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RESEARCH ARTICLE

On the ground state energy of the inhomogeneous Bose gas

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Within the self-consistent Hartree–Fock approximation, an explicit in this approximation expression for the ground state energy of inhomogeneous Bose gas is derived as a functional of the inhomogeneous density of the Bose–Einstein condensate. The results obtained are based on existence of the off-diagonal long-range order in the single-particle density matrix for systems with a Bose–Einstein condensate. This makes it possible to avoid the use of anomalous averages. The explicit form of the kinetic energy, which differs from one in the Gross–Pitaevski approach, is found. The obtained form of kinetic energy is valid beyond the Hartree–Fock approximation and can be applied for arbitrary strong interparticle interaction.

Keywords Bose condensation, elementary excitations, single-particle Green function, density-density Green function, thermodynamic energy

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Experimental observation of the Bose–Einstein condensate (BEC) in ultracold gases of alkali metals [1] is a strong motivation for theoretical studies of weakly nonideal Bose systems. Due to the presence of magnetic moment the alkali metal atoms can be confined in magnetic traps. Ultralow temperatures requiring to form the BEC are achieved by use laser cooling which leads to evaporation of atoms with high energy from a magnetic trap (see Ref. [2] for more details). The ultracold gas obtained in such a way is rarefied and is characterized by strong inhomogeneity [3]. For these reasons, the Gross–Pitaevskii equation [4, 5] corresponding to the "mean" field approximation and allowing the consideration of the effect of laser radiation [6] is widely used to describe the ultracold gas. Wherein, validity of the Gross–Pitaevskii equation is shown for the inhomogeneous system, containing a finite number of particles N in an infinite volume V [7]. The consideration of such system does not correspond to the thermodynamic limit transition ($N \to \infty$, $V \to \infty$, $N/V = const$). At the same time the derivation of the Gross–Pitaevskii equation for an inhomogeneous system in thermodynamic limit is based on the hypothesis of the "anomalous averages" existence (see Ref. [8]). As shown in Refs. [9–15] the description of homogeneous systems with BEC using of anomalous averages is dubious.

An alternative approach proposed in the present paper is based on applying the conventional diagram technique of the perturbation theory to an equilibrium system in a large but finite volume [16] and on existence of the off-diagonal long-range order (ODLRO) in the one-particle density matrix. Such approach allows the self-consistent consideration of BEC by transferring to the thermodynamic limit [17] (see Ref. [18] for more details). On this basis we establish in the present paper two new results: (i) the explicit expression for kinetic part of the ground state energy of Bose system with BEC in an external field, which is valid for arbitrary strong interaction between particles, (ii) the ground state energy of the system under consideration in the Hartree–Fock approximation, which differs from one in the theory, based on anomalous averages.

We use ODLRO to describe an inhomogeneous system of bosons with zero spin and mass m, which is in a static external field defined by the scalar potential $\varphi^{(ext)}(\boldsymbol{r})$. The Hamiltonian of such a system in the volume V is written as

$$\hat{H} = -\frac{\hbar^2}{2m}\int_V \mathrm{d}^3r\,\hat{\psi}^+(\boldsymbol{r})\Delta_{\boldsymbol{r}}\hat{\psi}(\boldsymbol{r}) + \frac{1}{2}\int_V \mathrm{d}^3r_1\int_V \mathrm{d}^3r_2\, v(\boldsymbol{r}_1-\boldsymbol{r}_2)\hat{\psi}^+(\boldsymbol{r}_1)\hat{\psi}^+(\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_1) + \int_V \mathrm{d}^3r\,\varphi^{(ext)}(\boldsymbol{r})\hat{\psi}^+(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}), \quad (1)$$

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where $\hat{\psi}^{+}(\boldsymbol{r})$ and $\hat{\psi}(\boldsymbol{r})$ are, respectively, the field operators of creation and annihilation satisfying the bosonic commutation relations, and $v(r)$ is the pair interaction potential of particles. To determine the average energy $E_V = \langle \hat{H} \rangle_V$ of a rarefied weakly nonideal gas in the macroscopic volume V, we can use the self-consistent Hartree–Fock approximation (see Ref. [19] for more details)

$$E_V = \int_V \mathrm{d}^3 r_1 \int_V \mathrm{d}^3 r_2 \left\{ \left[-\frac{\hbar^2}{2m} \Delta_{\boldsymbol{r}_2} \gamma_V(\boldsymbol{r}_1, \boldsymbol{r}_2) \right] \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) + \frac{1}{2} v(\boldsymbol{r}_1 - \boldsymbol{r}_2) n_V(\boldsymbol{r}_1) n_V(\boldsymbol{r}_2) + \frac{1}{2} v(\boldsymbol{r}_1 - \boldsymbol{r}_2) \gamma_V(\boldsymbol{r}_1, \boldsymbol{r}_2) \gamma_V(\boldsymbol{r}_2, \boldsymbol{r}_1) \right\} + \int_V \mathrm{d}^3 r \varphi^{(ext)}(\boldsymbol{r}) n_V(\boldsymbol{r}). \tag{2}$$

Here $\gamma_V(\boldsymbol{r}_1, \boldsymbol{r}_2) \equiv \langle \hat{\psi}^{+}(\boldsymbol{r}_1) \hat{\psi}(\boldsymbol{r}_2) \rangle_V$ is the single-particle density matrix, $n_V(\boldsymbol{r}) \equiv \langle \hat{\psi}^{+}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) \rangle_V$ is the inhomogeneous density of the system under consideration in the macroscopic volume V, and angle brackets mean averaging with the grand canonical Gibbs ensemble. As is known [20], the average values of physical quantities correspond to the state of thermodynamic equilibrium if the transition to the thermodynamic limit $V \to \infty$, $\langle \hat{N} \rangle_V \to \infty$, $\overline{n} = \lim_{V\to\infty} \langle \hat{N} \rangle_V / V = const$ is performed. Here $\langle \hat{N} \rangle_V = \int_V \mathrm{d}^3 r n_V(\boldsymbol{r})$ is the average total number of particles in the macroscopic volume V, and $\overline{n}$ is the average density of the number of particles in the thermodynamic limit [20]. For transition to the thermodynamic limit in the calculation of the average energy $E = \lim_{V\to\infty} E_V$, we represent the functions $\gamma_V(\boldsymbol{r}_1, \boldsymbol{r}_2)$ and $n_V(\boldsymbol{r})$ in the form of the Fourier series

$$\gamma_V(\boldsymbol{r}_1, \boldsymbol{r}_2) = \gamma_V\left(\boldsymbol{R} - \frac{\boldsymbol{r}}{2}, \boldsymbol{R} + \frac{\boldsymbol{r}}{2}\right) = \frac{1}{V} \sum_{\boldsymbol{p}} f_V(\boldsymbol{p}, \boldsymbol{R}) \exp(\mathrm{i}\boldsymbol{p}\boldsymbol{r}), \tag{3}$$

$$n_V(\boldsymbol{r}) = \gamma_V(\boldsymbol{r}, \boldsymbol{r}) = \frac{1}{V} \sum_{\boldsymbol{p}} f_V(\boldsymbol{p}, \boldsymbol{r}), \tag{4}$$

where $f_V(\boldsymbol{p}, \boldsymbol{R})$ is the inhomogeneous single-particle distribution function over momenta $\hbar \boldsymbol{p}$, $\boldsymbol{R} = (\boldsymbol{r}_2 + \boldsymbol{r}_1)/2$, $\boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1$. We note that, according to Eq. (3), the function $f_V(\boldsymbol{p}, \boldsymbol{R})$ completely defines the average kinetic energy $\langle \hat{K} \rangle_V$ of inhomogeneous system in the macroscopic volume V [21]

$$\langle \hat{K}_V \rangle = \int_V \mathrm{d}^3 r_1 \int_V \mathrm{d}^3 r_2 \left[-\frac{\hbar^2}{2m} \Delta_{\boldsymbol{r}_2} \gamma_V(\boldsymbol{r}_1, \boldsymbol{r}_2) \right] \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) = \frac{\hbar^2}{2mV} \int \mathrm{d}^3 R \sum_{\boldsymbol{p}} \left(p^2 - \mathrm{i}\boldsymbol{p}\nabla_{\boldsymbol{R}} - \frac{1}{4} \Delta_{\boldsymbol{R}} \right) f_V(\boldsymbol{p}, \boldsymbol{R}). \tag{5}$$

We further take into account that in the region of ultralow temperatures in rarefied boson gas the BEC appears. The presence of the BEC manifests itself as the ODLRO for the function $\gamma_V(\boldsymbol{r}_1, \boldsymbol{r}_2)$ [22–24]. The existence of the ODLRO for the considering inhomogeneous system is defined as

$$\lim_{|\boldsymbol{r}|\to\infty} \gamma_V\left(\boldsymbol{R} - \frac{\boldsymbol{r}}{2}, \boldsymbol{R} + \frac{\boldsymbol{r}}{2}\right) = n^{BEC}(\boldsymbol{R}) \neq 0. \tag{6}$$

Here $n^{BEC}(\boldsymbol{R})$ is inhomogeneous local density of the number of particles in the BEC [25]. Therefore, according to Eqs. (3) and (6) the function $f_V(\boldsymbol{p} = 0, \boldsymbol{R}) = n^{BEC}(\boldsymbol{R}) V$ is a macroscopic quantity, which defines the existence of the BEC.

As a result, after transition to the thermodynamic limit in Eqs. (3) and (4), we find

$$\gamma\left(\boldsymbol{R} - \frac{\boldsymbol{r}}{2}, \boldsymbol{R} + \frac{\boldsymbol{r}}{2}\right) = \lim_{V\to\infty} \gamma_V\left(\boldsymbol{R} - \frac{\boldsymbol{r}}{2}, \boldsymbol{R} + \frac{\boldsymbol{r}}{2}\right) = n^{BEC}(\boldsymbol{R}) + \gamma^{(over)}(\boldsymbol{r}, \boldsymbol{R}), \tag{7}$$

$$n(\boldsymbol{r}) = n^{BEC}(\boldsymbol{r}) + n^{(over)}(\boldsymbol{r}), \tag{8}$$

$$\gamma^{(over)}(\boldsymbol{r}, \boldsymbol{R}) = \lim_{V\to\infty} \frac{1}{V} \sum_{\boldsymbol{p}\neq 0} f_V(\boldsymbol{p}, \boldsymbol{R}) \exp(\mathrm{i}\boldsymbol{p}\boldsymbol{r}) = \int \mathrm{d}^3 p/(2\pi)^3 f^{(over)}(\boldsymbol{p}, \boldsymbol{R}) \exp(\mathrm{i}\boldsymbol{p}\boldsymbol{r}), \tag{9}$$

$$n^{(over)}(\boldsymbol{r}) = \lim_{V\to\infty} \frac{1}{V} \sum_{\boldsymbol{p}\neq 0} f_V(\boldsymbol{p}, \boldsymbol{r}) = \int \mathrm{d}^3 p/(2\pi)^3 f^{(over)}(\boldsymbol{p}, \boldsymbol{r}). \tag{10}$$

Here $\gamma^{(over)}(\boldsymbol{r}, \boldsymbol{R})$ and $n^{(over)}(\boldsymbol{r})$ are, respectively, the single-particle density matrix and the inhomogeneous density for "overcondensate" particles. The function $f^{(over)}(\boldsymbol{p}, \boldsymbol{r})$ is the distribution over momenta $\hbar \boldsymbol{p}$ under the condition $\boldsymbol{p} \neq 0$.

According to Eq. (8), the average density of the number of particles is $\overline{n} = \overline{n}^{BEC} + \overline{n}^{(over)}$. For ultracold inhomogeneous gases which can be considered as weakly nonideal ones, almost all gas particles at temperature tends to zero ($T \to 0$) are in the BEC: $\overline{n}^{BEC} \simeq \overline{n}$ [7, 26]. Such an approximation was used, in particular, in deriving the Gross–Pitaevskii equation [4, 5]. In the problem under consideration this means that for $T \to 0$ the "overcondensate" functions $f^{(over)}(\boldsymbol{p}, \boldsymbol{R})$, $n^{(over)}(\boldsymbol{R})$ equal zero and

$$\lim_{T\to 0} \gamma(\boldsymbol{r}, \boldsymbol{R}) = n^{BEC}(\boldsymbol{r}); \qquad \lim_{T\to 0} n(\boldsymbol{r}) = n^{BEC}(\boldsymbol{r}). \tag{11}$$

Therefore, for $T \to 0$ only the condensate with $\boldsymbol{p} = 0$ in Eq. (5) is essential. As a result, only the last term in Eq. (11) contributes to kinetic energy in the considering case. Moreover, for $\boldsymbol{p} = 0$, using Eqs. (4), (8) and

(10) we arrive at equality $f_V(0,\boldsymbol{R}) = Vn^{BEC}(\boldsymbol{R})$. Using Eq. (5), (11) and transferring to the thermodynamic limit in (2), we find the ground state energy as functional of the inhomogeneous BEC density

$$E_0[n^{BEC}] = \lim_{T\to 0}\lim_{V\to\infty} E_V = -\frac{\hbar^2}{8m}\int \mathrm{d}^3R\Delta_{\boldsymbol{R}} n^{BEC}(\boldsymbol{R}) + \int \mathrm{d}^3r\varphi^{(ext)}(\boldsymbol{r})n^{BEC}(\boldsymbol{r})$$
$$+\frac{1}{2}\int \mathrm{d}^3R\int \mathrm{d}^3rv(r)\left[n^{BEC}\left(\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\right)n^{BEC}\left(\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\right)+n^{BEC}(\boldsymbol{R})n^{BEC}(\boldsymbol{R})\right]. \tag{12}$$

The result obtained is based only on use of the ODLRO concept (4) for the single-particle density matrix within the self-consistent Hartree–Fock approximation. The hypotheses of the existence of anomalous averages in the considering method is not necessary.

Let us pay attention that, according to Eqs. (1), (5) and (11), the first two terms on the right-hand side of relation (12), corresponding to the average kinetic energy and the energy in the external field potential, respectively, are exact for the considering limit $T \to 0$, i.e., the form of these terms is also valid beyond the self-consistent Hartree–Fock approximation.

Since the inhomogeneous density $n^{BEC}(\boldsymbol{r})$ is the non-negative value we can represent it as $n^{BEC}(\boldsymbol{r}) = |\Phi(\boldsymbol{r})|^2$, where $\Phi(\boldsymbol{r})$ is so-called the wave function of BEC [8]. It is easily seen, that relation (12) for the energy of ground state of weakly nonideal Bose gas does not correspond to one from the equation of Gross–Pitaevskii [4, 5]. The difference is drastically essential for the first term in the right part (12), which is the explicit form for the kinetic energy of an nonhomogeneous BEC [see Eq. (5)]. The cause of this difference is conditioned by the applicability of the Gross–Pitaevskii equation only to the case of the finite number of bosons in infinite volume [7]. This system does not correspond to the description in thermodynamic limit which is considered in this paper.

According to the Gauss' theorem,

$$\int \mathrm{d}^3R\Delta_{\boldsymbol{R}} n^{BEC}(\boldsymbol{R}) = \oint \mathrm{d}\boldsymbol{S}\nabla_{\boldsymbol{R}} n^{BEC}(\boldsymbol{R}). \tag{13}$$

Therefore, if we neglect the surface integral over the infinitely-distant surface on the right-hand side of relation (13) the kinetic part of the ground state energy [the first term in Eq. (12)] for degenerate Bose gas equals zero: $\lim_{T\to 0}\lim_{V\to\infty}\langle \hat{K}\rangle_V = 0$. This result corresponds to thermodynamic limit for arbitrary interparticle interaction potential. The physical sense of this result is clear: in inhomogeneous system of bosons BEC particles cannot contribute to the kinetic energy, as well as in homogeneous one. Formal application of the Gross–Pitaevskii equation for determination of inhomogeneous thermodynamics [8] leads to non-zero contribution to the kinetic energy and is invalid.

According to Eq. (13), the ground state energy (12) for the inhomogeneous rarefied Bose gas in the self-consistent Hartree–Fock approximation is given by the relation

$$E_0[n^{BEC}] = \int \mathrm{d}^3r\varphi^{(ext)}(\boldsymbol{r})n^{BEC}(\boldsymbol{r})$$
$$+\frac{1}{2}\int \mathrm{d}^3R\int \mathrm{d}^3rv(r)\left[n^{BEC}\left(\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\right)n^{BEC}\left(\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\right)+n^{BEC}(\boldsymbol{R})n^{BEC}(\boldsymbol{R})\right]. \tag{14}$$

Then, without loss of generality, we can apply the density functional theory [27] widely used in describing inhomogeneous electron systems (see Ref. [28] for more details) to the system under consideration. According to Eq. (14), the universal functional of the inhomogeneous BEC density $F[n^{BEC}]$ in the self-consistent Hartree–Fock approximation is written as

$$F[n^{BEC}] = \frac{1}{2}\int \mathrm{d}^3R\int \mathrm{d}^3rv(r)\left[n^{BEC}\left(\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\right)n^{BEC}\left(\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\right)+n^{BEC}(\boldsymbol{R})n^{BEC}(\boldsymbol{R})\right]. \tag{15}$$

Then, within the Lagrange multiplier method taking into account the normalization condition $\int \mathrm{d}^3r(\boldsymbol{r})n^{BEC}(\boldsymbol{r}) = \langle \hat{N}\rangle$, we find the equation for determining the function $n^{BEC}(\boldsymbol{r})$

$$\delta F[n^{BEC}]/\delta n^{BEC}(\boldsymbol{r}) + \varphi^{(ext)}(\boldsymbol{r}) = \mu, \tag{16}$$

where μ is the chemical potential of the system under consideration. Substituting Eq. (15) into Eq. (16), we find the integral equation

$$\int \mathrm{d}^3 r_1 v(|\boldsymbol{r}-\boldsymbol{r}_1|) n^{BEC}(\boldsymbol{r}_1) + v_0 n^{BEC}(\boldsymbol{r}) + \varphi^{(ext)}(\boldsymbol{r}) = \mu, \tag{17}$$

where $v_0 = \int \mathrm{d}^3 r v(\boldsymbol{r})$. The solution of Eq. (17) has a form $n^{BEC}(\boldsymbol{r}) = n^{BEC}(\boldsymbol{r}, \mu, [\varphi^{(ext)}(\boldsymbol{r})])$ in agreement with the Grand canonical ensemble requirements.

We note, that relation (17) as applied to the homogeneous degenerate Bose gas leads to the result $\mu = 2\overline{n}v_0$ [11–13], in contrast with theory based on anomalous averages (see, e.g., Refs. [8, 29]).

As easy to show the relation for pressure of the homogeneous degenerate Bose gas P in Hartree–Fock approximation and in the mean-field approximation in anomalous average approach can be written in universal form

$$P^{(hom)}(\mu) = -\left(\frac{\partial E_0}{\partial V}\right)^{(hom)}_{\langle \hat{N} \rangle} = \frac{\mu \overline{n}(\mu)}{2}, \tag{18}$$

in spite the concrete relation for chemical potentials, energy and pressure as functions of the interaction potential and density are different.

The integral equation (17) can be simplified for slowly variable (in comparison with the characteristic length of the interaction potential) external field $\varphi^{(ext)}(\boldsymbol{r})$. In this case

$$\begin{aligned} &\int \mathrm{d}^3 r_1 v(|\boldsymbol{r} - \boldsymbol{r}_1|) n^{BEC}(\boldsymbol{r}_1) \\ &\quad = \int \mathrm{d}^3 R v(|\boldsymbol{R}|) n^{BEC}(\boldsymbol{r} + \boldsymbol{R}) \\ &\quad \simeq v_0 n^{BEC}(\boldsymbol{r}) + v_2 \Delta_{\boldsymbol{r}} n^{BEC}(\boldsymbol{r}), \end{aligned} \tag{19}$$

where

$$v_2 = \frac{1}{3} \int \mathrm{d}^3 R R^2 v(R). \tag{20}$$

Therefore, in the weakly inhomogeneous case the approximate solution of Eq. (17) can be found from the differential equation

$$v_2 \Delta_{\boldsymbol{r}} n^{BEC}(\boldsymbol{r}) + 2 v_0 n^{BEC}(\boldsymbol{r}) + \varphi^{(ext)}(\boldsymbol{r}) = \mu, \tag{21}$$

The presented results are valid for the system with short-range interaction potential between particles, when the values v_0 and v_2 (20) are finite. For the system of charged particles with Coulomb long-range interaction a special consideration is needed (see Ref. [30] and references therein).

Thus, the ground state energy of inhomogeneous BEC in thermodynamic limit is alternative to one following from Gross–Pitaevskii equation. This difference is conditioned by the application of anomalous averages for obtaining of GP equation. In the present consideration, based on ODLRO, the method of anomalous averages is avoided. The final choice between these alternative ways should be established on the basis of further theoretical investigations and comparison with the experimental measurements.

Wherein, it is necessary to take into account that the experiments for the degenerated Bose gas are performed in confining trap (see Ref. [31] and references therein). For this reason there are certain difficulties in the experimental data interpretation. Currently, the local density approximation (see Ref. [32] and references therein) is widely used. However, applicability of this approximation is limited by the smallness condition of the so called gradient corrections [an example is the first term in the left side (21)].

Besides, for the proper interpretation of experimental data the relation between the local pressure $P(\boldsymbol{r})$ and local density $n(\boldsymbol{r})$ should be correctly establish. For this purpose, the quasi-classic approximation for ideal gas is often used (fore more details see Ref. [32]). However, the applicability of this approximation is restricted, *strictly speaking*, the case of inhomogeneous ideal classical gas (see, e.g., Ref. [33]). This approximation cannot be used for description of the inhomogeneous degenerate Bose gas, since for such a system kinetic energy of BEC equals zero and it contribution to pressure is absent at $T = 0$.

Even for homogeneous gas with BEC, the relation (18) is invalid if quantum relation between pressure and density as well as interparticle interaction are not taken into account [8, 20, 29]. Consideration of the local pressure $P(\boldsymbol{r})$ dependence on local density $n(\boldsymbol{r})$ of nonideal Bose gas with BEC will be presented in detail in a separate publication.

We should also underline that chemical potential cannot be measured straightforward. This means that determination of chemical potential requires various approximated relations as, e.g., a formal generalization of Eq. (18) for inhomogeneous case by use the local density approximation

$$P(\boldsymbol{r}) = \frac{\mu n(\boldsymbol{r})}{2}, \tag{22}$$

However, the validity of the equality $\mu = 2\overline{n}v_0$ for chemical potential for the homogeneous case cannot be established on this basis, since the value of v_0 is unknown.

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