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Condensate fluctuations in the dilute Bose gas

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The fluctuations of a number of particles in the Bose-Einstein condensate are studied in the grand canonical ensemble with an effective single-mode Hamiltonian, which is derived from an assumption that the mode corresponding to the Bose-Einstein condensate does not asymptotically correlate with other modes. The fluctuations are evaluated in the dilute limit with a proposed simple method, which is beyond the mean-field approximation. The accuracy of the latter is estimated; it is shown that the mean-field scheme does not work for the single-mode Hamiltonian, while for the Hartree Hamiltonian it allows us to estimate the condensate fluctuations up to a numerical factor. As a hypothesis, a formula is proposed that relates the fluctuations in the canonical ensemble with that of the grand canonical one.

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I. INTRODUCTION

The observation of Bose-Einstein condensation (BEC) in trapped alkali-metal gases [1] has stimulated theoretical and experimental studies of the basic problems related to this phenomenon (see the reviews in Refs. [2–4]). In particular, the statistical properties of the condensate are of especial interest for interacting bosons. In the case of the ideal Bose gas, fluctuations of a number of particles in the Bose-Einstein condensate $\langle \delta\hat{N}_0^2\rangle \equiv \langle \hat{N}_0^2\rangle - \langle \hat{N}_0\rangle^2$ have been studied thoroughly in a box [5] and a harmonic trap [6] as well. However, in the case of the interacting gas, this problem is rather subtle and requires a more refined approach. So far there has been no uniform treatment of this problem in the literature [7–19]. It is not even clear what the value of the power γ is in dependence of the fluctuations on the total number of particles,

$$\langle \delta\hat{N}_0^2\rangle \propto N^{\gamma}, \tag{1}$$

in various Gibbs ensembles (compare, e.g., the different results of Refs. [10–12]). Apart from general theoretical interest, condensate fluctuations can be measured, in principle, by means of a scattering of series of short laser pulses [20].

In this paper we deal with the problem of fluctuations in the grand canonical ensemble and consider the global gauge symmetry U(1) of the Bose system to be broken. In principle, the properties of the dilute Bose gas in the grand ensemble are described quite well by the Bogoliubov model [21], with the condensate terms being treated as asymptotic c-numbers and with three- and four-boson terms being neglected in the Hamiltonian. However, the statistical properties of the Bose-Einstein condensate are beyond the Bogoliubov theory due to the c-number replacement. Consequently, in order to tackle this problem, we need other approximations or assumptions that keep the quantum nature of the condensate operators. Assuming that the condensate mode and other modes can be considered as quasi-independent, we obtain the usual thermodynamic fluctuations of the condensate with $\gamma=1$ in Eq. (1) and show that this result is consistent quite well with the Bogoliubov theory.

We consider a dilute Bose gas interacting with a short-range pairwise potential [i.e., the potential that goes to zero at $r\to\infty$ as $1/r^m$ ($m>3$) or faster]. The method used in our paper can be called the approximation of the quasi-independent mode. This assumption is nothing else but a generalization of Bogoliubov's relation (3) for the operators $\hat{a}_0$ and $\hat{a}_0^{\dagger}$ (see Sec. II below). As a result, we consider the condensate mode and the other ones to be uncorrelated. In the framework of this approximation, one can easily derive the effective single-mode Hamiltonian. Our consideration is primarily dedicated to the homogeneous case, except for Sec. IV B, where fluctuations in the Hartree model are discussed briefly in the nonhomogeneous case.

The paper is organized as follows. In Sec. II we review some important issues in the field of Bose-Einstein condensation, which might not be well known for a reader. In the next section we derive the effective single-mode Hamiltonian, which is employed for studying condensate fluctuations in the grand canonical ensemble. In Secs. IV A and IV B the fluctuations are evaluated in the framework of the mean-field approximation and beyond it. Possible corrections to the value of the fluctuations are discussed in Sec. IV C. In the last section the main results are summarized.

II. GENERAL REMARKS

Let us recall some important issues in the considered problem, following Bogoliubov's paper [22]. A number of bosons in the Bose-Einstein condensate can be defined as the macroscopic eigenvalue N_0 of the one-body density matrix $\langle\hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r}')\rangle$—that is, $\int d^3r'\langle\hat{\psi}^{\dagger}(\mathbf{r}')\hat{\psi}(\mathbf{r})\rangle\phi_0(\mathbf{r}')=N_0\phi_0(\mathbf{r})$, $\int d^3r|\phi_0(\mathbf{r})|^2=1$, where N_0 is proportional to the total number of bosons in the thermodynamic limit, while the other eigenvalues are proportional to the unit. The eigenfunction ϕ_0 is a one-body wave function of the Bose-Einstein condensate,

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obeying the Gross-Pitaevskii equation in the first approximation. One can easily introduce the condensate operators $\hat{a}_0$ and $\hat{a}_0^\dagger$ by expanding the Bose field operators in the complete set of eigenfunctions of the one-body matrix: $\hat{\psi}(\mathbf{r}) = \hat{a}_0\phi_0(\mathbf{r}) + \sum_{j\neq 0}\hat{a}_j\phi_j(\mathbf{r})$; then, the operator $\hat{N}_0 = \hat{a}_0^\dagger\hat{a}_0$ describes the number of particles in the condensate: $\langle\hat{N}_0\rangle = N_0$. For a homogeneous system the index j is associated with momentum $\mathbf{p}$, $\phi_{\mathbf{p}}(\mathbf{r}) = \exp(i\mathbf{p}\cdot\mathbf{r})/\sqrt{V}$ (V is the volume), and the condensate operators coincide with the Bose zero-momentum operators. Bogoliubov noticed [21,22] that in this case the operators $\hat{a}_0/\sqrt{V}$ and $\hat{a}_0^\dagger/\sqrt{V}$ should be very close to c-numbers, since they commute in the thermodynamic limit $V\to\infty$, $n=N/V=$const. This implies that

$$\lim_{V\to\infty}\left\langle\left(\frac{\hat{a}_0^\dagger}{\sqrt{V}} - \sqrt{n_0}e^{-i\varphi}\right)\left(\frac{\hat{a}_0}{\sqrt{V}} - \sqrt{n_0}e^{i\varphi}\right)\right\rangle = 0, \qquad (2)$$

where φ is an arbitrary phase and $n_0 = N_0/V$ denotes the density of the Bose-Einstein condensate. However, we always have the constraint $\langle\hat{a}_0\rangle = \langle\hat{a}_0^\dagger\rangle = 0$ due to global gauge invariance, which is equivalent to conservation of the total number of bosons (i.e., $[\hat{H},\hat{N}]=0$). Hence, the ground state is not stable with respect to an infinitesimally small perturbation that breaks the gauge symmetry. For a correct mathematical treatment of the homogeneous Bose system with broken symmetry, Bogoliubov proposed [22] to include the terms $-\nu(\hat{a}_0^\dagger e^{i\varphi} + \hat{a}_0 e^{-i\varphi})\sqrt{V}$ in the Hamiltonian, where the parameter $\nu > 0$ and $\nu\to 0$. Now the absolute minimum of the energy corresponds to the state with $\langle\hat{a}_0\rangle/\sqrt{V} = \langle\hat{a}_0^\dagger\rangle^*/\sqrt{V} = \sqrt{n_0}e^{i\varphi}$, because the gain in energy per particle, by Eq. (2), is equal to $2\nu\sqrt{n_0/n}$ in the limit $V\to\infty$ due to Bogoliubov's terms. We stress that the limit $\nu\to 0$ should be performed *after* the thermodynamic one. These two subsequent limits yield the well-defined order parameter $\langle\hat{\psi}(\mathbf{r})\rangle = \langle\hat{a}_0\rangle/\sqrt{V} = \sqrt{n_0}e^{i\varphi}$ with fixed phase φ. Thus, due to Bogoliubov's infinitesimal terms, the values of the *anomalous* averages (like $\langle\hat{\psi}\rangle$, $\langle\hat{\psi}\hat{\psi}\rangle$, and so on) change drastically, and such averages can be called, following Bogoliubov, quasiaverages (hereafter by the term "average" we mean "quasiaverage"). At the same time, the values of the *normal* averages (like $\langle\hat{\psi}^\dagger\hat{\psi}\rangle$ and so on) do not change. In particular, this is valid for the one-body $\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}')\rangle$ and two-body $\langle\hat{\psi}^\dagger(\mathrm{r}_1)\hat{\psi}^\dagger(\mathrm{r}_2)\hat{\psi}(\mathbf{r}_2')\hat{\psi}(\mathbf{r}_1')\rangle$ matrices. Hence, in the thermodynamic limit the eigenfunctions of the matrices do not change when the symmetry is broken. On the other hand, the anomalous averages have a transparent physical interpretation: $\langle\hat{\psi}(\mathbf{r})\rangle = \sqrt{N_0}\phi_0(\mathbf{r})$ is the eigenfunction of the one-body matrix associated with the maximum eigenvalue N_0, and $\langle\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}')\rangle$ is that of the two-body matrix with the eigenvalue $N_0(N_0-1)$ [23]. Hence, with the concept of broken symmetry we obtain a simple method of evaluating these eigenfunctions.

Equation (2) can be derived from Bogoliubov's principle of correlation weakening [22], which takes a particular form $\langle\hat{\psi}(\mathbf{r})\cdots\hat{\psi}^\dagger(\mathbf{r}_1)\cdots\hat{\psi}(\mathbf{r}_2)\cdots\rangle \simeq \langle\hat{\psi}(\mathbf{r})\rangle\langle\cdots\hat{\psi}^\dagger(\mathbf{r}_1)\cdots\hat{\psi}(\mathbf{r}_2)\cdots\rangle$ when $|\mathbf{r}-\mathbf{r}_1|\to\infty,\ldots$ and $|\mathbf{r}-\mathbf{r}_2|\to\infty$. Indeed, using the expression of the condensate operator in the homogeneous system, $\hat{a}_0 = \int \mathrm{d}^3r\,\hat{\psi}(\mathbf{r})/\sqrt{V}$, we obtain, in the thermodynamic limit,

$$\begin{aligned}\left\langle\frac{\hat{a}_0}{\sqrt{V}}\cdots\hat{\psi}^\dagger(\mathbf{r}_1)\cdots\hat{\psi}(\mathbf{r}_2)\cdots\right\rangle &= \frac{1}{V}\int \mathrm{d}^3r\langle\hat{\psi}(\mathbf{r})\cdots\hat{\psi}^\dagger(\mathbf{r}_1)\cdots\hat{\psi}(\mathbf{r}_2)\cdots\rangle\\ &= \frac{1}{V}\int \mathrm{d}^3r\langle\hat{\psi}(\mathbf{r})\rangle\langle\cdots\hat{\psi}^\dagger(\mathbf{r}_1)\cdots\hat{\psi}(\mathbf{r}_2)\cdots\rangle\\ &= \frac{\langle\hat{a}_0\rangle}{\sqrt{V}}\langle\cdots\hat{\psi}^\dagger(\mathbf{r}_1)\cdots\hat{\psi}(\mathbf{r}_2)\cdots\rangle. \end{aligned} \qquad (3)$$

One can indeed replace the condensate operators by the c-numbers, and this procedure, according to Bogoliubov, still yields *exact* values [22] of all thermodynamic quantities in the limit $V\to\infty$. Note that the above relations can easily be extended to the inhomogeneous case. For example, in order to consider the harmonic trap, it is sufficient to replace the volume V by $1/\overline{\omega}^3$ and define the thermodynamic limit as [24] $N\to\infty$, $N\overline{\omega}^3=$const (here $\overline{\omega} = \sqrt[3]{\omega_x\omega_y\omega_z}$ is the average harmonic frequency).

We stress once more that the replacement of $\hat{a}_0$ and $\hat{a}_0^\dagger$ by the c-numbers gives always the main asymptotics of the averages of these operators (if the Bose-Einstein condensate exists), and this method is sufficient for obtaining an exact value of any thermodynamic quantity (see Sec. 7 of Bogoliubov's paper [22]). However, the main asymptotic value is canceled when evaluating the condensate fluctuations $\langle\delta\hat{N}_0^2\rangle$, and, thus, we have to take into consideration here the quantum nature of the condensate operators. Nevertheless, Eq. (2) results in the constraint $\gamma < 2$ for the parameter γ in Eq. (1). The case $\gamma > 1$ implies that bosons in the Bose-Einstein condensate and beyond it are strongly correlated, and the extent of the correlation is nonthermodynamically large, since the thermodynamic fluctuations of any extensive observable are proportional to the total number of particles. The results $\gamma = 4/3$ and $\gamma = 1$ have been obtained in Refs. [10] and [11,12], respectively, in the Gibbs canonical ensemble. The results of Refs. [11,12] are consistent with ours for the grand canonical ensemble, while those of Ref. [10] are at variance with ours (see Sec. IV C below).

If the symmetry is broken (that is, if the ground state is a superposition of states with different numbers of particles), then it is rather difficult to define what the Gibbs canonical ensemble is. Indeed, within a variational scheme, we cannot use the restriction $N=$const directly and have to impose the additional condition $\langle\hat{N}\rangle = N$, which is equivalent to introducing the Lagrange term $-\mu\hat{N}$ in the Hamiltonian; this is nothing else but using the Gibbs grand canonical ensemble. So a reliable treatment of the canonical ensemble can be done in the framework of the number-conserving scheme (for recent developments of the scheme, see Refs. [25,26]). For that reason, in this paper we restrict ourselves to the grand ensemble.

III. APPROXIMATION OF THE QUASI-INDEPENDENT MODE

Let us describe the model and methods of calculation. In order to evaluate the mean square of the number fluctuations in the Bose-Einstein condensate, it sufficient to know the condensate density matrix $\hat{\rho}_c$. According to general rules of quantum mechanics, it can be obtained from the total density matrix $\hat{\rho}$ by taking the partial trace in the occupation number representation

$$\hat{\rho}_c = \underset{\substack{\cdots n_p \cdots \\ p\neq 0}}{\mathrm{Tr}}\, \hat{\rho} = \sum_{\substack{\cdots n_p \cdots \\ p\neq 0}} \langle \cdots n_p \cdots |\hat{\rho}| \cdots n_p \cdots \rangle, \tag{4}$$

where we denote $|\cdots n_p \cdots\rangle = \Pi_{p\neq 0}|n_p\rangle$ and the index p is associated with momentum in the homogeneous case. So $\hat{\rho}_c$ depends on the condensate operators $\hat{a}_0^\dagger$ and $\hat{a}_0$ only and acts only on states of the condensate—say, the Fock states $|N_0\rangle$ and their superpositions. By analogy with Eq. (4), one can also define the density matrix for all noncondensate states $\hat{\rho}_{\rm out} = \mathrm{Tr}_{N_0}\hat{\rho}$, which depends on the Bose operators $\hat{a}_p^\dagger$ and $\hat{a}_p$ with $p\neq 0$. Certainly, it is difficult to evaluate the density matrix of the Bose-Einstein condensate directly from Eq. (4) and one has to use additional assumptions.

As discussed in Sec. II, Eq. (3), a particular case of Bogoliubov's principle of correlation weakening is valid in the thermodynamic limit. This suggests that the state of the condensate mode is, in effect, independent of the other modes. It means that one can use the approximation for the density matrix $\hat{\rho} \simeq \hat{\rho}_c \hat{\rho}_{\rm out}$. The parameters of the matrices $\hat{\rho}_c$ and $\hat{\rho}_{\rm out}$ are assumed to be related in a self-consistent manner. The factorization of the total density matrix implies that the condensate and noncondensate subsystems are considered to be uncorrelated. Hence, we have $\langle \hat{A}\hat{B}\rangle \simeq \langle \hat{A}\rangle\langle \hat{B}\rangle$ for arbitrary $\hat{A}$ and $\hat{B}$, depending on the condensate and noncondensate operators, respectively. This is very consistent with the approximation [27]

$$\hat{A}\hat{B} \simeq \langle \hat{A}\rangle \hat{B} + \hat{A}\langle \hat{B}\rangle - \langle \hat{A}\rangle\langle \hat{B}\rangle. \tag{5}$$

Let us apply the approximation (5) for a homogeneous Bose system with the pairwise potential $V(r)$. In this case, the Hamiltonian reads, in terms of the Bose fields operators,

$$\hat{H} = \int d^3r\, \hat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m} - \mu\right)\hat{\psi}(\mathbf{r}) + \int d^3r d^3r'\, V(|\mathbf{r}-\mathbf{r}'|)\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}). \tag{6}$$

According to the above method, one should separate explicitly the condensate operators in the Hamiltonian by means of substitution $\hat{\psi}(\mathbf{r}) = \hat{a}_0/\sqrt{V} + \hat{\vartheta}(\mathbf{r})$ [here we denote $\hat{\vartheta}(\mathbf{r}) = \Sigma_{p\neq 0}\hat{a}_{\mathbf{p}} \exp(i\mathbf{p}\cdot\mathbf{r})/\sqrt{V}$] and employ the decomposition (5) to every operator containing the product of the condensate operators and $\hat{\vartheta}$ or $\hat{\vartheta}^\dagger$. As one can see, applying Eq. (5) to the Hamiltonian (6), we come to the approximation

$$\hat{H} \simeq \hat{H}_c + \hat{H}_{\rm out} + \text{const}, \tag{7}$$

and, hence, the density matrix of the grand canonical ensemble $\hat{\rho} \sim \exp(-\hat{H}/T)$ is really factorized (in this paper we include the term $-\mu\hat{N}$ in the Hamiltonian). By virtue of this factorization, the condensate fluctuations arise in the grand canonical ensemble due to the particle and temperature bath rather than the energy excitations. Here we derive the effective grand canonical Hamiltonian of the Bose-Einstein condensate:

$$\hat{H}_c = \frac{1}{2}\left(V_0\frac{\hat{a}_0^{\dagger 2}\hat{a}_0^2}{V} + A(\hat{a}_0^{\dagger 2} + \hat{a}_0^2) + 2(B-\mu)\hat{a}_0^\dagger\hat{a}_0 + 2C(\hat{a}_0^\dagger + \hat{a}_0)\sqrt{V}\right), \tag{8}$$

where V_0 is the zero component of the Fourier transform of the pairwise interaction $V(r)$, and we introduce by definition the coefficients

$$A = \int d^3r\, V(r)\langle \hat{\vartheta}(\mathbf{r})\hat{\vartheta}(0)\rangle,$$

$$B = V_0\langle \hat{\vartheta}^\dagger(0)\hat{\vartheta}(0)\rangle + \int d^3r\, V(r)\langle \hat{\vartheta}^\dagger(\mathbf{r})\hat{\vartheta}(0)\rangle,$$

$$C = \int d^3r\, V(r)\langle \hat{\vartheta}^\dagger(\mathbf{r})\hat{\vartheta}(\mathbf{r})\hat{\vartheta}(0)\rangle. \tag{9}$$

In the above expressions, the gauge symmetry is certainly assumed to be broken, and for the sake of simplicity, we put $\varphi=0$ in Bogoliubov's terms (see Sec. II); in this case, all the coefficients are real. In general, they depend on the density and temperature and will be evaluated below. It is worthwhile to note that A, B, and C tend to constant values in the thermodynamic limit. As to the Hamiltonian $\hat{H}_{\rm out}$, it is given by Eq. (6) but with c-numbers instead of the condensate operators [28], so we arrive at the standard asymptotically exact Hamiltonian with Bogoliubov's replacement. The coefficients (9) can be calculated by means of the Hamiltonian $\hat{H}_{\rm out}$.

When calculating the coefficients in the dilute limit, one can employ the results of our previous papers [23,29–31], based on an analysis of the two-body density matrix. One can show the following.

(i) The functions

$$\varphi(r) = 1 + \psi(r), \quad \varphi_{\mathbf{p}}(\mathbf{r}) = \sqrt{2}\cos(\mathbf{p}\cdot\mathbf{r}) + \psi_{\mathbf{p}}(\mathbf{r}) \quad (p\neq 0) \tag{10}$$

are eigenfunctions of the two-body density matrix, which belong to the continuous spectrum and describe the scattering of pairs of bosons in a medium of other bosons. The quantum number p can be associated with the relative momentum of that scattering [$\varphi(r)$ corresponds to zero momentum]. Their scattering parts $\psi(r)$ and $\psi_{\mathbf{p}}$, respectively, obey the boundary conditions $\psi(r)$, $\psi_{\mathbf{p}}(\mathbf{r}) \to 0$ at $r\to\infty$. The Fourier transforms of the scattering parts can be expressed in terms of the Bose operators:

$$\psi(k) = \frac{\langle \hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}\rangle}{n_0}, \quad \psi_{\mathbf{p}}(\mathbf{k}) = \sqrt{\frac{V}{2n_0}}\frac{\langle \hat{a}^{\dagger}_{2\mathbf{p}}\hat{a}_{\mathbf{p}+\mathbf{k}}\hat{a}_{\mathbf{p}-\mathbf{k}}\rangle}{n_{2p}}, \quad (11)$$

where $n_p=\langle \hat{a}^{\dagger}_{\mathbf{p}}\hat{a}_{\mathbf{p}}\rangle$ stands for the average occupation number of bosons.

(ii) The following limiting relations are valid:

$$\lim_{p\to 0}\varphi_{\mathbf{p}}(\mathbf{r}) = \sqrt{2}\varphi(r), \quad \lim_{n\to 0}\varphi(r) = \varphi^{(0)}(r), \quad (12)$$

where $\varphi^{(0)}(r)$ obeys the two-body Schrödinger equation, describing the scattering of two bosons in a vacuum with zero relative momentum. Now, using relations (11) and (12), one can obtain the coefficients (9) in the dilute limit $n\to 0$ after a small amount of algebra [32]:

$$A \simeq n_0[U^{(0)}(0) - V_0], \quad B \simeq 2(n-n_0)V_0,$$

$$C \simeq 2\sqrt{n_0}(n-n_0)[U^{(0)}(0) - V_0]. \quad (13)$$

Here $U^{(0)}(0)=\int d^3r\ \varphi^{(0)}(r)V(r)=4\pi\hbar^2 a/m$ stands for the scattering amplitude and a is the scattering length.

Now all averages of the operators $\hat{a}^{\dagger}_0$ and $\hat{a}_0$ and their products can be calculated in the grand ensemble by means of the matrix

$$\hat{\rho}_{\rm c} = \exp(-\hat{H}_{\rm c}/T)/Z_c, \quad (14)$$

with the grand partition function for the condensate

$$Z_c = \operatorname*{Tr}_{N_0}\exp(-\hat{H}_{\rm c}/T). \quad (15)$$

Note that the approximation of the quasi-independent mode was introduced earlier in Ref. [33]. The authors considered the quadratic terms only in operators $\hat{a}$ and $\hat{a}^{\dagger}$ in Eq. (8) (see the definition in Sec. IV B below) and obtained the condensate ground state, which turns out to be the coherent squeezed state in this case. However, this approach leads to additional approximations, which change drastically the final expression for the condensate fluctuations (see below). In order to avoid the additional approximations, we need to keep the four-boson Hartree term in the condensate Hamiltonian (8).

The model (8) yields the asymptotically exact value of the condensate density provided that the coefficients (9) are known. Indeed, it follows from Eq. (3) that the condensate operators can be replaced by their mean values $\langle \hat{a}_0/\sqrt{V}\rangle=\langle \hat{a}^{\dagger}_0/\sqrt{V}\rangle=\sqrt{n_0}$ in order to evaluate the main asymptotics of $\langle \hat{H}_{\rm c}\rangle$ in the thermodynamic limit. Then the condensate density can be found by minimization of $\langle \hat{H}_{\rm c}\rangle$ with respect to the c-number parameter n_0. The condition of this minimum can also be obtained from the initial Hamiltonian (6), since Bogoliubov's replacement is asymptotically exact [22] due to Eq. (3). Hence, the condensate density n_0 can be considered as a variational parameter whose value is obtained by minimization of the thermodynamic potential of the grand canonical ensemble. With the well-known expression for an infinitesimal change of the potential, $\delta\Omega=\langle \delta\hat{H}\rangle$, we have $\partial\Omega/\partial n_0=\langle \partial\hat{H}/\partial n_0\rangle=\partial\langle \hat{H}_{\rm c}\rangle/\partial n_0=0$. Here the second equality is due to the condensate operators being involved explicitly only in $\hat{H}_{\rm c}$. The last equation reads

$$\mu = V_0 n_0 + A + B + C/\sqrt{n_0}. \quad (16)$$

We come to the equation obtained by Bogoliubov and treated by him as asymptotically exact [see Eq. (7.16) of Ref. [22]], since its derivation is based only on the c-number replacement of the condensate operators. It can be rewritten as $\mu=\int d^3r'\ V(|\mathbf{r}-\mathbf{r}'|)\langle \hat{\psi}^{\dagger}(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})\rangle/\sqrt{n_0}$, where $\hat{\psi}(\mathbf{r})=\sqrt{n_0}+\hat{\vartheta}(\mathbf{r})$. This equation relates the equilibrium value of the condensate density n_0 with that of the chemical potential.

IV. CONDENSATE FLUCTUATIONS

A. Method of parameter differentiation

We adopt a standard method of evaluating the fluctuations from the Hamiltonian (8). One can derive a useful relation by differentiation of the expression for the average $\langle \hat{N}_0\rangle=\mathrm{Tr}(\hat{\rho}_{\rm c}\hat{N}_0)$ with respect to the chemical potential. If the Hamiltonian $\hat{H}_{\rm c}$ had commuted with $\hat{N}_0$, we would have $\langle \delta\hat{N}_0^2\rangle/N_0=T(\partial n_0/\partial\mu)_T/n_0$ from Eqs. (14) and (15), but the noncommutativity leads to corrections we need to estimate. One can apply the identity $\delta\exp\hat{\Gamma}=\int_0^1 dz\exp[z\hat{\Gamma}]\delta\hat{\Gamma}\exp[(1-z)\hat{\Gamma}]$ (here δ denotes variation) to the operator $\hat{\Gamma}=-\hat{H}_{\rm c}/T$ and use the first two terms of the expansion

$$e^{z\hat{\Gamma}}\hat{N}_0 e^{-z\hat{\Gamma}} = \hat{N}_0 + [\hat{\Gamma},\hat{N}_0]\frac{z}{1!} + [\hat{\Gamma},[\hat{\Gamma},\hat{N}_0]]\frac{z^2}{2!} + \cdots. \quad (17)$$

This yields

$$T\frac{\partial Z}{\partial\mu} = T\frac{\partial\,\mathrm{Tr}\,e^{\hat{\Gamma}}}{\partial\mu} = \mathrm{Tr}(e^{\hat{\Gamma}}\hat{N}_0),$$

$$T\frac{\partial\,\mathrm{Tr}(e^{\hat{\Gamma}}\hat{N}_0)}{\partial\mu} = \int_0^1 dz\,\mathrm{Tr}\Biggl(\Biggl[\hat{N}_0 + \frac{A}{T}(\hat{a}^{\dagger 2}_0 - \hat{a}_0^2) + \frac{C}{T}\sqrt{V}(\hat{a}^{\dagger}_0 - \hat{a}_0) + \cdots\Biggr]e^{\hat{\Gamma}}\hat{N}_0\Biggr).$$

In order to estimate the second term on the right-hand side (RHS) of the last equation, we note that $\mathrm{Tr}(\hat{a}^{\dagger 2}_0 e^{\hat{\Gamma}}\hat{N}_0)=[\mathrm{Tr}(\hat{a}^{\dagger 2}_0 e^{\hat{\Gamma}}\hat{N}_0)]^*=\mathrm{Tr}(\hat{N}_0 e^{\hat{\Gamma}}\hat{a}_0^2)$ owing to the reality of the coefficients in the Hamiltonian (8). Here we derive

$$\mathrm{Tr}[(\hat{a}^{\dagger 2}_0 - \hat{a}_0^2)e^{\hat{\Gamma}}\hat{N}_0] = \mathrm{Tr}(e^{\hat{\Gamma}}[\hat{a}_0^2,\hat{N}_0]) = 2\langle \hat{a}_0^2\rangle Z$$

and, in the same manner,

$$\mathrm{Tr}[(\hat{a}^{\dagger}_0 - \hat{a}_0)e^{\hat{\Gamma}}\hat{N}_0] = \langle \hat{a}_0\rangle Z.$$

Thus, we arrive at the asymptotic expression

$$\frac{\langle\delta\hat{N}_0^2\rangle}{N_0}=\frac{T}{n_0}\left(\frac{\partial n_0}{\partial\mu}\right)_T-\frac{2A}{T}-\frac{C}{T}\frac{1}{\sqrt{n_0}}+\cdots. \tag{18}$$

We stress that the chemical potential (16) is involved in implicit form in the coefficients A, B, and C, but it is clear from the above consideration that one should hold the coefficients constant when taking the derivation $\partial\mu/\partial n_0$ in Eq. (18). As a result, we obtain, from Eq. (16),

$$n_0(\partial\mu/\partial n_0)_T=V_0n_0-C/(2\sqrt{n_0}). \tag{19}$$

In the thermodynamic limit, Eq. (16) is the exact relation [22] for the chemical potential, and it can be applied [23] at any densities and for arbitrary strong pairwise potential [34]. By contrast, Eq. (18) cannot be employed in the strong-coupling regime, for which $V_0\to+\infty$, since the divergence appearing in the coefficients (13) is not canceled in this expression (18) [35]. However, one can use Eqs. (18) and (19) in the weak-coupling case, for Eq. (17) is in fact the expansion in terms of the coupling constant. Nevertheless, simple physical arguments (see Sec. V in the first paper of Ref. [29]) can help us to extend our results to the strong-coupling regime. Since the properties of dilute quantum gases are ruled by the scattering length, the final expression for condensate fluctuations should depend on the pairwise potential $V(r)$ through mediation of the scattering length in the strong-coupling case. From this expression one can derive the formula for the weak-coupling regime by means of the Born series for the scattering amplitude (length): $U^{(0)}(0)=4\pi\hbar^2a/m=U_0+U_1+\cdots$, where $U_0=V_0$ and $U_1=-(2\pi)^{-3}\int d^3k\,V_k^2/(2T_k)<0$, $T_k=\hbar^2k^2/(2m)$, and V_k is the Fourier transform of the pairwise interaction. Otherwise, the relation obtained in the weak-coupling case should involve some first terms of the Born series, but coefficients before the term $U_0=V_0$ are the same as before $U^{(0)}(0)$ in the strong-coupling case. Thus, in the "weak-coupling" formulas the substitution $V_0\to U^{(0)}(0)$ (and $U_1,U_2,\ldots\to0$) should be made to obtain the "strong-coupling" formulas. Performing this substitution in the coefficients (13) yields $A\to0$, $C\to0$, and Eqs. (18) and (19) result in a simple final answer:

$$\frac{\langle\delta\hat{N}_0^2\rangle}{N_0}=\frac{m}{4\pi^2n_0}\frac{T}{a}. \tag{20}$$

This equation is valid for sufficiently small depletion of the condensate—that is, when $T\ll T_c$. Note that the above consideration allows us to avoid [29,30] the divergence $U_1\to-\infty$ arising in the standard pseudopotential approximation $V_k=4\pi\hbar^2a/m$.

The result (20) is a direct consequence of the single-mode approximation (8). Indeed, when deriving the Hamiltonian (8), we neglect the correlations between the condensate and noncondensate particles; besides, the condensate depletion is small for the dilute Bose gas. Consequently, we can put

$$\langle\delta\hat{N}_0^2\rangle\simeq\langle\delta\hat{N}^2\rangle=T\left(\frac{\partial N}{\partial\mu}\right)_T\simeq\frac{mV}{4\pi\hbar^2}\frac{T}{a}. \tag{21}$$

Here the familiar expression is employed for the fluctuations of the total number of particles in the grand ensemble and the formula for the chemical potential, $\mu=4\pi\hbar^2an/m$, in leading order at the density, which follows from Eqs. (13) and (16). Note that this expression is nothing else but the relationship between the compressibility $\chi_T=(\partial n/\partial P)_T/n$ and the fluctuations of the total number of particles, where P stands for the pressure. Indeed, with the help of the thermodynamic relation $(\partial n/\partial P)_T=n(\partial n/\partial\mu)_T$ and the definition of the compressibility, it can be written in the form

$$\frac{\langle\delta\hat{N}_0^2\rangle}{N_0}\simeq\frac{\langle\delta\hat{N}^2\rangle}{N}=Tn\chi_T.$$

For the ideal Bose gas $a=0$, and we come to an infinitely large value of the fluctuations because of the nonphysical behavior of the compressibility of the ideal Bose gas [5,6]. Note that the fluctuations of the total number of particles in the grand canonical ensemble remain finite and approach zero as $T\to0$ when a is finite, however weak the interaction may be; this is also valid for the one- and two-dimensional Bose gases [19].

B. Mean-field calculations

It is interesting to compare the result (20) with the mean-field calculations for the condensate fluctuations. By separating the c-number part $\sqrt{z}$ in the condensate operator $\hat{a}_0=\sqrt{z}+\hat{a}$ (hence, $\langle\hat{N}_0\rangle=N_0=\langle\hat{a}^\dagger\hat{a}\rangle+z$), the fluctuation of the condensate in the grand ensemble can be represented in the form

$$\langle\delta\hat{N}_0^2\rangle=(x+1/2)^2+y^2-1/4+2z(x+1/2+y), \tag{22}$$

where the notations $x=\langle\hat{a}^\dagger\hat{a}\rangle$ and $y=\langle\hat{a}^\dagger\hat{a}^\dagger\rangle=\langle\hat{a}\hat{a}\rangle$ are introduced, and the decoupling $\langle\hat{a}^{\dagger2}\hat{a}^2\rangle=2x^2+y^2$ is employed in accordance with Wick's theorem.

Let us study the Hartree grand canonical Hamiltonian

$$\hat{H}_\mathrm{h}=\frac{V_0}{2V}\hat{a}_0^{\dagger2}\hat{a}_0^2-\mu\hat{a}_0^\dagger\hat{a}_0, \tag{23}$$

which is the model Hamiltonian (8) in the case of $A=B=C=0$. To evaluate the parameters x and y in Eq. (22), which correspond to the Hamiltonian (23), one can use the Gibbs-Bogoliubov inequality

$$\Omega\leqslant\Omega_0+\langle\hat{H}-\hat{H}_0\rangle_0. \tag{24}$$

Here $\langle\cdots\rangle_0$ means the averages in the grand Gibbs ensemble with the Hamiltonian $\hat{H}_0$, and Ω and Ω_0 are the grand thermodynamic potentials corresponding to the arbitrary Hamiltonians $\hat{H}$ and $\hat{H}_0$, respectively. Now, the basic idea is to choose $\hat{H}=\hat{H}_\mathrm{h}$ and

$$\hat{H}_0=\frac{1}{2}(A_0\hat{a}^{\dagger2}+A_0^*\hat{a}^2+2B_0\hat{a}^\dagger\hat{a}), \tag{25}$$

with arbitrary parameters A_0 and B_0, and minimize the RHS of Eq. (24) with respect to them. As a result, we find the stationary values of A_0 and B_0. Note that B_0 is always real, and we can put $A_0=A_0^*$ if all coefficients are real in the Hamiltonian $\hat{H}$. By using Bogoliubov's transformation, one can find the values x and y with the Hamiltonian (25):

$$x=\langle\hat{a}^{\dagger}\hat{a}\rangle_0=\frac{B_0}{2\varepsilon}\coth\frac{\varepsilon}{2T}-\frac{1}{2},$$

$$y=\langle\hat{a}\hat{a}\rangle_0=-\frac{A_0}{2\varepsilon}\coth\frac{\varepsilon}{2T}, \tag{26}$$

where $\varepsilon=\sqrt{B_0^2-|A_0|^2}$. We notice that at zero temperature this method is nothing else but the approximation of the coherent squeezed state (see, e.g., Ref. [36]) for the condensate mode.

It is more convenient to deal with the variables x and y rather than A_0 and B_0, since $\langle\hat{H}\rangle_0$ is easily expressed via x and y with Wick's theorem and $\mathrm{d}(\Omega_0-\langle\hat{H}_0\rangle_0)=-A_0\mathrm{d}y-B_0\,\mathrm{d}x$. Hence, we come to the minimum conditions

$$\partial\langle\hat{H}\rangle_0/\partial y=A_0,\quad \partial\langle\hat{H}\rangle_0/\partial x=B_0, \tag{27}$$

which should be solved in conjunction with

$$\partial\langle\hat{H}\rangle_0/\partial z=0. \tag{28}$$

For the Hartree Hamiltonian we have $\langle\hat{H}_{\mathrm{h}}\rangle_0=(V_0/2V)(2x^2+y^2+4xz+2zy+z^2)-\mu(z+x)$, and Eqs. (27) and (28) yield

$$x=\frac{1-y/z}{4\sqrt{-y/z}}\coth\frac{\mu\sqrt{-y/z}}{T}-\frac{1}{2},$$

$$y=-\frac{1+y/z}{4\sqrt{-y/z}}\coth\frac{\mu\sqrt{-y/z}}{T}, \tag{29}$$

where the asymptotic formula $V_0z/V\simeq\mu$ is utilized. The limits $x/z\to 0$ and $y/z\to 0$ at $V\to\infty$ follow from Eq. (2), since $z/V\simeq n_0$. If these limits were not fulfilled, the separation of the condensate operator into quantum and c-number parts would have made no sense. At zero temperature Eqs. (29) lead to $x\simeq -y\simeq z^{1/3}/2^{4/3}$ and $x+1/2+y\simeq 2^{-5/3}z^{-1/3}$, and Eq. (22) yields

$$\frac{\langle\delta\hat{N}_0^2\rangle}{N_0}\simeq\frac{3}{2^{5/3}}\frac{1}{N_0^{1/3}}. \tag{30}$$

This result was obtained for the Hartree model by another method in Refs. [4,8]. We note that the asymptotics (30) is in agreement with Eq. (20) at $T=0$, which reproduces only the exact limit $\langle\delta\hat{N}_0^2\rangle/N_0=0$ for $N_0\to\infty$. At nonzero temperature we obtain in the same manner $x\simeq -y\simeq\sqrt{T/\mu}\sqrt{z}/2$ and $x+1/2+y\simeq T/(2\mu)$, and, hence,

$$\frac{\langle\delta\hat{N}_0^2\rangle}{N_0}\simeq\frac{3}{2}\frac{T}{\mu}. \tag{31}$$

The replacement $V_0\to 4\pi\hbar^2a/m$, discussed in Sec. IV A, results in Eq. (20) but with the factor 3/2. Certainly, the previous relation (20) is valid, as based on the more general considerations than the mean-field expression (31). Note that the method of the previous section, applied to the Hartree Hamiltonian (23), also leads to the same correct result (20).

The mean-field scheme works even worse in the case of the Hamiltonian (8), for the subtle balance of the terms is broken in Eqs. (22), (27), and (28). As a result, the term $V_0=U_0$ vanishes in the limit $V\to\infty$, and the main contribution comes in the condensate fluctuations from the term U_1. Note that the approximations used in Ref. [33] lead to the same effect. Thus, the mean-field scheme, applied to the model Hamiltonian (8), is not consistent for calculating the fluctuations, because it does not reproduce the correct answer (20). Nevertheless, for a qualitative estimation of the condensate fluctuations, it is quite right to make use of the mean-field scheme, which reproduces the correct answer up to a factor of 3/2. Note that the Hartree Hamiltonian can be easily written down for the nonhomogeneous system (see Sec. 2.8 in Ref. [4]); the coefficients depend on the condensate wave function (the eigenfunction of the one-body density matrix), which is the solution of the Gross-Pitaevskii equation. So it is possible to estimate qualitatively the condensate fluctuations for the trapped system by means of Eqs. (30) and (31).

C. Next-to-leading order corrections for the fluctuations

In this paper we study the condensate fluctuations within the single-mode Hamiltonian (8). As is stressed in Sec. III it means that we neglect the correlations between the numbers of the particles in the condensate and beyond it; that is, we put $[\langle\hat{N}_0\hat{N}_{\mathrm{out}}\rangle-\langle\hat{N}_0\rangle\langle\hat{N}_{\mathrm{out}}\rangle]/V\simeq 0$ in the thermodynamic limit, where by definition $\hat{N}_{\mathrm{out}}=\hat{N}-\hat{N}_0=\Sigma_{p\neq 0}\hat{a}_{\mathbf{p}}^{\dagger}\hat{a}_{\mathbf{p}}$ is the operator of particles beyond the Bose-Einstein condensate. In Ref. [10] an opposite idea was accepted that $\langle\delta\hat{N}_0^2\rangle=\langle\delta\hat{N}_{\mathrm{out}}^2\rangle$ due to the restriction $N=$const in the canonical ensemble, but at the same time, Bogoliubov's scheme, which does not conserve the number of particles, was used there. This approach leads to nonthermodynamical fluctuations with $\gamma=4/3$ in Eq. (1). As discussed in Sec. II, the replacement of the condensate operators by the c-numbers implies that Bogoliubov's terms are involved in the Hamiltonian. Such a procedure leads to $[\hat{H},\hat{N}]\neq 0$ and can change the accepted relation $\langle\delta\hat{N}_0^2\rangle=\langle\delta\hat{N}_{\mathrm{out}}^2\rangle$. On the other hand, within the *conserving* scheme (when $[\hat{H},\hat{N}]=0$) the Bogoliubov transformation $\hat{b}_{\mathbf{p}}=u_p\hat{\alpha}_{\mathbf{p}}+v_p\hat{\alpha}_{-\mathbf{p}}^{\dagger}$ relates the creation $\hat{\alpha}_{\mathbf{p}}^{\dagger}$ and destruction $\hat{\alpha}_{\mathbf{p}}$ quasiparticle operators with not the particle operator $\hat{a}_{\mathbf{p}}$ but with $\hat{b}_{\mathbf{p}}=\hat{a}_{\mathbf{p}}\hat{a}_0^{\dagger}/\sqrt{N_0}$ [25,26,37]. Hence, the variance of the operator $\Sigma_{p\neq 0}\hat{b}_{\mathbf{p}}^{\dagger}\hat{b}_{\mathbf{p}}$ is no longer equal to the variance of the number of noncondensate bosons $\langle\delta\hat{N}_{\mathrm{out}}^2\rangle$. For this reason, the approach [10] is implicitly based on the assumption that $[\langle\hat{N}_0^2\hat{N}_{\mathrm{out}}^2\rangle-\langle\hat{N}_0\hat{N}_{\mathrm{out}}\rangle^2]/N_0^2\simeq\langle\hat{N}_{\mathrm{out}}^2\rangle-\langle\hat{N}_{\mathrm{out}}\rangle^2$ in leading order. A justification of this assumption is needed, since it may occur that the main contribution to the LHS comes from the term $\langle\hat{N}_{\mathrm{out}}^2(\hat{N}_0^2-N_0^2)\rangle/N_0^2$, which may be proportional to $V^{4/3}$. The question remains open what approximation is more correct, the approximation of the quasi-independent mode or the nonconserving approximation in conjunction with $\langle\delta\hat{N}_0^2\rangle=\langle\delta\hat{N}_{\mathrm{out}}^2\rangle$. Note that our result (20) does not contradict to that of the papers [11,12], in which the fluctuations were investigated in the canonical ensemble within the number-conserving simple scheme. We stress that the Bogoliubov model, based on the c-number replacement, is consistent with any value of $\gamma<2$, so all the approaches [10] and [11,12] and ours do not contradict to the Bogoliubov's c-number replacement. Thus, we are able to use the single-mode Hamiltonian (8) until a decisive answer has been given what is the value of the correlator $[\langle\hat{N}_0\hat{N}_{\mathrm{out}}\rangle-\langle\hat{N}_0\rangle\langle\hat{N}_{\mathrm{out}}\rangle]/V$ within the number-conserving scheme [38].

Let us formulate the hypothesis for the interacting Bose gas that in the framework of *the number-conserving scheme* the relation $\langle\hat{N}_0\hat{N}_{\mathrm{out}}\rangle/V\simeq\langle\hat{N}_0\hat{N}_{\mathrm{out}}\rangle_c/V$ should be fulfilled; here, $\langle\cdots\rangle$ and $\langle\cdots\rangle_c$ stand for the averages in the grand canonical and canonical ensembles, respectively. This hypothesis is reasonable, since transitions of bosons from the condensate state to the noncondensate ones and back occur in the whole volume, and thus the boundary conditions seem to be of no importance here. In addition, we have the relations $\langle\hat{N}_0\hat{N}\rangle_c=N_0N$ and $\langle\hat{N}_0\hat{N}\rangle-N_0N=T(\partial N_0/\partial\mu)_T$; the latter can be derived by differentiating $\langle\hat{N}_0\rangle$ with respect to the chemical potential (within the number-conserving scheme we do not face the difficulties discussed in Sec. IV A). Thus, from the accepted hypothesis we obtain

$$\frac{\langle\delta\hat{N}_0^2\rangle}{N_0}=\frac{T}{n_0}\left(\frac{\partial n_0}{\partial\mu}\right)_T+\frac{\langle\delta\hat{N}_0^2\rangle_c}{N_0}. \tag{32}$$

Here the derivative $(\partial\mu/\partial n_0)_T$ is not related to the formula (19), which concerns the single-mode Hamiltonian (8), because the averages in Eq. (32) correspond to the full Hamiltonian with the pairwise potential; one should calculate it from the thermodynamic expression for the chemical potential. In particular, in the temperature region $n_0U^{(0)}(0)\ll T\ll T_{\mathrm{c}}$ [here T_{c} is the transition temperature of the ideal Bose gas and $U^{(0)}(0)=4\pi\hbar^2a/m$] we have

$$n_0\left(\frac{\partial\mu}{\partial n_0}\right)_T\simeq n_0U^{(0)}(0)\left[1-6\sqrt{\pi}\frac{(n_0a^3)^{1/2}T}{n_0U^{(0)}(0)}\right],$$

where $(n_0a^3)^{1/2}T/[n_0U^{(0)}(0)]\ll 1$ (see, e.g., Ref. [39]). On the other hand, the number-conserving approach of Ref. [11] yields

$$\frac{\langle\delta\hat{N}_0^2\rangle_c}{N_0}\simeq 2\sqrt{2}\sqrt{\pi}(n_0a^3)^{1/2}\left(\frac{T}{n_0U^{(0)}(0)}\right)^2$$

in that temperature region [40]. Thus, with the proposed equation (32) we obtain the relation

$$\frac{\langle\delta\hat{N}_0^2\rangle}{N_0}\simeq\frac{T}{n_0U^{(0)}(0)}\left[1+(6+2\sqrt{2})\sqrt{\pi}\frac{(n_0a^3)^{1/2}T}{n_0U^{(0)}(0)}\right], \tag{33}$$

which contains the correction term in comparison with Eq. (20).

V. SUMMARY

Starting from the approximation of the quasi-independent mode, we derive the single-mode Hamiltonian (8) and obtain the condensate fluctuations (20) for the grand canonical ensemble in the dilute limit. This relation is derived beyond the mean-field approximation. The mean-field scheme, applied to the Hamiltonian (8), leads to incorrect results. For the Hartree Hamiltonian (23), the mean-field approximation results in Eq. (31) at nonzero temperature, which differs from the correct relation (20) by a factor of 3/2. With the help of the proposed hypothesis and the estimations of Ref. [11], the next-to-leading term is obtained for the condensate fluctuations (33).

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