Bose–Einstein condensate and excited single-particle states

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Abstract. On the basis of the second quantization formalism in the framework of the self-consistent Hartree–Fock approximation, it is shown that to describe the Bose–Einstein condensate in an inhomogeneous weakly nonideal gas of bosons, it is necessary to take into account excited single-particle states. It has been established that the description of the corresponding excited states essentially depends on the degree of inhomogeneity of the boson system. If all gas particles are in a Bose–Einstein condensate, then the resulting equations correspond to the stationary Gross–Pitaevskii equation.
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1. INTRODUCTION

Experiments on the observation of the Bose–Einstein condensate (BEC) in ultracold rarefied gases of alkali metals [1–3] have stimulated a great theoretical and experimental interest in this phenomenon [4–7]. Ultracold gases provide a unique opportunity to study various quantum effects at the macroscopic level.

For this purpose, the non-stationary Gross–Pitaevsky (GP) equation [8, 9] considering an external field [10], is widely used.

However, when using the GP equation, the following circumstances must be taken into account. On the one hand, the derivation of the GP equation is based on the use of the hypothesis of the existence of "quasi-averages" and the representation of the creation and annihilation operators with zero momentum as c-numbers (see [11, 12] for more details).

Although the stationary GP equation is very successfully used to describe vortex structures in the BEC, where an external field is absent [8, 9], the results of its application, on the whole, do not correspond to the equilibrium theory of Bogoliubov [11, 13] for a homogeneous boson gas, within which the number of particles in the BEC N_0 differs on the total number of particles N (see also [14]).

On the other hand, when describing a homogeneous system with BEC, there are certain doubts regarding the hypothesis of the existence of "quasi-averages" and the representation of the creation and annihilation operators as c-numbers. This procedure formally does not correspond to the commutation relations for these operators in the framework of the standard diagram technique of quantum statistical mechanics, where the average value of one operator of creation or annihilation of a particle for an arbitrary state equals zero. The respective doubts and the alternative approach, free from the hypothesis about "quasi-averages" are considered, in particular, in [15–18].

An alternative description of an equilibrium rarefied inhomogeneous gas of bosons in the ground state can be based on the use of the multi-configurational time-dependent Hartree method for bosons (MCTDHB). The method was first introduced as the best mean-field (BMF) method in [19–21], with the generalized time-independent theory treated in [22] and the time-dependent in [23].

Another variant of description is associated with the use of the self-consistent Hartree–Fock approximation (SHFA), when for both systems with an integer (bosons) or semi-integer (fermions) spin values can be considered from a unified standpoint (see [24–26] and references therein). In this paper, within the framework of the SHFA, we will show the possibility of taking into account the difference between the number of particles in the BEC N_0 and the total number of particles N when describing the ground state of an inhomogeneous boson gas. In doing so, we will discuss the question of approaching the thermodynamic limit, which is essential in the study of a weakly inhomogeneous system of bosons.

2. SELF-CONSISTENT HARTREE–FOCK APPROXIMATION AND STATIONARY GROSS–PITAEVSKY EQUATION

We consider an equilibrium inhomogeneous system consisting of N bosons with zero spin, which are in a macroscopic but finite volume V in a static external field with a scalar potential $v^{(ext)}(\mathbf{r})$. This system is characterized by the Hamiltonian

$$\hat{H} = \int_V d^3r \hat{\Psi}^+(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + v^{(ext)}(\mathbf{r}) + \frac{1}{2}\int_V d^3r_1 U(\mathbf{r}_1 - \mathbf{r})\hat{\Psi}^+(\mathbf{r}_1)\hat{\Psi}(\mathbf{r}_1) \right\} \hat{\Psi}(\mathbf{r}), \quad (1)$$

where $U(\mathbf{r})$ is the potential energy of the pair interaction of bosons.

In the representation of occupation numbers, the field operators $\hat{\Psi}^+(\mathbf{r})$ and $\hat{\Psi}(\mathbf{r})$ can be written as $\hat{\Psi}^+(\mathbf{r}) = \sum_k \varphi_k^*(\mathbf{r})\hat{a}_k^+$ and $\hat{\Psi}(\mathbf{r}) = \sum_k \varphi_k(\mathbf{r})\hat{a}_k$. Here $\varphi_k(\mathbf{r})$ is a complete system of one-particle wave functions characterized by some set of quantum numbers k: $\int_V d^3r \varphi_k^*(\mathbf{r})\varphi_l(\mathbf{r}) = \delta_{k,l}$, $\hat{a}_k^+$ and $\hat{a}_k$ are boson creation and annihilation operators respectively, in the state described by the one-particle wave function $\varphi_k^*(\mathbf{r})$.

In this case, the system under consideration is characterized by the wave function $\Phi(N_0, N_1 ... N_\alpha ...)$ in the representation of occupation numbers in the Fock space, where $N_k = 0, 1, 2...$ is the number of particles (occupation number) in a state with a set of quantum numbers k so that the wave function Φ satisfies the equation $\hat{H}\Phi = E_\Phi \Phi$. Further, to describe a weakly nonideal system of bosons, we will use SHFA.

Then, in accordance with the Wick–Bloch–Dominicis theorem [27] applied to quantum mechanics, the expected value of the normal product of the same number of creation and annihilation operators is represented as the sum of all possible pair products

$$\langle \Phi^{SHFA} \mid \hat{a}_k^+ \hat{a}_l \mid \Phi^{SHFA} \rangle = N_l \delta_{kl}, \quad \sum_k N_k = N. \tag{2}$$

In turn, the energy E_Φ^{SHFA} corresponding to the wave function Φ^{SHFA} in the SHFA has the form

$$E_\Phi^{SHFA} = \langle \Phi^{SHFA} \mid \hat{H} \mid \Phi^{SHFA} \rangle =$$
$$\sum_k N_k \int_V d^3 r \varphi_k^*(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m}\Delta_\mathbf{r} + v^{ext}(\mathbf{r}) \right\} \varphi_k(\mathbf{r}) +$$
$$\frac{1}{2} \sum_k N_k(N_k - 1) \int_V d^3 r \int_V d^3 r_1 U(\mathbf{r}_1 - \mathbf{r}) \times$$
$$\mid \varphi_k(\mathbf{r}) \mid^2 \mid \varphi_k(\mathbf{r}_1) \mid^2 +$$
$$\frac{1}{2} \sum_k \sum_{l \neq k} N_k N_l \int_V d^3 r \int_V d^3 r_1 U(\mathbf{r}_1 - \mathbf{r}) \times$$
$$\{ \mid \varphi_k(\mathbf{r}) \mid^2 \mid \varphi_l(\mathbf{r}_1) \mid^2 + \gamma_k(\mathbf{r}_1, \mathbf{r}) \gamma_l(\mathbf{r}, \mathbf{r}_1) \}, \tag{3}$$

where $\gamma_k(\mathbf{r}_1, \mathbf{r}_1) = \varphi_k^*(\mathbf{r}_1)\varphi_k(\mathbf{r})$.

Note that a state with a wave function Φ^{SHFA} for a given number of particles N (2) corresponds to a well-defined set of nonzero occupation numbers $\{N_k\}$. This means that if the corresponding set $\{N_k\}$ satisfying condition (2) is known, the energy of the considered system E_Φ^{SHFA} in a given external field $v^{(ext)}(\mathbf{r})$ is a functional of the wave functions: $E_\Phi^{SHFA} = E_\Phi^{SHFA}[\varphi_k]$. To determine the ground state energy E_0^{SHFA} of such a system it is naturally to apply the inequality

$$E_0^{SHFA} \leq E_\Phi^{SHFA}[\varphi_0] \tag{4}$$

However, to use inequality (4) in the variational procedure adopted in quantum mechanics (see, e.g., [28]), a set of nonzero occupation numbers $\{N_k\}$ corresponding to the ground state of the considered boson system should be known. Here the fundamental difference between the boson and the fermion systems is manifested. For fermions, due to the Pauli principle, the admissible values of N_k are 0 or 1. In other words, to find the energy of the ground E_0^{SHFA} for the boson system, we should consider the energy $E_\Phi^{SHFA}[\varphi_k]$ not only as a functional of wave functions φ_k, but also as a function of the occupation numbers N_k, i.e. $E_\Phi^{SHFA} = E_\Phi^{SHFA}([\varphi_k], N_k)$ according to condition (2). A similar statement is valid for the wave functions $\varphi_k = \varphi_k(\mathbf{r}, \{N_l\})$.

The “traditional” assumption is that in a weakly nonideal boson gas, the ground state corresponds to the presence of all particles in the same single-particle state (see, e.g., [11–13]). Thus, it is assumed that accounting for the interaction between bosons (the last two terms on the right-hand side of (3)) does not affect the situation that takes place for non-interacting bosons (taking into account only the first term on the right-hand side of (3)). This means that in the ground state of the considered inhomogeneous system of bosons

$$N_0 = N; \qquad N_{k \neq 0} = 0, \tag{5}$$

where N_0 — the number of particles in a single-particle state with the lowest energy ε_0 (BEC).

Then, varying equality (3) taking into account (4), (5), we arrive at the conclusion that the one-particle wave function $\varphi_0(r)$ corresponding to the ground state in SHFA satisfies the stationary nonlinear equation

$$\left\{ -\frac{\hbar^2}{2m}\Delta_\mathbf{r} + v^{ext}(\mathbf{r}) + \right.$$
$$\left. (N-1) \int_V d^3 r_1 U(\mathbf{r}_1 - \mathbf{r}) \mid \varphi_0(\mathbf{r}_1) \mid^2 \right\} \varphi_0(\mathbf{r}) = \varepsilon_0 \varphi_0(\mathbf{r}) \tag{6}$$

Equation (6) directly follows from inequality (4), considered as a condition for the minimum of functional (3) with regard to (5). This result can be obtained from the coordinate representation for the many-particle wave function in the form of a product of one-particle wave functions (see [24] for more details).

In the case of $N \gg 1$, we can replace the one-particle wave functions $\varphi_k(\mathbf{r})$ in (5) by the so-called BEC wave function of the form

$$\Phi_0^{BEC}(\mathbf{r}) = \sqrt{N}\varphi_0(\mathbf{r}), \tag{7}$$

which, as is easy seen, satisfies the stationary equation

$$\left\{ -\frac{\hbar^2}{2m}\Delta_\mathbf{r} + v^{ext}(\mathbf{r}) + \right.$$
$$\left. \int_V d^3 r_1 U(\mathbf{r}_1 - \mathbf{r}) \mid \Phi_0^{BEC}(\mathbf{r}) \mid^2 \right\} \Phi_0^{BEC}(\mathbf{r}) = \varepsilon_0 \Phi_0^{BEC}(\mathbf{r}),$$
$$\int_V d^3 r \mid \Phi_0^{BEC}(\mathbf{r}) \mid^2 = N. \tag{8}$$

This equation for $U(\mathbf{r}) = U_0\delta(\mathbf{r})$ turns into the stationary Gross–Pitaevsky equation ($\delta(\mathbf{r})$ is the Dirac δ-function).

Thus, putting the wave function BEC $\Phi_0^{BEC}(\mathbf{r})$ (7) into consideration is a formal mathematical trick that allows only the exclusion of the number of particles N from the nonlinear Schrödinger equation (6), transferring the value of N to the normalization condition (8). The one-particle wave function $\varphi_0(\mathbf{r})$ (6), corresponding to the ground state of one particle in the self-consistent field of the remaining $N-1$ particles, taking into account their indistinguishability (identity), has a direct physical meaning.

It immediately follows from (8) that

$$N\varepsilon_0 = \int_V d^3 r \Phi_0^{*BEC}(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m}\Delta_\mathbf{r} + v^{ext}(\mathbf{r}) + \right.$$
$$\left. \int_V d^3 r_1 U(\mathbf{r}_1 - \mathbf{r}) \mid \Phi_0^{BEC}(\mathbf{r}) \mid^2 \right\} \Phi_0^{BEC}(\mathbf{r}). \tag{9}$$

In this case, the energy of the ground state of the boson system, according to (4)–(8), is given by

$$E_0^{SHFA} = N\varepsilon_0 - \frac{1}{2}\int_V d^3r_1 \int_V d^3r_2 U(\mathbf{r}_1 - \mathbf{r}_2)\times \mid \Phi_0^{BEC}(\mathbf{r}_1) \mid^2 \mid \Phi_0^{BEC}(\mathbf{r}_2) \mid^2 . \quad (10)$$

Therefore, the energy of the ground state E_0^{SHFA} of the boson system in the considered approximation is not determined only by the value of $N\varepsilon_0$ (9).

At first glance, given that the energies E_0^{SHFA} and ε_0 are functions of the number of particles N, to solve this problem, we can use the equality that directly follows from (8)–(10) under the condition $N \gg 1$ [18].

$$\frac{dE_0^{SHFA}(N)}{dN} = \varepsilon_0(N) \quad (11)$$

However, two essential circumstances should be taken into account. First, the number of particles N is a discrete quantity, so its minimum change $\triangle N$ is equal to $\triangle N_{min} = 1$. At the same time, equality (11) makes sense if we assume that the number of particles N is a continuous quantity. Second, the integration of equation (11) implies setting the value $E_0^{SHFA}(N)$ at a certain number of particles (meaning the boundary condition for equation (11)) at $N \gg 1$. In addition, the energy $\varepsilon_0(N)$ essentially depends on the boundary conditions for the wave functions in (6) and (8).

Thus, in the general case, the energy $\varepsilon_0(N)$, found from the stationary Gross–Pitaevsky equation, does not determine the energy of the ground state of a finite inhomogeneous degenerate Bose gas, although the wave function Φ_0^{BEC} (7) corresponds to this state.

The corresponding problems are well-known in statistical thermodynamics in connection with the determination of the chemical potential (see [29] for more details). It is necessary to take into account the procedure for approaching the thermodynamic limit (see, e.g., [30]) to solve them when describing systems in a state of thermodynamic (statistical) equilibrium.

$$Lim_T : N \to \infty, \quad V \to \infty, \quad \overline{n} = \frac{N}{V} = const < \infty \quad (12)$$

where $\overline{n}$ is the average density of the number of particles in the system occupying the volume V. In this case, the quantity $\overline{n}$ can be considered as a continuous variable (see [25] for more details).

3. EXCITED STATES IN THE SELF-CONSISTENT HARTREE–FOCK APPROXIMATION

As noted above, condition (5) generally only holds if the interaction between bosons is not taken into account. Thus, strictly speaking, when considering interacting bosons, it is necessary to take into account the possibility that, in order to determine the energy of the ground state, it is necessary to take into account also the excited one-particle states.

When using SHFA, we mean the analogy with considering a system of interacting fermions (e.g., an inhomogeneous system of electrons (see [28] for more details)). In other words, we will assume that the occupation numbers N_l in the functions $E_\Phi^{SHFA} = E_\Phi^{SHFA}([\varphi_k], N_l)$ and $\varphi_k = \varphi_k(\mathbf{r}, N_l)$ are known. This means that the ground state is determined not by a single one-particle wave function φ_0 (see above), but by a set of wave functions φ_k, including excited one-particle states.

Assuming that the numbers N_k are known, we vary equality (4) by the method of indefinite Lagrange multipliers. Taking into account the normalization condition $\int_V d^3r \mid \varphi_0(\mathbf{r}) \mid^2 = 1$, one can come to the conclusion that the one-particle wave function $\varphi_0(\mathbf{r})$, corresponding to the ground state within the SHFA, satisfies the stationary nonlinear and non-local equation

$$\Big\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + v^{ext}(\mathbf{r}) + (N_0 - 1)\int_V d^3r_1 U(\mathbf{r}_1 - \mathbf{r}) \mid \varphi_0(\mathbf{r}_1) \mid^2 \Big\} \varphi_0(\mathbf{r}) + \sum_{k\neq 0} N_k \int_V d^3r_1 U(\mathbf{r}_1 - \mathbf{r})\{\mid \varphi_k(\mathbf{r}_1) \mid^2 \varphi_0(\mathbf{r}) + \gamma_k(\mathbf{r}_1, \mathbf{r})\varphi_0(\mathbf{r}_1)\} = \varepsilon_0\varphi_0(\mathbf{r}_1). \quad (13)$$

In the case of $N \gg 1$, we can replace in (13) the one-particle wave functions $\varphi_k(\mathbf{r})$ by functions of the form (see (7))

$$\Phi_k(\mathbf{r}) = \sqrt{N}\varphi_k(\mathbf{r}), \qquad \int_V d^3r \mid \Phi_k(\mathbf{r}) \mid^2 = N, \quad (14)$$

and rewrite Eq. (13) in the form

$$\Big\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + v^{ext}(\mathbf{r}) + \int_V d^3r_1 U(\mathbf{r}_1 - \mathbf{r})\times \Big[n_0 \mid \Phi_0(\mathbf{r}_1) \mid^2 + \sum_{k\neq 0} n_k \mid \Phi_k(\mathbf{r}_1) \mid^2\Big]\Big\} \Phi_0(\mathbf{r}) + \sum_{k\neq 0} n_k \int_V d^3r_1 U(\mathbf{r}_1 - \mathbf{r})\times \Phi_k^*(\mathbf{r}_1)\Phi_k(\mathbf{r})\Phi_0(\mathbf{r}_1) = \varepsilon_0\Phi_0(\mathbf{r}), \quad (15)$$

where $n_k = N_k/N$ is the relative number of particles ("concentration" of particles) in a state with a set of quantum numbers k:

$$\sum_k n_k = 1, \quad (16)$$

To determine the wave function $\Phi_1(\mathbf{r})$ corresponding to the first excited state, we proceed similarly, but in addition to the normalization condition, we also take into account the orthogonality condition:

$$\int_V d^3r \mid \Phi_1(\mathbf{r}) \mid^2 = N, \qquad \int_V d^3r \Phi_1^*(\mathbf{r})\Phi_0(\mathbf{r}) = 0. \quad (17)$$

When conditions (17) are satisfied for the energy of the first excited state E_1^{SHFA} of such a system, we can apply the inequality (see, e.g., [28])

$$E_1^{SHFA} \le E_\Phi^{SHFA}[\Phi_1] \quad (18)$$

Thus, the wave function $\Phi_1(\mathbf{r})$ for the first excited state is determined by equation

$$\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + v^{ext}(\mathbf{r}) + \int_V d^3r_1 U_(\mathbf{r}_1 - \mathbf{r})\times\right.$$
$$\left.\left[n_1 \mid \Phi_1(\mathbf{r}_1)\mid^2 + \sum_{k\neq 1} n_k \mid \Phi_k(\mathbf{r}_1)\mid^2\right]\right\}\Phi_1(\mathbf{r}) +$$
$$\sum_{k\neq 1} n_l \int_V d^3r_1 U(\mathbf{r}_1 - \mathbf{r}) \times$$
$$\Phi_k^*(\mathbf{r}_1)\Phi_k(\mathbf{r})\Phi_1(\mathbf{r}_1) = \varepsilon_1 \Phi_1(\mathbf{r}) \quad (19)$$

In a similar way, we find equations for the wave functions of various states $\Phi_k(\mathbf{r})$, which are orthogonal to each other and normalized to the total number of particles N

$$\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + v^{ext}(\mathbf{r}) + \int_V d^3r_1 U_(\mathbf{r}_1 - \mathbf{r})\times\right.$$
$$\left.\left[n_k \mid \Phi_k(\mathbf{r}_1)\mid^2 + \sum_{l\neq k} n_l \mid \Phi_l(\mathbf{r}_1)\mid^2\right]\right\}\Phi_k(\mathbf{r}) +$$
$$\sum_{l\neq k} n_l \int_V d^3r_1 U(\mathbf{r}_1 - \mathbf{r}) \times$$
$$\Phi_l^*(\mathbf{r}_1)\Phi_l(\mathbf{r})\Phi_k(\mathbf{r}_1) = \varepsilon_k \Phi_k(\mathbf{r}), \quad (20)$$

In this case, according to (3), the energy of the ground state of an inhomogeneous system of bosons within the SHFA is given by

$$E_0^{SHFA} = N\sum_k n_k\varepsilon_k$$
$$-\frac{1}{2}\sum_k n_k \int_V d^3r \int_V d^3r_1 U_(\mathbf{r}_1 - \mathbf{r})\left[n_k \mid \Phi_k(\mathbf{r}_1)\mid^2 + \right.$$
$$\left.\sum_{l\neq k} n_l \mid \Phi_l(\mathbf{r}_1)\mid^2\right] \mid \Phi_k(\mathbf{r})\mid^2 -$$
$$\frac{1}{2}\sum_k n_k \int_V d^3r \int_V d^3r_1 U(\mathbf{r}_1 - \mathbf{r})\times$$
$$\Phi_k^*(\mathbf{r}_1)\Phi_k(\mathbf{r})\sum_{l\neq k} n_l \Phi_l^*(\mathbf{r})\Phi_l(\mathbf{r}_1). \quad (21)$$

As noted above, for fixed N under a given external field $v^{(ext)}(\mathbf{r})$, the quantities ε_k, $\Phi_k(\mathbf{r})$ and E_0^{SHFA} depend on the set of particle concentrations $\{n_k\}$, the values of which are assumed as known. However, in fact, these values are unknown a priori.

This means that it is necessary to proceed to the final stage, i.e., — the determination of the ground state energy E_0 as a minimum of the value E_0^{SHFA} (21), considered as a function of the set of particle concentrations $\{n_k\}$:

$$E_0 = min_{\{n_k\}} E_0^{SHFA}(\{n_k\}). \quad (22)$$

This problem can be solved by standard methods of mathematical analysis, taking into account the normalization condition (16) for fixed values of N under a given external field $v^{(ext)}(\mathbf{r})$.

The corresponding computational procedure was implemented for the one-dimensional case in [20], and in [21] for the one-dimensional, two-dimensional and three-dimensional cases for certain potentials of the external field $v^{(ext)}$ and the number of particles N in the framework of the BMF-method, the implementation of which leads to the results, similar to those presented above when approaching the limit $V \to \infty$.

It is assumed that the system of bosons is in an external field, which ensures its finite state, localized in a limited region of space. This means that the system under consideration is characterized by a discrete energy spectrum, and its wave functions rather quickly (exponentially) tend to zero as it moves away from the localization region. In this regard, the following remark should be made.

Although expression (21) for the energy of the ground state does not explicitly contain the potential of the external field $v^{ext}(\mathbf{r})$, this result makes sense only in the presence of an external field that ensures the spatial localization of the system under consideration as a whole. Formally, this is related to applying the orthogonality condition to the one-particle wave functions $\Phi_k(\mathbf{r})$ in the derivation. The ground state energy E_0, like the wave functions $\Phi_k(\mathbf{r})$, the energy levels ε_k, and the concentration n_k are functionals of the external field potential $v^{ext}(\mathbf{r})$:

$$E_0 = E_0[v^{ext}], \quad \Phi_k = \Phi_k[v^{ext}],$$
$$\varepsilon_k = \varepsilon_k[v^{ext}], \quad n_k = n_k[v^{ext}]. \quad (23)$$

In other words, each quantity in (15) fundamentally depends on the form and parameters of the potential $v^{ext}(\mathbf{r})$.

In addition, it is necessary to solve the problem of the boundary conditions for the wave functions $\Phi_k(\mathbf{r})$ appearing in the system of equations (20) on the boundaries of the macroscopic volume V. In this case, the results have physical meaning after excluding the quantity V from consideration, i.e. after approaching the limit $V \to \infty$.

According to the above consideration, we "tacitly" considered that the system of bosons is in an external field $v^{(ext)}(\mathbf{r})$, which ensures the spatial localization of a given total number of bosons N in a relatively small region of space compared to the macroscopic volume V, with taking into account the subsequent tendency to the limit $V \to \infty$. In this case, as boundary conditions for the wave functions $\psi_k(\mathbf{r})$ in relations (20), (21), we can use zero values for the wave functions at "infinity": $\psi_k(\mid \mathbf{r} \mid) \to \infty$, which provides the normalization condition and corresponds to the consideration of localized states with a discrete energy spectrum. But such a system is characterized by a zero value of the average density of the number of bosons $\overline{n}$:

$$\overline{n} = \lim_{V\to\infty}\frac{N}{V} = 0. \quad (24)$$

This means that the system under consideration has no thermodynamic limit (see (12)). Usually, the procedure that ensures the transition to the thermodynamic limit (12) is implemented using the Gibbs grand canonical distribution based on the assumption that the system under consideration, being a part of a "big" system (the so-called

"Universe"), is in thermodynamic equilibrium with it, which is determined by the given values of the chemical potential and temperature (see, for example, [31]). Thus, the total number of particles in the system under consideration is not fixed but is determined by the given values of the chemical potential and temperature. This means that the bosons of the system under consideration can lie outside the volume V, which must be taken into account when setting the boundary conditions on the surface that limits the volume V for the wave functions describing the corresponding states of the bosons. Traditionally, when considering homogeneous systems, the so-called periodic boundary conditions are used in this case (see [31] for more details). However, the results obtained in this work are based on the use of the condition on a given total number of particles N. Thus, the corresponding results, generally speaking, do not correspond to the consideration using the Gibbs grand canonical distribution.

4. CONCLUSIONS

Within this approach, two options for further consideration are possible:

- based on the grand canonical Gibbs distribution, which corresponds to the traditional consideration of the equilibrium properties of the boson gas, including the Bogoliubov hypothesis of "quasi-averages";

- on the basis of the Gibbs microcanonical distribution, when the equilibrium state of the bosonic system is not determined by the thermostat surrounding this system, but is its "true" state.

The difference between these variants is related to the degree of inhomogeneity of the system of bosons under consideration, which is determined by the parameters (characteristics) of the external field potential. In the case of strong inhomogeneity, the equilibrium system of bosons, which contains a macroscopic but finite number N of particles located in an unlimited space, does not have a thermodynamic limit. Then, the resulting system of equations should be considered as nonlinear Schrödinger equations for spatially localized systems with a fixed finite number of particles and a discrete energy spectrum. In turn, in the limit of weak inhomogeneity, we can use the traditional approach based on the concept of chemical potential. In this case, according to Pitaevskii [12], the corresponding consideration corresponds to the semiclassical approximation.

The obtained theoretical results show that the consequent accounting of the excited states in the degenerate Bose system permits finding the ground state energy of the degenerate Bose system. In the framework of Hartree–Fock approximation, assuming that BEC occupied only one single-particle state, we arrive at the stationary Gross–Pitaevskii equation (8). It is shown, however, that in this case, there is no need to assume the existence of anomalous averages. In general, similarly to the homogeneous case [11, 13, 14], the BEC in the inhomogeneous external field can be distributed on different single-particle states. The appropriate ground state energy due to interaction between particles can be found by the numerical solution of the obtained non-linear integral equations (20), (21). The numerical solution of these equations is a separate and complex problem. On this basis, it will be clarified whether the energy of the ground state corresponds to the distribution of particles over a set of single-particle states and what these states are.

The results of the relevant studies will be presented in separate publications.

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