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*Short notes*

# Nonstationary equation for the one-particle wave function of the Bose–Einstein condensate

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Based on the self-consistent Hartree–Fock approximation, the nonstationary equation is obtained for the one-particle wave function describing the Bose–Einstein condensate in a rarefied gas of spin-zero bosons. A rarefied gas of bosons is exposed to the static external field, which ensures its finite ground state. The derived equation allows one to correctly determine the ground state energy in the stationary case.

Keywords: degenerate Bose gas, Bose–Einstein condensate, self-consistent Hartree–Fock approximation, ground state energy.

The experimental observation of the Bose–Einstein condensate (BEC) in ultracold gases of alkali metals [1] gave a powerful impact for theoretical studies of weakly nonideal Bose systems. Due to the presence of magnetic moments, alkali metal atoms can be kept in magnetic traps. To achieve the ultralow temperatures required for the formation of BEC, laser cooling and the evaporation of the highest energy atoms from a magnetic trap are used (see [2] for more details). The resulting ultracold gas is usually rarefied and strongly inhomogeneous [3]. In view of the inhomogeneity of the system, the nonstationary Gross–Pitaevsky (GP) equation [4, 5] is widely used to describe such a gas at zero temperature with regard to the effect of laser radiation [6]. However, this equation does not allow to directly determine the ground state energy of a Bose gas [7, 8].

In the case of an ultracold gas of spinless bosons of mass $m$, located in a static external field $\varphi^{(\mathrm{ext})}(\mathbf{r})$, the GP equation for the BEC wave function $\Psi(\mathbf{r},t)$ has the form

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}\Psi(\mathbf{r},t)+\varphi^{(\mathrm{ext})}(\mathbf{r})\Psi(\mathbf{r},t)+ +U_0\left|\Psi(\mathbf{r},t)\right|^2\Psi(\mathbf{r},t), \tag{1}$$

where $U_0$ is a constant that determines the intensity of the pair interaction of bosons:

$$U(\mathbf{r})=U_0\delta(\mathbf{r})$$
$$\int d^3r\left|\Psi(\mathbf{r},t)\right|^2=N, \tag{2}$$

$N$ is the number of particles in the considerated degenerate Bose gas, equal to the number of particles in the BEC [4, 5]. The derivation of the GP equation is usually based on the exact equation of motion for the field operators of creation $\hat{\Psi}^+(\mathbf{r},t)$ and annihilation $\hat{\Psi}(\mathbf{r},t)$ in the Heisenberg representation:

$$i\hbar\frac{\partial\hat{\Psi}(\mathbf{r},t)}{\partial t}=-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}\hat{\Psi}(\mathbf{r},t)+\varphi^{(\mathrm{ext})}(\mathbf{r})\hat{\Psi}(\mathbf{r},t)+ +U_0\hat{\Psi}^+(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t), \tag{3}$$

with the subsequent formal replacement of these operators by their average (expected) values [4, 5]:

$$\hat{\Psi}^+(\mathbf{r},t)\to\left\langle\hat{\Psi}^+(\mathbf{r},t)\right\rangle\equiv\Psi^*(\mathbf{r},t),$$
$$\hat{\Psi}(\mathbf{r},t)\to\left\langle\hat{\Psi}(\mathbf{r},t)\right\rangle\equiv\Psi(\mathbf{r},t). \tag{4}$$

However, the use of formal substitution (4) raises certain doubts (see [9–13] and the references therein). In this regard, A. Leggett [7] drew attention to the fact that the derivation of the GP equation can be derived using the well-known self-consistent Hartree–Fock approximation (SCHF). At the same time, he also pointed out that in this case the GP equation (1) contains a some contradiction, which was already mentioned above: the stationary GP equation does not directly determine the energy of the ground state of a degenerate Bose gas (see also [8]). Indeed, in a stationary state, for which the BEC wave function has the form

$$\Psi(\mathbf{r},t)=\psi(\mathbf{r})\exp(-i\mathcal{E}t/\hbar), \tag{5}$$

the "stationary" wave function $\psi(\mathbf{r})$ satisfies the stationary GP equation:

$$\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\varphi^{(\mathrm{ext})}(\mathbf{r})+U_0\left|\psi(\mathbf{r})\right|^2\right\}\psi(\mathbf{r})=\mathcal{E}\psi(\mathbf{r}). \tag{6}$$

Physically, $\mathcal{E}$ must coincide with the ground state energy $\mathcal{E}_0$ per particle. However, in the approximation corresponding to the GP equation, the ground state energy $\mathcal{E}_0$ is determined by the relation

$$N\mathcal{E}_0=\int d^3r\psi^*(\mathbf{r})\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\varphi^{(\mathrm{ext})}(\mathbf{r})+\frac{1}{2}U_0\left|\psi(\mathbf{r})\right|^2\right\}\psi(\mathbf{r}). \tag{7}$$

It is easy to verify the validity of (7), if we take into account that with regard to Eq. (4), the expected value of the Hamiltonian $\hat{H}$ for the system under consideration

$$\hat{H}=\int d^3r\hat{\Psi}^+(\mathbf{r})\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\varphi^{(\mathrm{ext})}(\mathbf{r})+\frac{1}{2}U_0\hat{\Psi}^+(\mathbf{r})\hat{\Psi}(\mathbf{r})\right\}\hat{\Psi}(\mathbf{r}) \tag{8}$$

leads to the ground state energy $N\mathcal{E}_0$.

In this case, to derive the stationary GP equation (6), it is reasonable to assume that the stationary many-particle wave function for a degenerate Bose gas in the ground state can be represented in the form

$$\psi_0(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=\prod_{i=1}^{N}\chi_0(\mathbf{r}_i),\quad \int d^3r\left|\chi_0(\mathbf{r})\right|^2=1, \tag{9}$$

where $\chi_0(\mathbf{r})$ is the one-particle stationary wave function. To determine the wave function $\chi_0(\mathbf{r})$, the variational principle should be used for calculating the energy of the ground state of the system with the Hamiltonian

$$\hat{H}=\sum_{i=1}^{N}\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i}+\varphi^{(\mathrm{ext})}(\mathbf{r}_i)+\frac{1}{2}U_0\sum_{j\neq i}^{N}\delta(\mathbf{r}_i-\mathbf{r}_j)\right\}. \tag{10}$$

Then it is easy to verify [7] that the function $\chi_0(\mathbf{r})$ satisfies the equation

$$\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\varphi^{(\mathrm{ext})}(\mathbf{r})+U_0(N-1)\left|\chi_0(\mathbf{r})\right|^2\right\}\chi_0(\mathbf{r})=\mathcal{E}\psi(\mathbf{r}). \tag{11}$$

Equation (11) defines the stationary wave function $\chi_0(\mathbf{r})$ for one boson with zero spin in the self-consistent field of the other $(N-1)$ bosons. Provided that $N\gg 1$, the stationary GP equation (6) immediately follows from (11), if we assume that the stationary wave function of the BEC is determined by the relation

$$\psi(\mathbf{r})\cong\sqrt{N}\chi_0(\mathbf{r}). \tag{12}$$

A similar result within the SCHF approach can be obtained using the secondary quantization formalism [8].

To obtain the appropriate nonstationary equation (for the one-dimensional case in the absence of an external field, such an equation was first derived for in Ref. 14), it is natural to assume that for a degenerate Bose gas the nonstationary many-particle wave function in the coordinate representation $\Psi_0(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N;t)$ satisfying the Schrödinger equation

$$i\hbar\frac{\partial\Psi_0}{\partial t}=\sum_{i=1}^{N}\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i}+\varphi^{(\mathrm{ext})}(\mathbf{r}_i)+\frac{1}{2}U_0\sum_{j\neq i}^{N}\delta(\mathbf{r}_i-\mathbf{r}_j)\right\}\Psi_0, \tag{13}$$

by analogy with (9) can be represented in the form (see, e.g., [7])

$$\Psi_0(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N;t)=\prod_{i=1}^{N}\chi_0(\mathbf{r}_i,t),\quad \int d^3r\left|\chi_0(\mathbf{r},t)\right|^2=1. \tag{14}$$

Substituting (14) into (13), one obtains

$$i\hbar\sum_{i=1}^{N}\frac{\partial\chi_0(\mathbf{r}_i,t)}{\partial t}\Lambda_i(\{\mathbf{r}_{k\neq i}\},t)=$$
$$=\sum_{i=1}^{N}\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i}+\varphi^{(\mathrm{ext})}(\mathbf{r}_i)+\frac{1}{2}U_0\sum_{j\neq i}^{N}\delta(\mathbf{r}_i-\mathbf{r}_j)\right\}\times$$
$$\times\chi_0(\mathbf{r}_i,t)\Lambda_i(\{\mathbf{r}_{k\neq i}\},t), \tag{15}$$

where the function $\Lambda_i(\{\mathbf{r}_{k\neq i}\},t)=\prod_{j\neq i}^{N}\chi_0(\mathbf{r}_j,t)$ does not depend on the spatial variable $\mathbf{r}_i$. Further, within the framework of the accepted consideration, very significant assumptions are made to obtain a nonstationary equation [7].

In particular, by virtue of the condition $N\gg 1$, it is assumed that the quantity $\sum_{j\neq i}^{N}\delta(\mathbf{r}_i-\mathbf{r}_j)$ can be considered as the local inhomogeneous density of the gas at the point $\mathbf{r}_i$. Moreover, it is accepted that this value can be replaced by its expected value [by analogy with the statement (4)].

Under the validity of such assumptions, it is argued that Eq. (15) is satisfied if the one-particle wave function $\chi_0(\mathbf{r},t)$ satisfies the following equation:

$$i\hbar\frac{\partial\chi_0(\mathbf{r},t)}{\partial t}=-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}\chi_0(\mathbf{r},t)+\varphi^{(\text{ext})}(\mathbf{r})\chi_0(\mathbf{r},t)+ + NU_0\left|\chi_0(\mathbf{r},t)\right|^2\chi_0(\mathbf{r},t), \quad (16)$$

which is equivalent to the nonstationary GP equation (1) up to the replacement $\Psi(\mathbf{r},t)\cong\sqrt{N}\chi_0(\mathbf{r},t)$ [see (12)] [7].

Meanwhile, as shown in [14], for the case of a one-dimensional problem in the absence of an external field, there is no need for the assumptions made in [7].

To derive a closed equation for the function $\chi_0(\mathbf{r}_i,t)$, it is sufficient to multiply equation (15) by the function $\Lambda_i^*(\{\mathbf{r}_{k\neq i}\},t)$ and integrate over all spatial variables $\mathbf{r}_i$, except for the selected $\mathbf{r}_i$. As a result, omitting the index $(i)$ and accounting that

$$\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\ldots=\sum_{i=1}^{N}\sum_{j>i}^{N}\ldots, \quad (17)$$

we get

$$i\hbar\frac{\partial\chi_0(\mathbf{r},t)}{\partial t}+i\hbar(N-1)\left\langle\chi_0\left|\frac{\partial\chi_0}{\partial t}\right.\right\rangle\chi_0(\mathbf{r},t)=-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}\chi_0(\mathbf{r},t)+ +\varphi^{(\text{ext})}(\mathbf{r})\chi_0(\mathbf{r},t)+(N-1)U_0\left|\chi_0(\mathbf{r},t)\right|^2\chi_0(\mathbf{r},t)+ +(N-1)\left\langle\chi_0\left|\hat{\mathcal{H}}\right|\chi_0\right\rangle\chi_0(\mathbf{r},t), \quad (18)$$

where the angular brackets define the procedure for calculating the expected values:

$$\langle\psi|\varphi\rangle\equiv\int d^3r\,\psi^*(\mathbf{r},t)\varphi(\mathbf{r},t),$$
$$\langle\psi|\hat{A}|\varphi\rangle\equiv\int d^3r\,\psi^*(\mathbf{r},t)\hat{A}\,\varphi(\mathbf{r},t), \quad (19)$$

and the operator $\hat{\mathcal{H}}$ in the coordinate representation is equal

$$\hat{\mathcal{H}}=-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\varphi^{(\text{ext})}(\mathbf{r})+\frac{1}{2}U_0(N-2)\left|\chi_0(\mathbf{r},t)\right|^2. \quad (20)$$

It is convenient to rewrite Eq. (18) in the form similar to the nonstationary GP equation (16) for the one-particle wave function:

$$i\hbar\frac{\partial\chi_0(\mathbf{r},t)}{\partial t}=\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\varphi^{(\text{ext})}(\mathbf{r})+(N-1)E(t)+ +U_0(N-1)\left|\chi_0(\mathbf{r},t)\right|^2\right\}\chi_0(\mathbf{r},t), \quad (21)$$

$$E(t)=\left\langle\chi_0\left|\hat{\mathcal{H}}\right|\chi_0\right\rangle-i\hbar\left\langle\chi_0\left|\partial\chi_0/\partial t\right.\right\rangle. \quad (22)$$

Next, we substitute (20) into (21), multiply by the function $\chi_0^*(\mathbf{r},t)$ and integrate over the spatial variable $\mathbf{r}$. Thus, we obtain

$$i\hbar\left\langle\chi_0\left|\frac{\partial\chi_0}{\partial t}\right.\right\rangle-\left\langle\chi_0\left|-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\varphi^{(\text{ext})}(\mathbf{r})\right|\chi_0\right\rangle= =\frac{1}{2}\left\langle\chi_0\left|U_0(N-1)\left|\chi_0(\mathbf{r},t)\right|^2\right|\chi_0\right\rangle. \quad (23)$$

The nonstationary equation for the one-particle wave function of the Bose–Einstein condensate in the form (21) directly follows from Eqs. (21)–(23) with $E(t)$ equal to

$$E(t)=-\frac{1}{2}\left\langle\chi_0\left|U_0\left|\chi_0(\mathbf{r},t)\right|^2\right|\chi_0\right\rangle. \quad (24)$$

Let us emphasize that the obtained relations, as well as the method of their derivation, are in full agreement with the results obtained for the first time in Ref. 14 and reproduce them for the one-dimensional case in the absence of an external field. Equations (21)–(24) indicate that describing behavior of one boson, it is necessary to take into account the self-consistent change in the behavior of the other bosons, which is not reduced to the traditional “mean field” effect (see [14] for more details).

In a stationary state, when the wave function $\chi_0(\mathbf{r},t)$ can be represented as

$$\chi_0(\mathbf{r},t)=\mathrm{X}_0(\mathbf{r})\exp(-i\varepsilon_0 t/\hbar), \quad (25)$$

the quantity $E(t)$ is described by

$$E(t)=E_0=\left\langle\mathrm{X}_0\left|\hat{\mathcal{H}}\right|\mathrm{X}_0\right\rangle-\varepsilon_0. \quad (26)$$

As a result, according to Eqs. (18)–(26), we obtain a stationary equation that determines the function $\mathrm{X}_0(\mathbf{r})$ and the energy $\varepsilon_0$:

$$\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\varphi^{(\text{ext})}(\mathbf{r})+(N-1)\times \times\left(U_0\left|\mathrm{X}_0(\mathbf{r})\right|^2+\left\langle\mathrm{X}_0\left|\hat{\mathcal{H}}\right|\mathrm{X}_0\right\rangle\right)\right\}\mathrm{X}_0(\mathbf{r})=N\varepsilon_0\mathrm{X}_0(\mathbf{r}). \quad (27)$$

It is easy to show that the energy $\varepsilon_0$ coincides with the energy of the ground state $\mathcal{E}_0$ per particle in the considerated boson gas [see (5)], that was required to prove. Taking into account Eq. (26), it is seen that the function $\mathrm{X}_0(\mathbf{r})$ corresponds to the solution of the stationary GP equation (11).


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## Нестаціонарне рівняння для одночастинкової хвильової функції бозе-ейнштейнівського конденсату

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На основі самоузгодженого наближення Хартрі–Фока отримано нестаціонарне рівняння для одночастинкової хвильової функції, що описує конденсат Бозе–Ейнштейна в розрідженому газі спін-нульових бозонів. Розріджений газ бозонів піддається впливу статичного зовнішнього поля, що забезпечує його кінцевий основний стан. Отримане рівняння дозволяє правильно визначити енергію основного стану у стаціонарному випадку.

Ключові слова: вироджений бозе-газ, конденсат Бозе–Ейнштейна, самоузгоджене наближення Хартрі–Фока, енергія основного стану.