}-\mathbf{q}|)U(q)}{\sqrt{\tilde{T}_q^2+2n\tilde{T}_qU(q)}}-\frac{\Phi(|\mathbf{k}-\mathbf{q}|)U(q)}{T_q}\right).$$

Performing the "scaling" substitution (39) in the integral and then taking the zero-density limit in the integrand, for $n\to 0$ we find

$$I=-\alpha\Phi(k),\quad \alpha=\frac{\sqrt{nm^3}}{\pi^2\hbar^3}U^{3/2}(0).\qquad(61)$$

From Eqs. (60) and (61) it now follows that

$$U(k)-U^{(0)}(k)=\alpha\Phi(k)-\int\frac{d^3q}{(2\pi)^3}\frac{\Phi(|\mathbf{k}-\mathbf{q}|)}{2T_q}[U(q)-U^{(0)}(q)],\qquad(62)$$

where $U^{(0)}(k)$ obeys Eq. (60) with $n=0$, i.e., the standard Lippmann-Schwinger equation. Introducing the new quantity $\xi(q)=-[U(q)-U^{(0)}(q)]/(2T_q)$, for its Fourier transform $\xi(r)$ we find an equation that is nothing else but the Schrödinger equation (9) with $\varphi^{(0)}(r)$ replaced by $\alpha+\xi(r)$. As $\xi(r)\to 0$ when $r\to\infty$, we can conclude that $\xi(r)=\alpha\psi^{(0)}(r)$. Hence, for $n\to 0$ we get

$$U(k)\simeq U^{(0)}(k)\left(1+\gamma(k,n)\frac{8}{\sqrt{\pi}}\sqrt{na^3}\right).\qquad(63)$$

Here $\gamma(k,n)\to 1$ when $n\to 0$, and the scattering length a is defined by Eq. (11). The result derived for the in-medium scattering amplitude $U(k)$ coincides with the low-density expansion for the effective potential found within the effective-interaction approach at zero temperature [see Eq. (4.27) in the review [18]]. This shows once more that there are actual parallels between our model and the approach of Ref. [4]. However, these parallels are accompanied by significant differences. First, in general the in-medium Lippmann-Schwinger equation (60) is not a variant of the t matrix equation, which is frequency dependent, contrary to Eq. (60). Second, Eq. (60) has been found beyond any diagram technique by means of a variational procedure whose consequence is that the pair wave functions "generating" in-medium scattering amplitudes coincide with the pair wave functions involved in $g(r)$. On the contrary, this is not true for the effective-interaction scheme, which implies plane waves for $\varphi_{\mathbf{p}}(\mathbf{r})$ in the pair distribution function (see the discussion in Sec. V) and certainly goes beyond the plane-wave approximation when calculating the t matrix corresponding to a pair of particles with nonzero total momentum. Third, in Eqs. (57)–(60) we deal with $\tilde{T}_k$ rather than with T_k, appearing in the effective-interaction scheme. For more information, see also the discussion in [10]. Now, returning to Eq. (63), we can conclude that for $r\lesssim R$ [R is the radius of the interaction potential $\Phi(r)$; for strongly singular potentials R is of the order of the scattering length a] and $n\to 0$ we obtain the following in-medium renormalization:

$$\varphi(r)\simeq\varphi^{(0)}(r)\left(1+\frac{8\sqrt{na^3}}{\sqrt{\pi}}\right).\qquad(64)$$

Thus, the correlation hole coming from the repulsion of bosons at small particle separations becomes less marked with an increase of the density of the surrounding bosons, which is mainly the result of the Bose-Einstein statistics. For the pair distribution function at small boson densities we have $g(r)\propto[\varphi^{(0)}(r)]^2$ [see the expression (83)]. So, for strongly singular potentials, when $\varphi^{(0)}(r=0)=0$, the correct strong-coupling result $g(r=0)=0$ occurs for a dilute Bose gas if Eqs. (2), (8), and (51) are taken as the basic relations.

It is interesting to note that for the effective-interaction approach [4] an upper cutoff in the momentum space at $p_c \simeq \hbar/a$ is usually made. Thus, one could expect that owing to the uncertainty relation in-medium renormalization would be essential when $a \lesssim r$ in real space. Equation (64) shows that this is not the case. As is seen, $\varphi(r)$ at small separations is really a solution of the bare Schrödinger equation (see Sec. I) but differs from $\varphi^{(0)}(r)$ by the multiplier $(1+8\sqrt{na^3}/\sqrt{\pi})$. We also remark that unusual overscreening takes place for $\varphi(r)$ when $r\rightarrow\infty$. Indeed, Eq. (58) yields

$$\lim_{k\rightarrow 0} k\psi(k) = -\frac{1}{2}\sqrt{\frac{mU(0)}{n}}.$$

The last relation implies that for the condensate-condensate pair wave function we have $\psi(r)=\varphi(r)-1 \propto 1/r^2$ for $r\rightarrow\infty$, in contrast to the bare wave function $\psi^{(0)}(r)=\varphi^{(0)}(r)-1\propto 1/r$ for $r\rightarrow\infty$ [see Eq. (10)].

VIII. LOW-DENSITY EXPANSIONS

Now, to verify that a subtle balance of the terms coming from the short-range particle correlations plays a significant role in the problem of the strong-coupling Bose gas, let us calculate low-density expansions of the basic thermodynamic quantities. The relation for the condensate depletion

$$\zeta = \frac{n-n_0}{n} = \int \frac{d^3q}{(2\pi)^3}\,\frac{n_q}{n} = \frac{8\sqrt{na^3}}{3\sqrt{\pi}} + \cdots \qquad (65)$$

can be obtained from Eq. (57) with the ''scaling'' substitution given by Eq. (39).

The low-density expansion for the energy can be derived in four different ways.

A. The chemical potential

The first way of obtaining the energy expansion deals with the chemical potential μ and starts from the following relation for μ valid in the presence of the Bose condensate [8]:

$$\mu = \frac{1}{\sqrt{n_0}}\int d^3r'\,\Phi(|\mathbf{r}-\mathbf{r}'|)\langle \hat{\psi}^{\dagger}(\mathbf{r}')\,\hat{\psi}(\mathbf{r}')\,\hat{\psi}(\mathbf{r})\rangle. \qquad (66)$$

Here $\hat{\psi}^{\dagger}(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$ stand for the Bose field operators. This relation follows from the well-known expression for an infinitesimal change of the grand canonical potential $\delta\Omega = \langle \delta(\hat{H}-\mu\hat{N})\rangle$ and the necessary condition of the minimum of Ω with respect to the order parameter $N_0 : \partial\Omega(N_0,\mu,T)/\partial N_0 = 0$, the Hamiltonian depending on the number of condensed particles owing to the substitution $\hat{a}_0^{\dagger}=\hat{a}_0=\sqrt{N_0}$. Equations (5) and (66) lead to [24]

$$\mu = n_0 U(0) + \sqrt{2}\int \frac{d^3q}{(2\pi)^3}\,n_q U_{\mathbf{q}/2}(\mathbf{q}/2), \qquad (67)$$

where $U(0)$ is defined by Eq. (53), and

$$U_{\mathbf{p}}(\mathbf{k}) = \int d^3r\,\varphi_{\mathbf{p}}(\mathbf{r})\Phi(r)\exp(-i\mathbf{k}\cdot\mathbf{r}). \qquad (68)$$

Using the substitution (39) in the integral and taking into consideration Eqs. (55), (63), and (65), we can rewrite Eq. (67) for $n\rightarrow 0$ as

$$\mu = nU(0)(1+\zeta+\cdots) = \frac{4\pi\hbar^2 an}{m}\left(1+\frac{32}{3\sqrt{\pi}}\sqrt{na^3}+\cdots\right). \qquad (69)$$

This, together with the thermodynamic relation $\mu = \partial[n\varepsilon(n)]/\partial n$, yields the following result:

$$\varepsilon = \frac{2\pi\hbar^2 an}{m}\left(1+\frac{128}{15\sqrt{\pi}}\sqrt{na^3}+\cdots\right), \qquad (70)$$

known since the familiar paper by Lee and Yang [25] and found with the binary collision expansion method.

B. Direct calculation of the energy

The method of this subsection is direct and starts from the expression (8). Inserting Eq. (2) into Eq. (6) and using the substitution (39) in the integral, we can rewrite the pair distribution function for $n\rightarrow 0$ in the form

$$g(r) \simeq (1+2\zeta)\varphi^2(r), \qquad (71)$$

where the relation (55) is implied. Note that this expression is not valid at sufficiently large r as the boundary condition $g(r)\rightarrow 1$ for $r\rightarrow\infty$ is not satisfied. However, here we are not interested in the long-range behavior of $g(r)$ because we use Eq. (71) when integrating $g(r)$ multiplied by the short-range potential $\Phi(r)$. Equation (71) makes it possible to represent Eq. (8) for $n\rightarrow 0$ as

$$\varepsilon \simeq \frac{n}{2}(1+2\zeta)U(0) + \int \frac{d^3q}{(2\pi)^3}\left(T_q\frac{n_q}{n} + \frac{n}{2}(1+2\zeta)U(q)\psi(q)\right). \qquad (72)$$

Taking the term proportional to ζ in the integral in Eq. (72), we can rewrite it for $n\rightarrow 0$ in the form

$$I = n\zeta\int \frac{d^3q}{(2\pi)^3}U(q)\psi(q) \simeq n\zeta\int\frac{d^3q}{(2\pi)^3}U^{(0)}(q)\psi^{(0)}(q) = -n\zeta\frac{4\pi\hbar^2}{m}b, \qquad (73)$$

where the vacuum scattering amplitude $U^{(0)}(q)$ and the characteristic length b are given by Eqs. (59) and (22), respectively. Using the substitution (39) in the residual part of the integral in Eq. (72),

$$\int \frac{d^3q}{(2\pi)^3}\left(T_q\frac{n_q}{n}+\frac{n}{2}U(q)\psi(q)\right),$$

and taking into account Eqs. (57), (58), (63), and (65), we arrive at Eq. (70) but with the second term multiplied by the factor $\lambda=1-5b/(8a)$. Now the question arises which variant we should prefer, Eq. (70) or Eq. (70) with the factor $\lambda=1-5b/(8a)$, and what is the reason for this ambiguous situation?

To answer this question, let us reconsider the procedure of calculating ε given in this subsection. As was mentioned earlier, Eqs. (57) and (58) used in our calculations are consistent with Eq. (26) rather than with Eq. (51). Being characteristic of the Bogoliubov model, Eq. (26) is accurate to the leading order in $(n-n_0)/n$ and differs from Eq. (51) by the supracondensate-condensate term neglected in the Bogoliubov relation. The problem of the λ factor turns out to be directly related to this term. It can be taken into account by representing Eq. (51) for $n\to 0$ in the form

$$n_k(n_k+1)=(1+2\zeta)\psi^2(k). \tag{74}$$

Solving this equation with respect to n_k and noticing Eq. (58), one can obtain

$$n_k=\frac{1}{2}\left(\frac{\sqrt{[\widetilde{T}_k+nU(k)]^2+2\zeta n^2U^2(k)}}{\sqrt{\widetilde{T}_k^2+2n\widetilde{T}_kU(k)}}-1\right). \tag{75}$$

Now, restarting from Eq. (72) and making use of the system of Eqs. (75) and (58) instead of that of Eqs. (57) and (58), we arrive at Eq. (70). The term given by Eq. (73) is now canceled due to the correcting term $2\zeta n^2U^2(k)$ involved in Eq. (75). So we face a rather complicated situation: namely, to get the correct result (70) in the direct calculations starting from Eq. (8), we have to abandon Eq. (57) in favor of Eq. (75), while for $\psi(k)$ we can exploit Eq. (58). The most important point here is the uniform convergence of the integral in Eq. (72) provided Eq. (75) is used. This allows for employing Eq. (75) together with Eq. (58) in spite of the fact that the latter has been found in the leading order in $(n-n_0)/n$. The higher-order corrections to Eq. (58) do not influence the result of calculating the integral in Eq. (72) if we limit ourselves to the leading and next-to-leading orders in na^3. It is worth noting that replacing Eq. (75) by Eq. (57) does not influence Eqs. (65) and (69). So the preliminary result for ε found in [3] and corresponding to Eq. (70) with the second term multiplied by the factor $\lambda=1-5b/(8a)$ has to be abandoned in favor of Eq. (70).

The analysis carried out in this section demonstrates the crucial role of the subtle balance of the terms coming from the boson scattering (or, in other words, from the short-range boson correlations). Disturbance of this fine interplay, which seems to be insignificant, can nevertheless lead to wrong conclusions. We stress that the strong-coupling model of Ref. [3] is balanced because it takes into consideration the supracondensate-condensate scattering waves in *both* the pair distribution function and the relation connecting the momentum distribution with the pair wave functions. On the contrary, the effective-interaction approach is not balanced with respect to the supracondensate-condensate scattering waves, which are missed in the pair distribution function but make a contribution to the dressed potential (see Sec. V). Exactly this problem is the basis for the so-called ultraviolet divergence occurring in the effective-interaction approach.

C. Energy expansion through the Hellmann-Feynman theorem

As shown in Sec. V, the effective-interaction approach results in an irrelevant picture of the short-range boson correlations. This is why it cannot yield the correct individual values of the interaction ε_{int} and kinetic ε_{kin} energies by direct calculations based on Eq. (8). Recall that we have the following definitions: these energies are defined by

$$\varepsilon_{int}=\frac{1}{N}\left\langle\sum_{i\neq j}\frac{\gamma}{2}\Phi(|\mathbf{r}_i-\mathbf{r}_j|)\right\rangle=\frac{n}{2}\int d^3r\,\gamma\Phi(r)g(r), \tag{76}$$

$$\varepsilon_{kin}=\frac{1}{N}\left\langle-\sum_i\frac{\hbar^2\nabla_i^2}{2m}\right\rangle=\int\frac{d^3k}{(2\pi^3)}T_k\frac{n_k}{n}, \tag{77}$$

where $\langle\cdots\rangle$ stands for the statistical average with respect to the ground state, and the auxiliary parameter γ is the coupling constant. The total energy per particle (8) is given by the sum of ε_{int} and ε_{kin} at $\gamma=1$:

$$E/N=\varepsilon=\varepsilon_{kin}+\varepsilon_{int}. \tag{78}$$

Our model provides the correct short-range behavior of the pair distribution function $g(r)$. So we can first evaluate $\varepsilon_{int}(\gamma)$, and then obtain the total energy (8) by means of the well-known expression often called the Hellmann-Feynman theorem, which is just the variational theorem for the ground state obeying the N-body Schrödinger equation

$$\delta E=\langle\delta\hat{H}\rangle. \tag{79}$$

In Eq. (79) δE and $\delta\hat{H}$ are infinitesimal changes of the average energy $(E=\langle\hat{H}\rangle)$ and the Hamiltonian

$$\hat{H}=-\sum_i\frac{\hbar^2\nabla_i^2}{2m}+\frac{1}{2}\sum_{i\neq j}\gamma\Phi(|\mathbf{r}_i-\mathbf{r}_j|), \tag{80}$$

respectively. The relations (76), (77), (79), and (80) lead to the important equations

$$\varepsilon_{int}=\gamma\frac{\partial\varepsilon}{\partial\gamma},\quad \varepsilon_{kin}=-m\frac{\partial\varepsilon}{\partial m}. \tag{81}$$

From the first expression in Eq. (81) it follows that

$$\varepsilon=\int_0^1 d\gamma\frac{\varepsilon_{int}(\gamma)}{\gamma}. \tag{82}$$

To evaluate $\varepsilon_{int}(\gamma)$ in the leading and next-to-leading orders in na^3, it is convenient to rewrite Eq. (71) as

$$g(r)\simeq w(na^3)[\varphi^{(0)}(r)]^2, \tag{83}$$

where Eqs. (64) and (65) are taken into account and $w(na^3)$ is given by

$$w(na^3)=1+\frac{64}{3\sqrt{\pi}}\sqrt{na^3}. \tag{84}$$

The range of particle separations for which Eq. (83) is correct coincides with that of Eq. (71) (see the discussion there). Keeping in mind Eqs. (21), (23), (76), (82), and (83), we obtain

$$\varepsilon \simeq \frac{2\pi\hbar^2 n}{m}\int_0^1 d\gamma \frac{\partial a}{\partial \gamma} w(na^3(\gamma)) = \frac{2\pi\hbar^2 n}{m}\int_0^a da' w(na'^3).$$

Thus, using Eq. (84), we arrive at Eq. (70) again.

D. Energy expansion through the virial theorem

This method was proposed by Bogoliubov in his original paper [6] in order to obtain the leading-order term in the energy expansion. Here we consider this method in a more general form. As in Sec. VIII C, we start from the expression for the pair distribution function $g(r,n)$ which is assumed to be a known function of the density n. The basic idea is to derive the differential equation for $\varepsilon(n)$.

On the one hand, from the virial theorem we get the following expression for the pressure:

$$P = \frac{2}{3}\varepsilon_{kin}(n)n - \frac{n^2}{6}\int d^3r \frac{d\Phi(r)}{dr} r g(r,n), \tag{85}$$

where $\varepsilon_{kin}(n)$ is given by Eq. (77). On the other hand, we have the thermodynamic relation

$$P = n^2 \frac{\partial \varepsilon(n)}{\partial n} \tag{86}$$

valid at zero temperature. Here $\varepsilon(n)$ is the energy per particle (8), which can be written as

$$\varepsilon(n) = \varepsilon_{kin}(n) + \frac{n}{2}\int d^3r g(r,n)\Phi(r). \tag{87}$$

The system of Eqs. (85)–(87) yields a differential equation for $\varepsilon(n)$ whose general solution is of the form

$$\varepsilon = C_0 n^{2/3} - \frac{1}{6}\int d^3r \left(\frac{d\Phi(r)}{dr} r + 2\Phi(r)\right)\chi(r,n), \tag{88}$$

where the function $\chi(r,n)$ stands for

$$\chi(r,n) = n^{2/3}\int_0^n dn' \frac{g(r,n')}{n'^{2/3}} \tag{89}$$

and C_0 is the integration constant. Note that Eqs. (88) and (89) are valid for both the Bose and Fermi systems because we have not used the type of statistics when deriving these equations. For a Fermi system the constant C_0 is not equal to zero, while for a Bose system we should put $C_0 = 0$ provided Bose-Einstein condensation takes place. Substituting Eq. (83) in Eq. (89), from Eq. (88) we get

$$\varepsilon = J\frac{n^{2/3}}{6}\int_0^n dn' \frac{w(n'a^3)}{n'^{2/3}}, \tag{90}$$

where

$$J = -\int d^3r \left(\frac{d\Phi(r)}{dr} r + 2\Phi(r)\right)[\varphi^{(0)}(r)]^2 = U^{(0)}(0).$$

The last equation can be derived after a little algebra with the help of Eqs. (9)–(12). As is seen, Eq. (90) together with Eq. (84) leads to the low-density expansion (70).

Thus, all four ways of calculating ε within the strong-coupling model developed in Ref. [3] leads to Eq. (70).

E. Interaction and kinetic energies

For any physical quantity there usually exist various calculating procedures leading to the same result provided the model considered is consistent. By contrast, in the presence of a thermodynamic inconsistency different ways of calculating any thermodynamic quantity are able to produce different results [26,27]; one of them can be reasonable but others are completely inadequate. Such a situation is realized when evaluating the interaction and kinetic energies via the effective-interaction method. This is demonstrated below.

The interaction (76) and kinetic (77) energies of a dilute Bose gas can be evaluated on the basis of the Hellmann-Feynman theorem with the help of Eq. (70). Representing this expansion for ε in the form

$$\varepsilon = \frac{2\pi\hbar^2 an}{m} f(na^3), \tag{91}$$

and keeping in mind Eqs. (81) and (23), one can derive

$$\varepsilon_{int} = \frac{2\pi\hbar^2(a-b)n}{m}\left(f(na^3) + 3na^3\frac{df(na^3)}{d(na^3)}\right), \tag{92}$$

$$\varepsilon_{kin} = \frac{2\pi\hbar^2 bn}{m}\left[f(na^3) + 3na^3\left(1-\frac{a}{b}\right)\frac{df(na^3)}{d(na^3)}\right]. \tag{93}$$

According to Eq. (70) $f(x) = 1 + 128\sqrt{x}/(15\sqrt{\pi})$, which together with Eqs. (92) and (93) yields

$$\varepsilon_{int} = \frac{2\pi\hbar^2(a-b)n}{m}\left(1 + \frac{64}{3\sqrt{\pi}}\sqrt{na^3} + \cdots\right), \tag{94}$$

$$\varepsilon_{kin} = \frac{2\pi\hbar^2 bn}{m}\left[1 + \frac{64}{3\sqrt{\pi}}\sqrt{na^3}\left(1-\frac{3a}{5b}\right) + \cdots\right]. \tag{95}$$

As is seen from Eqs. (91)-(93), terms involving b are present in the expressions for the kinetic and interaction energies and mutually canceled in the total energy ε. We emphasize that the reasoning of this paragraph can be fulfilled for both the effective-interaction approach and the model developed by the present authors.

Our approach is fully consistent, which makes it possible to derive Eqs. (94) and (95) in another way using direct calculations. Indeed, Eq. (76) taken at $\gamma = 1$ in conjunction with Eqs. (21) and (83) results in Eq. (94). Notice that the supracondensate-condensate scattering waves make a significant contribution to the next-to-leading term of the low-density expansion for ε_{int}. It is also not difficult to find the low-density expansion for the kinetic energy (95) with the help of Eqs. (63), (65), and (75).

In contrast, due to the thermodynamic inconsistency, the effective-interaction scheme does not allow for obtaining Eqs. (94) and (95) directly, beyond the Hellmann-Feynman theorem taken with Eq. (70). Let us show this for the pseudopotential approach discussed in Sec. V. To evaluate the kinetic energy in this case, one can start from Eq. (77) and use the Bogoliubov formula (35) with the pseudopotential substitution (47). In so doing the divergent integral $\int d^3k/k^2$ should be ignored (see the discussion in Sec. V). Similarly, the interaction energy at $\gamma=1$ can be derived from Eqs. (25), (35), (36), and (47) using the same regularization. However, to simplify the calculations, we adopt another way leading to the same results and based on the low-density expansion (42), found within the Bogoliubov model. The original Bogoliubov scheme is fully consistent, which implies equivalence of different ways of calculating any thermodynamic quantity. Therefore, we can first find the kinetic and interaction energies by using the Hellmann-Feynman theorem together with Eq. (42) and then replace a_0 by a and a_1 by 0 in the derived expressions. From the definition (16) it follows that

$$\gamma\frac{\partial a_0}{\partial\gamma}=m\frac{\partial a_0}{\partial m}=a_0,\quad \gamma\frac{\partial a_1}{\partial\gamma}=m\frac{\partial a_1}{\partial m}=2a_1.$$

Hence, within the Bogoliubov model we can arrive at

$$\varepsilon_{int}=\frac{2\pi\hbar^2 n}{m}\left(a_0+2a_1+a_0\frac{64}{3\sqrt{\pi}}\sqrt{na_0^3}+\cdots\right),\qquad(96)$$

$$\varepsilon_{kin}=\frac{2\pi\hbar^2 n}{m}\left(-a_1-a_0\frac{64}{5\sqrt{\pi}}\sqrt{na_0^3}+\cdots\right),\qquad(97)$$

provided Eqs. (42) and (81) are taken into consideration. Now, replacing a_0 by a and substituting 0 for a_1 (the latter allows for escaping the ultraviolet divergence; see Sec. V), we obtain the following expressions:

$$\varepsilon_{int}=\frac{2\pi\hbar^2 an}{m}\left(1+\frac{64}{3\sqrt{\pi}}\sqrt{na^3}+\cdots\right),\qquad(98)$$

$$\varepsilon_{kin}=-\frac{2\pi\hbar^2 an}{m}\frac{64}{5\sqrt{\pi}}\sqrt{na^3}+\cdots,\qquad(99)$$

which should be compared with the correct results given by Eqs. (94) and (95). As is seen, the sum of the rhs of Eqs. (98) and (99) gives the rhs of Eq. (70) but at the expense of a negative value of the kinetic energy (99). Notice that the Bogoliubov model is free from this nonphysical feature because $a_1<0$, which leads to $\varepsilon_{kin}>0$ at sufficiently small densities. Thus, Eqs. (98) and (99), found within the pseudopotential model, are inadequate. The reason is obvious: the pseudopotential scheme allows for restoring the functional dependence on the scattering length a in Eqs. (98) and (99) while it completely ignores the additional length b that cannot be involved in the pseudopotential model due to the ultraviolet divergence.

Note that in the case of the hard-sphere interaction (18) we get $a=b$ from the solution of the Schrödinger equation (9). Then, in the general case of Eq. (91) the relations $\varepsilon_{int}=0$, $\varepsilon_{kin}=\varepsilon$ come from Eqs. (92) and (93). Thus we arrive at an interesting property of the Bose gas with the pairwise potential (18): namely, although the Bose gas is strongly interacting, the interaction energy is equal to zero. Hence, the total energy of a dilute Bose gas made of hard spheres is exactly equal to the kinetic energy. One can see that this result is rather general: *for the hard-sphere potential* (18) *the interaction energy is equal to zero for any density.* Indeed, $\Phi(r)$ given by Eq. (18) can be thought of as the limiting case of the repulsive potential

$$\Phi(r)=\begin{cases}V_0, & r<a\\ 0, & r>a.\end{cases}$$

It is clear that saturation takes place when $V_0\gg\varepsilon$: further increase of the parameter V_0 does not change the energy per particle, ε. Hence, according to Eqs. (76) and (81), $\varepsilon_{int}=0$ because $\partial\varepsilon/\partial\gamma=0$ at $\gamma=1$ in the limit $V_0\to+\infty$. Notice that, even taken in the order linear in the density *n*, Eqs. (98) and (99) lead to the opposite case $\varepsilon_{int}\simeq\varepsilon$, $\varepsilon_{kin}\simeq0$. This incorrect redistribution of the energy of a dilute Bose gas in the pseudopotential approach is also noted in [28], where the leading order of the low-density energy expansion is considered.

Note that the relation Eq. (23) enables us to obtain the length *b* in an experimental way by the isotopic shift of the scattering length *a*:

$$b=a\left(1-\frac{\partial\ln a}{\partial\ln m}\right)\simeq a\left(1-\frac{\Delta a}{a}\frac{m}{\Delta m}\right).$$

Hence, we are able to evaluate the interaction (94) and kinetic (95) energies per particle via quantities that can be found experimentally.

IX. CONCLUSION

In conclusion, we remark that this paper concerns the thermodynamics of a dilute Bose gas with a strongly repulsive interaction in the leading and next-to-leading orders of the low-density expansion. The strong-coupling generalization of the Bogoliubov model proposed by the present authors is shown to reproduce the result (70) of Lee and Yang [25] found via the binary collision expansion method. Contrary to the effective-interaction approach of Ref. [4], the model considered in this paper is thermodynamically consistent and free of ultraviolet divergences. These advantages are due to accurate treatment of the short-range spatial boson correlations, whose picture is inadequate within the effective-interaction scheme. The present paper thus demonstrates that the effective-interaction scheme, which is reduced to the Bogoliubov model with an effective pairwise potential, is not acceptable for investigating a dilute strongly interacting Bose gas. In addition to the arguments mentioned above, this also follows from the results for the kinetic and interaction energies found in this paper.

In some sense the strong-coupling model discussed can be considered as a generalization of the Brueckner approach taken in its representation given by Bethe and Goldstone [29]. The new essential point is that the in-medium pair wave functions are calculated *in conjunction* with the particle momentum distribution on the basis of the variational procedure. So, to go further, additional investigations should be carried out to establish more accurate approximations of the relation connecting the boson momentum distribution with the scattering parts of the in-medium pair wave functions. In particular, this improvement is needed to clarify to what extent the correct spectrum of elementary excitations in a dilute Bose gas differs from the well-known prediction of the effective-interaction approach. Of course, the region of intermediate momenta is implied, rather than the linear phonon sector, which should be the same according to the thermodynamic prescription. This problem is closely related to investigation of long-range spatial boson correlations beyond the effective-interaction approach.

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