On a fragmented condensate in a uniform Bose system

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According to the well-known analysis by Nozières, the fragmentation of the condensate increases the energy of a uniform interacting Bose system. Therefore, at \( T = 0 \) the condensate should be nonfragmented. We perform a more detailed analysis and show that the result by Nozières is not general. We find that, in a dense Bose system, the formation of a crystal-like structure with a fragmented condensate is possible. The effect is related to a nonzero size of real atoms. Moreover, the wave functions studied by Nozières are not eigenfunctions of the Hamiltonian and, therefore, do not allow one to judge with confidence about the structure of the condensate in the ground state. We have constructed the wave functions in such a way that they are eigenfunctions of the Hamiltonian. The results show that the fragmentation of the condensate (quasicondensate) is possible for a finite one-dimensional uniform system at low temperatures and a weak coupling.

1 Introduction

The Bose–Einstein condensation (BEC) is a beautiful purely quantum property [1, 2, 3]. The early history of the ideas on a condensate can be found in review [4]. BEC in gases and fluids is intensively studied experimentally and theoretically [5, 6, 7, 8, 9, 10]. However, some open questions remain in this field. In particular, in addition to the one-particle condensate, the two-particle condensate can exist in a Bose system with repulsive interaction [11, 12, 13, 14, 15, 16, 17]. It is not quite clear whether the existence of the three-particle and higher condensates is possible. According to the calculation with regard for the two- and three-particle correlations, the three-particle and higher condensates are absent in a three-dimensional (3D) Bose liquid [16].

Of high interest is also the question whether a condensate can be fragmented. The condensate in a stationary system of \( N \) identical structureless bosons is called fragmented [7, if
the diagonal expansion of the single-particle density matrix

$$F_1(\mathbf{r}, \mathbf{r}') = \sum_{j=1}^{\infty} \lambda_j \phi_j^*(\mathbf{r}') \phi_j(\mathbf{r})$$

contains two or more macroscopic natural occupations $\lambda_j$: for example, $\lambda_1, \lambda_2 \sim N$. Here, the natural orbitals $\phi_j(\mathbf{r})$ form the complete collection of orthonormal functions, and $\lambda_j$ are the occupation numbers of the single-particle states $\phi_j(\mathbf{r})$. We use the normalization of the function $F_1(\mathbf{r}, \mathbf{r}')$, for which $\lambda_1 + \ldots + \lambda_\infty = N$. Pollock [18] and Nozières [19] argued that the energy $E^{(2)}$ of a uniform system with two condensates should be higher than the energy $E^{(1)}$ of a system with one condensate. Indeed, for the repulsive point interaction $U(|\mathbf{r}_j - \mathbf{r}_l|) = 2c \delta(|\mathbf{r}_j - \mathbf{r}_l|)$ the difference $E^{(2)} - E^{(1)}$ is close to the exchange energy [19, 20]:

$$E^{(2)} - E^{(1)} \simeq 2cN_1N_2 \int \phi_1^2(\mathbf{r})\phi_2^2(\mathbf{r})d\mathbf{r} > 0. \quad (2)$$

Here, we assume the following: All $N$ atoms of the system with one condensate are in the state $\phi_0(\mathbf{r})$. For the system with two condensates, $N_1$ atoms are in the state $\phi_1(\mathbf{r})$, $N_2$ atoms occupy the state $\phi_2(\mathbf{r})$, $N_1 + N_2 = N$, and $\phi_1^2(\mathbf{r}) \simeq \phi_2^2(\mathbf{r}) \simeq \phi_0^2(\mathbf{r})$. In this case, the fragmentation of the condensate costs a macroscopic energy [18, 19]. If the condensates are separated in the $\mathbf{r}$-space, then the overlapping of the functions $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$ is small. Therefore, to find the value of $E^{(2)} - E^{(1)}$, it is necessary to consider additional terms. The analysis shows that, for the Bose gas in a double-well potential of a trap, the state with two condensates, which are localized at different minima of a trap, is energy-gained [20, 21]. The other examples of a fragmented condensate can be found in [7, 22]. The solutions with a fragmented condensate were obtained for one-dimensional (1D) and two-dimensional (2D) Bose gases in a trap [23, 24, 25, 26, 27, 28, 29, 30]. The fragmentation of the condensate of quasiparticles is discussed in review [31].

In the present work, we will analyze the problem of the fragmentation of the condensate in more details than in [18, 19]. We will show that the fragmentation of the condensate is possible even for a uniform system (analogous result was obtained previously [32] without general analysis of the problem of fragmentation). In this case, the condensates are not separated in the $\mathbf{r}$-space, in contrast to the solutions in [20, 21, 23, 24, 25, 26, 27, 28, 29, 30]. We will consider the problem step by step, by passing from a more crude description to an accurate one. In Sections 2 and 3, we will show that the approach by Pollock-Nozières [18, 19] has two weak places: point interatomic potential and Hartree–Fock wave functions. We will see that the use of a nonpoint potential leads to the possibility of a crystal-like solution with fragmented condensate (Sect. 2). The transition from Hartree–Fock wave functions to the more accurate collective description is considered in Sect. 3. The solutions with fragmented condensate in Sections 2 and 3 are approximate. In Sect. 4, we will find the accurate solution for a fragmented condensate in the 1D Bose gas.
2 Periodic Bose system: quasi-single-particle approach

In this section, we will carry on the analysis similar to the analysis by Pollock [18] and by Nozières [19] and will take into account the nonpointness (nonzero interaction radius) of real particles. Consider the periodic system of $N$ bosons with repulsive interaction ($\nu(0) > 0$). The exact Hamiltonian of the system reads

\[
\hat{H} = -\frac{\hbar^2}{2m} \int d\mathbf{r} \hat{\psi}^+(\mathbf{r}, t) \Delta \hat{\psi}(\mathbf{r}, t) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r'} U(|\mathbf{r} - \mathbf{r'}|) \hat{\psi}^+(\mathbf{r}, t) \hat{\psi}^+(\mathbf{r'}, t) \hat{\psi}(\mathbf{r}, t) \hat{\psi}(\mathbf{r'}, t),
\]

(3)

\[
U(|\mathbf{r} - \mathbf{r'}|) = \frac{1}{V} \sum_\mathbf{k} \nu(\mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r'})},
\]

(4)

where $\mathbf{k} = 2\pi \left( \frac{j_x}{L_x}, \frac{j_y}{L_y}, \frac{j_z}{L_z} \right)$, $j_x, j_y, j_z = 0, \pm 1, \pm 2, \ldots$, $L_x, L_y, L_z$ are the sizes of the system, and $V = L_x L_y L_z$. In this section, we consider an isolated quantum-mechanical system, being in some pure state $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$. In view of this, we use the quantum-mechanical average [33]: $\langle \hat{A} \rangle = \int d\mathbf{r}_1 \ldots d\mathbf{r}_N \Psi^* \hat{A} \Psi$.

2.1 Solutions with one, two, and three condensates

If all atoms are in one condensate of atoms with zero momentum, then we have the wave function of the system

\[
\Psi = C_1 (\hat{a}_0^+)^N |\text{vac}\rangle,
\]

(5)

the second-quantized operator

\[
\hat{\psi}(\mathbf{r}, t) = \hat{a}_0 / \sqrt{V},
\]

(6)

and $\hat{a}_0^+ \hat{a}_0 = \hat{N}$. In this case,

\[
\hat{H}^{(1)} = \frac{\nu(0)(\hat{N}^2 - \hat{N})}{2V}, \quad E^{(1)} = \langle \hat{H}^{(1)} \rangle = \frac{\nu(0)(N^2 - N)}{2V},
\]

(7)

where $E^{(1)}$ is the energy of the system. Let the atoms be distributed over three states:

\[
\Psi = C_3 (\hat{a}_0^+)^{N_0} \cdot (\hat{a}_k^+)^{N_k} \cdot (\hat{a}_{-k}^+)^{N_{-k}} |\text{vac}\rangle,
\]

(8)

\[
\hat{\psi}(\mathbf{r}, t) = V^{-1/2} (\hat{a}_0 + \hat{a}_k e^{i\mathbf{k} \cdot \mathbf{r}} + \hat{a}_{-k} e^{-i\mathbf{k} \cdot \mathbf{r}}),
\]

(9)

$\hat{a}_0^+ \hat{a}_0 = \hat{N}_0$, $\hat{a}_k^+ \hat{a}_k = \hat{N}_k$, $\hat{a}_{-k}^+ \hat{a}_{-k} = \hat{N}_{-k}$, $\hat{N}_0 + \hat{N}_k + \hat{N}_{-k} = \hat{N}$ (it is seen from the analysis by Bogoliubov [2] that the states $e^{i\mathbf{k} \cdot \mathbf{r}}$ and $e^{-i\mathbf{k} \cdot \mathbf{r}}$ are coupled [this is indicated by terms $\hat{b}_k^+ \hat{b}_{-k}^+$ and $\hat{b}_{-k} \hat{b}_{-k}$ in Eq. (37) below]; therefore, we consider them together). In this case, $N_0 = \langle \hat{N}_0 \rangle$, ...
$N_k = \langle \hat{N}_k \rangle$, $N_{-k} = \langle \hat{N}_{-k} \rangle$. The numbers $N_k$ and $N_{-k}$ can be macroscopic or microscopic. Then

$$F_1(r, r') = \langle \hat{\psi}(r', t) \hat{\psi}(r, t) \rangle = N_0 \frac{1}{V} + N_k \frac{e^{i k (r-r')}}{V} + N_{-k} \frac{e^{-i k (r-r')}}{V}. \tag{10}$$

We have obtained the diagonal expansion (11) with $\lambda_0 = N_0$, $\lambda_k = N_k$, and $\lambda_{-k} = N_{-k}$. That is, the definition of a fragmented condensate on the basis of formulae like (8), (9) is equivalent to that on the basis of (11).

In order to find the Hamiltonian (3) with the operator $\hat{\psi}(r, t)$ (9), we should take into account in the operator $\hat{\psi}(r, t) \hat{\psi}(r', t) \hat{\psi}(r', t)$ the terms

$$\frac{1}{\sqrt{2}} \left\{ \hat{a}_k^+ \hat{a}_k^+ \hat{a}_k \hat{a}_k^+ \hat{a}_{-k} \hat{a}_{-k}^+ \right. \left. + \hat{a}_k^+ \hat{a}_{-k} \hat{a}_k \hat{a}_{-k}^+ \left( e^{i 2k (r-r')} + e^{-i 2k (r-r')} + 2 \right) \right.$$

$$\left. + \hat{a}_0^+ \hat{a}_0^+ \hat{a}_0 + \hat{a}_0^+ \hat{a}_0^+ \hat{a}_k \hat{a}_{-k}^+ \hat{a}_{-k} \left( e^{i k (r-r')} + e^{-i k (r-r')} + 2 \right) \right.$$

$$\left. + (\hat{a}_0^+ \hat{a}_0^+ \hat{a}_k \hat{a}_{-k} + \hat{a}_k^+ \hat{a}_{-k}^+ \hat{a}_0 \hat{a}_0) \left( e^{i k (r-r')} + e^{-i k (r-r')} \right) \right\}. \tag{11}$$

Using the formulae $\hat{a}_0^+ \hat{a}_0^+ \hat{a}_0 = N_0^2 - \hat{N}_0$, $\nu(-k) = \nu(k)$ and Eqs. (3), (4), (11), we get the Hamiltonian and the energy of the system:

$$\hat{H}^{(1+2)} = \hat{H}^{(1)} + (\hat{N}_k + \hat{N}_{-k}) \left[ K(k) + \frac{\hat{N}_0 \nu(k)}{V} \right] \frac{\nu(2k)}{V} + \hat{N}_k \hat{N}_{-k} + \hat{H}_{\text{scat}}, \tag{12}$$

$$\hat{H}_{\text{scat}} = \frac{\nu(k)}{V} (\hat{a}_0^+ \hat{a}_0^+ \hat{a}_k \hat{a}_{-k} + \hat{a}_k^+ \hat{a}_{-k}^+ \hat{a}_0 \hat{a}_0), \tag{13}$$

$$E^{(1+2)} = \langle \hat{H}^{(1+2)} \rangle = E^{(1)} + (N_k + N_{-k}) [K(k) + n_0 \nu(k)] + N_k N_{-k} \frac{\nu(2k)}{V}, \tag{14}$$

where $n_0 = \frac{N_0}{V}$, $K(k) = \frac{h^2 k^2}{2m}$. This three-condensate solution (1 + 2) yields immediately two two-condensate solutions. We set $N_0 = 0$ and $N_{-k} = N - N_k$. Then the solution (1 + 2) transits to the solution (0 + 2):

$$\Psi = C_{02} (\hat{a}_k^+)^{N_k} \cdot (\hat{a}_{-k}^+)^{N_{-k}} |\text{vac}\rangle, \tag{15}$$

$$\hat{\psi}(r, t) = V^{-1/2} (\hat{a}_k e^{i kr} + \hat{a}_{-k} e^{-i kr}), \tag{16}$$

$$\hat{H}^{(0+2)} = \hat{H}^{(1)} + (\hat{N}_k + \hat{N}_{-k}) K(k) + \frac{\nu(2k)}{V} \hat{N}_k \hat{N}_{-k}, \tag{17}$$

$$E^{(0+2)} = E^{(1)} + NK(k) + N_k (N - N_k) \nu(2k)/V. \tag{18}$$

If we set $N_{-k} = 0$ and $N_0 = N - N_k$ in the three-condensate solution, we find another solution with two condensates:

$$\Psi = C_{11} (\hat{a}_0^+)^{N_0} \cdot (\hat{a}_k^+)^{N_k} |\text{vac}\rangle, \tag{19}$$

$$\hat{\psi}(r, t) = V^{-1/2} (\hat{a}_0 + \hat{a}_k e^{i kr}), \tag{20}$$
\[ \hat{H}^{(1+1)} = \hat{H}^{(1)} + \hat{N}_k \left[ K(k) + \frac{\hat{N}_0 \nu(k)}{V} \right], \]
\[ E^{(1+1)} = E^{(1)} + N_k [K(k) + n_0 \nu(k)] - N_k^2 \nu(k)/V. \]

We note that formulae (19)–(22), written in a different form, were previously obtained by Pollock [18]. Work [18] is little known, but it contains the Nozières’ result and was published much earlier than the work by Nozières [19]. Formulae (12)–(22) allow us to make some interesting conclusions.

2.2 Analysis of solutions: when is the fragmentation possible?

For \( K(k) \approx 0 \) and \( \nu(2k) = \nu(k) = \nu(0) > 0 \), we obtain \( E^{(1+2)} \approx E^{(1)} + (N_k + N_{-k})n_0 \nu(0) + N_kN_{-k} \nu(0)/V > E^{(1)} \). Thus, we arrive at the Pollock-Nozières’ conclusion [18, 19]: the fragmentation of the condensate increases the energy of the system. If \( N_0 = 0 \) or \( N_{-k} = 0 \), the conclusion is the same. However, the equality \( \nu(k) = \nu(0) \) holds at any \( k \) only for the point interaction. As known, the point potential allows one to properly describe the long-wave properties of a system. Below, we will get solutions with fragmented condensate, for which the fragments \( N_k, N_{-k} \) of a condensate are short-wave solutions. In order to properly describe the short-wave properties of a system, we need to use a nonpoint potential. Indeed, any real interatomic potential has a nonzero radius \( r_0 \sim 1 \text{Å} \). In this case, \( \nu(k) \sim -0.1 \nu(0) < 0 \) at \( k \sim \pi/r_0 \). The real potentials have a complicated form (for \(^4\text{He}-\)atoms, see [34, 35]). Very approximately, we can consider an atom as a semitransparent ball:

\[ U(r) \approx \begin{cases} U_0 > 0 & r \leq d_0, \\ 0 & r > d_0, \end{cases} \]

where \( d_0 = 2r_0 \approx 2–3 \text{Å}, U_0 \sim 10^3–10^6 \text{K} \). We note that the simple model potential (23) allows us to qualitatively correctly reproduce the behavior of the Fourier-transform \( \nu(k) \) of a real complicated potential. In the 3D case, the Fourier transform of the potential (23) is

\[ \nu(k) = 4\pi U_0 d_0^3 f_3(kd_0), \]

where \( f_3(g) = (\sin g - g \cos g)/g^3 \). In the 1D case, we have

\[ \nu(k) = 2U_0 d_0 f_1(kd_0), \quad f_1(g) = \frac{\sin g}{g}. \]

The functions \( f_1(g) \) and \( f_3(g) \) are oscillatory (see Fig. 1).

If the values of \( k \) lie near the first minimum of the function \( \nu(k) \) and if \( n_0 \) is large, we have \( K(k) + n_0 \nu(k) < 0 \). Then it is seen from Eq. (14) that the relation \( E^{(1+2)} < E^{(1)} \) becomes possible. In this case, the average value of the energy of the state \((1 + 2)\) is less than for the state \(1\) (with one condensate). Therefore, the fragmentation of the condensate is...
Fig. 1: [Color online] The functions $f_1(g)$ (dashed line) and $f_3(g)$ (solid line). The function $f_1(g)$ is multiplied by 1/4.

possible. If $N_{-k} = 0$ or $N_0 = 0$, the conclusion is the same. Note that the considered states are uniform. In particular, for the state with three condensates, the particle number density $n(r)$ is constant:

$$n(r) = \langle \hat{\psi}^+(r, t) \hat{\psi}(r, t) \rangle = V^{-1} \langle \hat{a}_0^+ \hat{a}_0 + \hat{a}_k^+ \hat{a}_k + \hat{a}_{-k}^+ \hat{a}_{-k} \rangle = N/V. \quad (26)$$

Consider the conditions, under which the fragmentation is possible, in more details. In order to determine the smallest value of the function $E^{(1+2)}(N_k, N_{-k}) \quad (14)$, we need to find the minimum of this function in the internal domain of the phase space ($0 < N_k, N_{-k} < N; N_k + N_{-k} < N$) and the boundary values of the function (one boundary corresponds to $N_{-k} = 0$, and another one is set by the equality $N_k + N_{-k} = N$). The extremum corresponds to

$$N_k = N_{-k} = \frac{K(k) + n\nu(k)}{4n\nu(k) - n\nu(2k)}N. \quad (27)$$

In this case,

$$E^{(1+2)} = E^{(1)} + N_k(K(k) + n\nu(k)). \quad (28)$$

It is a minimum, if $\nu(k) < 0$. We see that $E^{(1+2)} < E^{(1)}$, if $K(k) + n\nu(k) < 0$. Next, we consider the boundary region $N_k + N_{-k} = N$, which is equivalent to the analysis of the above-presented solution (0 + 2). We need to determine a minimum of the function $E^{(0+2)}(N_k)$ at $0 < N_k < N$ and to compare it with the boundary value $E^{(0+2)}(N_k = 0) = E^{(1)} + NK(k)$. The minimum corresponds to the relations $N_k = N_{-k} = N/2, \nu(2k) < 0$. At this point of the minimum,

$$E^{(0+2)} = E^{(1)} + N(K(2k) + n\nu(2k))/4. \quad (29)$$

This value is less than the energies $E^{(1)} + NK(k)$ and $E^{(1)}$, if $K(2k) + n\nu(2k) < 0$. Eventually, we study another boundary region of function (14): $N_{-k} = 0$. This is equivalent to the

\[\text{Fig. 1: [Color online] The functions } f_1(g) \text{ (dashed line) and } f_3(g) \text{ (solid line). The function } f_1(g) \text{ is multiplied by 1/4.} \]
Fig. 2: [Color online] Smallest values of the function $E^{(1+2)}(N_k, N_{-k}, k)/E^{(1)}$ at the given density $n$ in the 1D (squares) and 3D (circles) cases. They are found numerically from Eqs. (7), (14) and $N_0 = N - N_k - N_{-k}$ for the potentials (24), (25) and all possible values of $N_k, N_{-k}$, and $k$ ($0 < k < \infty$, $0 \leq N_k \leq N$, $0 \leq N_{-k} \leq N$ under the condition $N_k + N_{-k} \leq N$). The values of $n_c$ in the 1D and 3D cases are presented in the text. We also show smallest values of $E^{(1+1)}(N_k, k)/E^{(1)}$ for the given $n$ in the 1D (stars) and 3D (rhombus) cases, determined from Eq. (31). At $n/n_c \leq 1$ the smallest $E^{(1+2)}(N_k, N_{-k}, k)$ and $E^{(1+1)}(N_k, k)$ are equal to $E^{(1)}$.

The analysis of the solution $(1 + 1)$, obtained in [18] and above. The energy $E^{(1+1)}(N_k)$ has a minimum at

$$\frac{N_k}{N} = \frac{K(k) + n\nu(k)}{2n\nu(k)}$$

(30)

and $\nu(k) < 0$. This implies that the solution with $N_k > 0$ exists at $K(k) + n\nu(k) < 0$. At the minimum, we have

$$E^{(1+1)}(N_k) = E^{(1)} + N\left(\frac{K(k) + n\nu(k)}{2n\nu(k)}\right)^2$$

(31)

If $\nu(k) < 0$, we obtain $E^{(1+1)} < E^{(1)}$. On the edges $(N_k = 0; N)$ the energy is higher: $E^{(1+1)} = E^{(1)}; E^{(1)} + NK(k)$.

Thus, in all three cases, we obtain the condition $n > n_c$, where the critical density $n_c$ is the smallest positive density, for which the equality $K(k) + n\nu(k) = 0$ holds at some $k$. We found numerically that $n_c \approx 84.2C_{1D}/d_0, g_c \approx 4.0781$ in the 1D case, and $n_c \approx 1091.45C_{3D}/d_0^3, g_c \approx 5.4486$ in the 3D case. Here, $C_{1D} = \frac{\hbar^2}{4mU_0d_0^2}, C_{3D} = \frac{C_{1D}}{2\pi}$, and $g_c$ is the value of $g = kd_0$ for which the equality $K(k) + n\nu(k) = 0$ yields $n = n_c$.

We obtained numerically the smallest value of the energy $E^{(1+2)}(N_k, N_{-k}, k)$ (14) as a function of $N_k, N_{-k}, k$ at a fixed $N = N_0 + N_k + N_{-k}$ in the 3D and 1D cases, by using the potentials (24) and (25), respectively. The analysis shows that at $n \leq n_c$ the smallest $E^{(1+2)}(N_k, N_{-k}, k)$ corresponds to $N_k = N_{-k} = 0$. In this case, $N_0 = N, E^{(1+2)}(N_k, N_{-k}, k)$ coincides with $E^{(1)}$, and the fragmentation is absent. At $n > n_c$ the small-
est \( E^{(1+2)}(N_k, N_{-k}, k) \) is less than \( E^{(1)} \) and coincides with the energy \( E^{(0+2)} \) with \( k \approx k_c = \frac{3\hbar}{2d_0} \). This value of \( E^{(1+2)} \) is shown in Fig. 2.

Thus, at \( n > n_c \), it is energy-gained for the state (3), (6) with a single condensate to transit into the state \((0 + 2)\) (15), (16) with two condensates \((N_k = N_{-k} = N/2, N_0 = 0)\), condensate value of \( k \) depends weakly on \( n \) and is close to \( k_c / 2 \).

Note the following important point. In the above solutions we considered only a few \( k \)-harmonics in the operator \( \hat{\psi} \) and in the Hamiltonian. Of course, for the accurate description of the system all \( k \)-harmonics should be taken into account. Are the above obtained solutions \( E^{(1+2)} \) (14), \( E^{(0+2)} \) (18), and \( E^{(1+1)} \) (22) close to the exact ones involving all \( k \)-harmonics? We saw above that, at \( n < n_c \), the state (5) with one condensate is energy-gained. As an accurate generalization of solution (5)–(7), we indicate Bogoliubov’s solution [2]. Under a weak coupling, Bogoliubov ground-state energy \( E_0 \) is very close to \( E^{(1)} \) (7). In this case, function (5) is an eigenfunction of the corresponding “truncated” Hamiltonian (7). Therefore, we suppose that if the wave function of the system describes properly the structure of the condensate and is an eigenfunction of the corresponding truncated Hamiltonian, and if the coupling is weak or intermediate, then the corresponding “truncated” energy of the system is close to the exact eigenenergy. In particular, the functions (15) and (19) are eigenfunctions of the truncated Hamiltonians (17) and (21), respectively. No accurate generalization of solutions (15) and (19) has been found. We expect that, for a weak and intermediate couplings, energies (18) and (22) are close to the exact ones, which can be determined in an accurate approach like Bogoliubov one [2]. Note that the function (8) is not an eigenfunction of the Hamiltonian \( \hat{H}^{(1+2)} \) (12) due to the term \( \hat{H}_{\text{scat}} \).

### 2.3 Physical properties of solutions

For real systems, the average distance \( \bar{r} \) between atoms should be larger than the atomic size: \( \bar{r} \geq d_0 \). The strong overlapping of atoms \( (\bar{r} \ll d_0) \) is possible only at very high external pressures; this case is omitted here.

We now make estimates for the 1D case. Let us introduce the dimensionless Lieb-Liniger’s parameter \[ 36 \] \( \gamma = \frac{m\nu(0)}{\hbar^2 n} = \frac{1}{qC_{1D}^2 84.2} \), where \( q = n / n_c \). For \(^4\)He atoms, we have \( d_0 \approx 2 \) Å, then \( C_{1D} \approx \frac{K_{1,34}}{1.34d_0} \). The condition \( \bar{r} = 1 / n \geq d_0 \) yields the inequalities \( n = qn_c \leq 1 / d_0 \), \( C_{1D} \leq 1 / (q84.2) \), and \( \gamma \geq 42.1q \). Since \( q \geq 1 \), we get \( \gamma \approx 1 \) corresponding to the strong coupling regime. For such \( \gamma \), the solution for the ground-state energy is close to the solution for impenetrable bosons \( (\gamma = \infty) \) \( E_0^{(\infty)} = \frac{N}{6} (\pi\hbar n)^2 \) [37]. The relations \( \frac{E^{(0+2)}}{E_0^{(\infty)}} \approx \frac{E^{(1+1)}}{E_0^{(\infty)}} \approx \frac{E^{(1)}}{E_0^{(\infty)}} = \frac{1.5\gamma}{\pi^2 d_0 C_{1D}} \geq \frac{1.584.2q}{\pi^2 d_0} \geq 13 \) imply that the energies \( E^{(0+2)} \) (29) and \( E^{(1+1)} \) (31) are much larger than the ground-state energy of a system of point bosons with the same \( \nu(0) \). In other words, the above-considered states \((0 + 2)\) and \((1 + 1)\) with two condensates are highly excited states of the system. However, we are mainly interested in the structure of a condensate for the ground state.
In the 3D case, there are no exact solutions like [36, 37]. Therefore, the estimates give less information. From the above-presented formulae $C_{3D} = \frac{C_{1D}}{2\pi} \approx \frac{K_k\rho}{2\pi \cdot 1.34 U_0}$ and $n_c \approx 1091.45 C_{3D}/d_0^3$, we get the critical density and the critical average interatomic distance: $n_c \approx \frac{1}{d_0} \frac{130 K_k\rho U_0}{U_0}$, $\bar{r}_c \approx n_c^{-1/3} \approx \frac{d_0}{U_0} \left( \frac{U_0}{K_k \rho} \right)^{1/3}$. The value of $U_0$ is usually determined by means of fitting of a potential $U(r)$ to get the best description of several experimental properties of a substance. In addition, $U_0$ can be determined by means of the calculation of the potential by the known structural factor $S(k)$. For $^4$He atoms these methods give very different estimates: $U_0 \sim 10^6 K_k \rho$ [34, 35] and $U_0 \sim 10^3 K_k \rho$ [38, 39], respectively. From whence, we obtain $\bar{r}_c \approx 20d_0$ and $\bar{r}_c \approx 2d_0$. The requirement $n \geq n_c$ yields $\bar{r} \leq \bar{r}_c \approx (2 \div 20)d_0$. Such densities correspond to a fluid, a crystal or a dense gas. In this case, Bogoliubov’s criterion [2] is not satisfied. We note that the magnitude and the sign of the scattering length $a$ can be varied with the help of the Feshbach resonance [8].

For a periodic system, $k$ is quantized: $k = 2\pi \left( \frac{L_x}{L_x}, \frac{L_y}{L_y}, \frac{L_z}{L_z} \right)$. Let $k = 2\pi \left( \frac{L_x}{L_x}, \frac{L_y}{L_y}, \frac{L_z}{L_z} \right)$ for the solutions (16) and (20). Then there exists the smallest vector $s = \left( \frac{L_x}{L_x}, \frac{L_y}{L_y}, \frac{L_z}{L_z} \right)$, for which $\hat{\psi}(r+s,t) = \hat{\psi}(r,t)$ for any $r$ (the last equality holds for any of the components of the vector $s$ as well). We have obtained a one-dimensional crystal-like solution. Indeed, let us put the axis $x$ along $k$. Then formula (9) takes the form $\hat{\psi}(r,t) = V^{-1/2} (\hat{a}_0 + \hat{a}_ke^{ikx} + \hat{a}_{-k}e^{-ikx})$, and for the two-particle density matrix $F_2(r_1, r_2| r_1, r_2) = \text{const} |\psi^+(r_1, t)\hat{\psi}^+(r_2, t)\hat{\psi}(r_1, t)\hat{\psi}(r_2, t)|\Psi$ we get $F_2(r_1, r_2| r_1, r_2) = \text{const} [N_{-k}(N_{-k} - 1) + N_k(N_k - 1) + 2N_{-k}N_k(1 + \cos [2k(x_1 - x_2)]) + 2N_0(N_{-k} + N_k)(1 + \cos [k(x_1 - x_2)]) + N_0(N_0 - 1)]$. This function has two periods and depends only on the coordinates $x_1, x_2$. By setting $N_0 = 0$ or $N_{-k} = 0$ in this formula, we obtain $F_2(r_1, r_2| r_1, r_2)$ for solutions (16) or (20), respectively. These are 1D solutions with one period. The 1D and 2D systems can be considered similarly. If the ground state of a natural crystal does contain a condensate, its structure is seen from the formula $\hat{\psi}(r+s, t) = \hat{\psi}(r,t)$ and the corresponding expansion of the operator $\hat{\psi}(r,t)$ in basis functions. We may expect that, for periodic boundary conditions (BCs), the principal harmonic of the condensate is characterized by the wave vector $k = 2\pi \left( \frac{1}{s_x}, \frac{1}{s_y}, \frac{1}{s_z} \right)$.

Interestingly, our crystal-like solution corresponds to a constant density. Moreover, it is easy to show that any pure stationary state of a periodic system of spinless particles is characterized by a constant density. Indeed, let $\hat{\psi}(r,t) = V^{-1/2} \sum_k \hat{a}_ke^{ikr}$. Then

$$n(r) = \langle \hat{\psi}^+(r,t)\hat{\psi}(r,t) \rangle = V^{-1} \sum_k \langle \hat{a}_k^+ \hat{a}_k \rangle = V^{-1} \sum_k N_k = N/V. \quad (32)$$

In this case, the crystalline properties should be manifested in the two-particle density matrix $F_2(r_1, r_2| r_1, r_2)$ and in the structural factor $S(k)$.

Can we observe the fragmented condensate experimentally? We showed above that the fragmented condensate in the 1D case corresponds to a highly excited state and, therefore, can hardly be produced. In the 3D case, the periodic BCs are not possible. For zero BCs, the basis functions are sines. Therefore, the degeneracy $e^{ikr} \leftrightarrow e^{-ikr}$ is removed, and the condensate...
Fig. 3: [Color online] Values of $N_k/N$ corresponding to the smallest value of $E^{(1+1)}/E^{(1)}$ at the given density $n$. The solutions for the 1D and 3D cases are presented (they coincide for each $n$, in the limits of errors). The smallest value of $E^{(1+1)}/E^{(1)}$ is determined numerically by means of the comparison of the values of $E^{(1+1)}(N_k, k)/E^{(1)}$, obtained from Eq. (31), for different $k$.

$(0 + 2)$ should be replaced by a single (nonfragmented) condensate $(0 + 1)$. However, the two-condensate state $(1 + 1)$ should conserve its structure under zero BCs as well. If such state is sufficiently close to the ground one, it should be observable. Unfortunately, we do not know whether this state, with regard for the necessary corrections considered in the following sections, is close to the ground one. But our above estimates do not forbid the latter. In Figs. 2 and 3 we present the smallest value (31) of the function $E^{(1+1)}(N_k, k)$ and the corresponding $N_k/N$ (30) for the given density (at $n = n_c$ the smallest $E^{(1+1)}(N_k, k)$ corresponds to $g = g_c$; the value of $g$ increases insignificantly with $n$; here, $g = kd_0$). At large $n$ the quantity $N_k$ approaches the asymptotic value $N_k = N/2$. Apparently, our conclusions are qualitatively valid also for the atoms in a harmonic trap.

We note that the crystal-like solutions were previously obtained numerically for the ground state of a 1D system of dipolar bosons [40, 41, 42, 43, 44, 45]. The crystallization occurs at the densities exceeding some critical value. In this case, the field of a trap was considered [43, 45] or was not [40, 41, 42, 44]. Note the interesting comparison of the solutions for point and dipolar interatomic interactions which was executed in [46] for strong coupling. The main difference of the solutions in [40, 41, 42, 43, 44, 45, 46] from the above-obtained ones consists in that our solution contains a condensate. The ground state in works [42, 43, 45], where the occupation numbers were calculated, does not contain a condensate. This difference is probably related to the circumstance that our 1D solutions correspond to highly excited states, whereas the authors of works [40, 41, 42, 43, 44, 45] ascribed the solutions to the ground state. According to the theorem of nodes, if the wave function of the ground state
has no nodes and corresponds to a crystal \[40, 41, 42, 43, 44, 45\], then a highly excited state with a lot of nodes and a similar crystal structure must exist. Our 1D solutions should correspond to it.

The Pollock-Nozieres’ results \[18, 19\] are important. However, the above analysis shows that, for a high-density uniform periodic system, Pollock-Noziéres’ argument does not work: the fragmentation of a condensate in such system is possible.

3 Periodic Bose system: collective description

In Section 2 we described a system of \(N\) interacting bosons with the quasi-single-particle (Hartree–Fock) wave functions of the form

\[\Psi_{\{n_k\}} = \text{const} (\hat{a}_{k_1}^+)^{n_{k_1}} (\hat{a}_{k_2}^+)^{n_{k_2}} \cdots |\text{vac}\rangle, \tag{33}\]

where \(n_{k_1} + n_{k_2} + \ldots = N\) and \(\{n_k\} \equiv (n_{k_1}, n_{k_2}, \ldots)\). The key point consists in that such wave functions are not eigenfunctions of the exact Hamiltonian (3). Therefore, the energies obtained in Sect. 2 are not eigenenergies. Indeed, Hamiltonian (3) can be written in the form

\[
\hat{H} = \sum_q K(q) \hat{a}_q^+ \hat{a}_q + \sum_{k_{q_1}, q_2} \nu(k) \frac{\nu(0)}{2V} \hat{a}_{k+q_1}^+ \hat{a}_{-k+q_2}^+ \hat{a}_{q_1} \hat{a}_{q_2} \\
= \sum_q K(q) \hat{N}_q + \sum_q \frac{\nu(0)}{2V} \hat{N}_q (\hat{N}_q - 1) + \sum_{k \neq 0} \frac{\nu(k)}{2V} \hat{N}_{k+q} \hat{N}_q \\
+ \sum_{q_1, q_2 \neq q} \frac{\nu(0)}{2V} \hat{N}_{q_1} \hat{N}_{q_2} + \sum_{k \neq 0, q_1, q_2 \neq q} \frac{\nu(k)}{2V} \hat{a}_{k+q_1}^+ \hat{a}_{q_1} \hat{a}_{q_2}^+ \hat{a}_{k+q_2}. \tag{34}\]

First four terms on the right-hand side of (34) do not change function (33). But the last term transfers this function into a superposition of the infinite number of various terms of the form (33). It means that the quasi-single-particle approach allows one to approximately study the possibility of the fragmentation of the condensate, but it does not allow one to find the ground state of the system. We need a more subtle method allowing one to determine the eigenfunctions and eigenenergies of the Hamiltonian.

In this section, we propose such method and consider one example of a solution with fragmented condensate.

The above analysis shows that a part of atoms must be outside the condensates. Therefore, one needs to consider the harmonics \(\hat{a}_k\) with all possible \(k\) in the operator \(\hat{\psi}(r, t)\) and the Hamiltonian \(\hat{H}\) (3), (34). However, in the crude approximation it is allowable to consider that all atoms of the system are in one or several condensates. In this case, the wave functions should be eigenfunctions of the truncated Hamiltonian written in the corresponding approximation for \(\hat{\psi}(r, t)\). To obtain such functions, we use the Landau idea \[47\] according to which the weakly excited states of a system of many interacting particles can be described.
in the language of noninteracting quasiparticles. This means that the exact Hamiltonian \[31\), \(33\] must be reduced to the diagonal form

\[ \hat{H} = E_0 + \sum_k E(k) \hat{c}_k^+ \hat{c}_k. \] (35)

In this case, the eigenfunctions of the Hamiltonian take the form

\[ \Psi_{\{n_k\}} = C(\hat{c}_{k_1}^+)^{n_{k_1}} \ldots (\hat{c}_{k_p}^+)^{n_{k_p}} \Psi_0. \] (36)

Here, \( \Psi_0 \) is the wave function for the state without quasiparticles, \( \hat{c}_k^+ \) and \( \hat{c}_k \) are the operators of creation and annihilation of a quasiparticle, and \( n_{k_j} \) is the number of quasiparticles with quantum number \( k_j \). It is clear that \( \hat{H} \Psi_{\{n_k\}} = E_{\{n_k\}} \Psi_{\{n_k\}} \), where \( E_{\{n_k\}} = E_0 + \sum_k n_k E(k) \). Such method allows one to find the operator structure of eigenfunctions and the eigenenergies \( E_{\{n_k\}} \) for lowest levels accurately.

The analysis below is carried on in such a way that the wave functions are eigenfunctions of the Hamiltonian. For a Bose gas under periodic BCs, we now compare two states: (i) the state, in which each of \( N \) atoms has the zero momentum, and (ii) the state, in which \( N_0 + N_k + N_{-k} = N \). For the state (i) we have the wave function \( \Psi = C_1(\hat{a}_0^+)^N |\text{vac}\rangle \), which is an eigenfunction of the Hamiltonian \( \hat{H}^{(1)} \) with the eigenenergy \( E^{(1)} \). For the state (ii) let \( \hat{\psi}(r, t) = V^{-1/2}(\hat{a}_0 + \hat{a}_k e^{i k r} + \hat{a}_{-k} e^{-i k r}) \) and \( N_k, N_{-k} \approx N \) (the latter condition is necessary for the diagonalization of the Hamiltonian). The numbers \( N_k \) and \( N_{-k} \) can be macroscopic or microscopic. The solution for the Hamiltonian is given by formula \(12\), where we neglect the term \( \sim \hat{N}_k \hat{N}_{-k} \). We also make replacements \( \hat{a}_{\pm k} \rightarrow e^{-i \omega t/h} \hat{b}_{\pm k} \), \( \hat{a}_0 \rightarrow e^{-i \omega t/h} \hat{b}_0 \). In the approximation \( \hat{N}_k, \hat{N}_{-k} \ll \hat{N} \) we have \( \hat{N}_0 = N_0, \hat{N} \approx N \). Then relation \(12\) leads to the Bogoliubov formulae \[2\]:

\[ \hat{H}^{(1+2)} \approx \frac{N_0 n_0 \nu(0)}{2} + [K(k) + n_0 \nu(k) + n_0 \nu(0)] \hat{b}_k^+ \hat{b}_k + [K(-k) - n_0 \nu(-k) + n_0 \nu(0)] \hat{b}_{-k}^+ \hat{b}_{-k} \]

\[ + \frac{b_0^2}{2V} [\nu(k) \hat{b}_k^+ \hat{b}_{-k} + \nu(-k) \hat{b}_{-k}^+ \hat{b}_k] + \frac{(b_0^2)^2}{2V^2} [\nu(k) \hat{b}_k \hat{b}_{-k} + \nu(-k) \hat{b}_{-k} \hat{b}_k] \] (37)

where \( E(k) = \sqrt{K^2(k) + 2 n_0 \nu(k) K(k)} \) \[2\]. Using the eigenfunctions \(36\), we now find the ground-state energy in the quasiparticle representation \[2,48,49\] as the statistical average \( \langle \hat{H}^{(1+2)} \rangle \) over the state without quasiparticles:

\[ E_{0}^{(1+2)} = E_{0}^{(1)} - A(k), \] (38)

\[ A(k) = \frac{(N - N_0)(n - n_0) \nu(0)}{2} + K(k) + n_0 \nu(k) - E(k) \approx K(k) + n_0 \nu(k) - E(k), \] (39)

where \( E_{0}^{(1)} = \frac{N_0 \nu(0)}{2} \) is the energy of the system, in which all atoms are in the condensate \( \psi(r, t) = V^{-1/2} a_0 \). In the calculation of \( \langle \hat{H}^{(1+2)} \rangle \), we considered \( N \) to be fixed and used
the Gibbs canonical distribution. For $K(k) + n_0\nu(k) > |n_0\nu(k)|$ we have $A(k) > 0$ and $E_0^{(1+2)} < E_0^{(1)}$. Therefore, the *fragmented condensate is possible.*

These solutions imply that, at $K(k) + n_0\nu(k) > |n_0\nu(k)|$, the condensate should be fragmented, and the numbers $N_k$, $N_{-k}$ can be macroscopic. However, more accurate analysis requires the consideration of all $k$-harmonics. In this case, the Hamiltonian $\hat{H}^{(1+2)}$ transits in the known Bogoliubov Hamiltonian [2]. Bogoliubov formulae for the equilibrium occupation numbers $N_k = \langle \hat{a}_k^+\hat{a}_k \rangle$ and $N_{-k} = \langle \hat{a}_{-k}^+\hat{a}_{-k} \rangle$ imply that the numbers $N_k$ and $N_{-k}$ can be macroscopic only for a 1D system, see also [32].

Moreover, the Bogoliubov energy $E_0$ of the ground state satisfies the inequality $E_0 < E_0^{(1)}$. Therefore, we conclude that it is energetically favorable for a weakly interacting Bose system with fixed $N$ that a part of atoms has a nonzero momentum.

Next, in Sect. 2 we noted that $\nu(k)$ can be negative. Despite this, the Bogoliubov solution satisfies the inequality $K(k) + n_0\nu(k) > |n_0\nu(k)|$ for all $k$, because the Bogoliubov model works at small $|n_0\nu(0)|$ [2], and since $|\nu(k)| \leq |\nu(0)|$ for any realistic potential. Since $n_0 \approx n$, and since $|\nu(k)|$ is not small for $k \lesssim 1/d_0$ (where $d_0$ is the size of an atom), the smallness of the quantity $|n_0\nu(k)|$ means the smallness of $n$. Thus, the analysis in Sect. 3 is applicable only to systems with low density. Such analysis cannot verify the validity of the solutions with fragmentation from Sect. 2, since these solutions correspond to a high density ($n > n_c$), which breaks the Bogoliubov criterion [2].

To verify the validity of the crystal-like solutions with fragmented condensate, which are obtained in Sect. 2, it is necessary to diagonalize the Hamiltonian for a condensate of corresponding structure, by considering all $k$-harmonics and preserving the terms $\sim \hat{N}_k\hat{N}_{-k}$. Since the functions (15) and (19) are eigenfunctions of the corresponding truncated Hamiltonians, it is quite probable that the exact condition of fragmentation is close to the condition $K(k) + n\nu(k) < 0$ obtained in Sect. 2.

Furthermore, it follows from the formula

$$\hat{\psi}(\mathbf{r}, t) = V^{-1/2}e^{-i\omega t/h}(\hat{b}_0 + \hat{b}_ke^{ikr} + \hat{b}_{-k}e^{-ikr})$$

(40)

that the system is uniform:

$$n(\mathbf{r}) = \langle \hat{\psi}^+(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t) \rangle = \langle \hat{b}_0^+\hat{b}_0 + \hat{b}_k^+\hat{b}_k + \hat{b}_{-k}^+\hat{b}_{-k} + \hat{b}_ke^{2i\omega r} + \hat{b}_{-k}e^{-2i\omega r} \rangle / V = N/V.$$  

Here, we used the Bogoliubov transformations, which yield $\langle \hat{b}_k^+\hat{b}_k \rangle = 0$.

The Bogoliubov method [2, 48] allows one to describe the weakly excited states of an equilibrium Bose system. Note that the method works for sufficiently large $N$: $N \gtrsim N_{cr}$. For a 1D system, the Bogoliubov solutions [2, 49] agree with the exact ones [36, 50, 51, 52, 53] at $N \gtrsim 100$ under periodic BCs and at $N \gtrsim 1000$ under zero BCs. Therefore, $N_{cr} \approx 100$ for periodic BCs, and $N_{cr} \approx 1000$ for the zero ones.

We note that, for real gases in a trap, it is necessary to consider quasiparticles and the variability of the number of particles. In this case, one needs to average over the grand
canonical ensemble [54].

We mention the work by Nozières and Saint James [15], where a pair condensation and a fragmentation of the condensate were studied within the variation method considering the finite size of particles and the anomalous averages. This method differs significantly from our one. In this case, a solution with a fragmented condensate was not found in [15].

We also mention the interesting work by Streltsov [26], in which it was shown that the ground state of a 1D Bose gas is fragmented, if the repulsive interatomic interaction is strong and the interaction radius is comparable with the system size. Our analysis in Sect. 3 is valid only at weak coupling. But the solutions in Sect. 2 are applicable in the case of strong coupling and hint that the fragmentation found in [26] is related to the nonpointness of atoms.

Thus, in this section we have studied the solution (1 + 2) (12)–(14) from Sect. 2 within a more accurate approach. We have required additionally that $N_k, N_{-k} \neq 0$ and $N_k, N_{-k} \ll N$, which prohibits solutions (0 + 2) and (1 + 1) from Sect. 2. With the account for all k-harmonics, our analysis yields the Bogoliubov Hamiltonian. Therefore, it is necessary to use Bogoliubov’s criterion for the density [2], which gives $n \ll n_c$. Under such condition, the inequality $A(k) > 0$ holds, and the fragmentation into three condensates $(0, k, -k)$ is energy-gained. However, according to Sect. 2, a one-condensate solution is energy-gained at $n \ll n_c$. In the analysis in Sect. 3, the fragmentation is energy-gained at $n \ll n_c$ due to the “anomalous” averages $\langle \hat{b}_k^+ \hat{b}_{-k}^+ \rangle$, $\langle \hat{b}_k \hat{b}_{-k} \rangle$. In Sect. 2, instead of the averages $\langle \hat{b}_k^+ \hat{b}_{-k}^+ \rangle$, $\langle \hat{b}_k \hat{b}_{-k} \rangle$ we considered the normal quantum-mechanical average $\langle \hat{H}_{\text{scat}} \rangle$, which is zero in the quasi-single-particle representation. Because of this, the possibility of a fragmentation for small $n$ was lost in Sect. 2. If we consider all k-harmonics in Sect. 2, the anomalous averages will not appear nevertheless, since they arise only within the collective approach. Therefore, the collective approach is basically more accurate than the quasi-one-particle one.

According to the analysis in Sect. 3, the fragmentation of the condensate is possible in a 1D Bose gas at $T = 0$ and a weak coupling. We have found no fragmentation in 2D and 3D Bose gases (here, the conclusion by Pollock and Nozières is proper). Interestingly, the condition of fragmentation $K(k) + n\nu(k) < 0$ (see Sect. 2) obtained in the quasi-single-particle approach is opposite to the condition $K(k) + n_0\nu(k) > |n_0\nu(k)|$ following from the collective approach (Sect. 3). The nonpointness of atoms favors the fragmentation in the first case and counteracts in the second one. We note that the condition $K(k) + n_0\nu(k) > |n_0\nu(k)|$ was obtained for the ground state and the weak coupling, whereas the condition $K(k) + n\nu(k) < 0$ is true in the case of strong coupling and non-ground state.

4 One-dimensional Bose gas under zero boundary conditions

In Sections 2 and 3 we have found the solutions containing only three k-harmonics. Below, we will determine the structure of the condensate in the collective approach involving all k-harmonics. We use zero BCs: $\hat{\psi}(x, t) = 0$ at $x = 0, L$. A similar problem was solved nu-
merically in the case of strong coupling at $T = 0$, $N \lesssim 100$ [26]. We will consider analytically a system with weak coupling, $T \geq 0$, and $N \gtrsim 1000$. Previously, with the help of the Bogoliubov method we constructed the description of weakly excited states of a Bose gas under zero BCs and found the density matrix $F_1(x, x')$ [49]. We emphasize that the Bogoliubov method describes well a finite 1D system at a weak coupling and $T \to 0$. This follows from the facts that the criterion of applicability of the method is satisfied [49], the solutions for $E_0$ and $E(k)$ coincide with the solutions in the exactly solvable approach based on the Bethe ansatz [36, 50, 51, 52, 53], and the solution for $F_1(x, x')|_{T=0}$ is close to the solution for a periodic system, obtained by different methods (see references in [49]). The solution for the density matrix of a 1D Bose gas under zero BCs reads [49]:

$$F_1(x, x') = \bar{F}_1(x, x') + \sum_{l=1,2,\ldots,\infty} \chi_l \varphi_2^*(x') \varphi_2(x),$$

$$\bar{F}_1(x, x') = f_0^*(x') f_0(x) + \frac{2}{L} \sum_{j=1,2,\ldots} \chi_{2j-1} \sin (k_{2j-1} x') \sin (k_{2j-1} x),$$

$$\chi_j = \frac{1}{\sqrt{y_j^4 + 4 y_j^2}} \left( \frac{2}{\sqrt{y_j^4 + 4 y_j^2 + y_j^2 + 2}} + \frac{y_j^2 + 2}{e^{y_j^2 + 4 y_j^2 - 1}} \right),$$

$$f_0(x) = \frac{4 \sqrt{n_0}}{\pi} \sum_{j=1,2,\ldots,\infty} \frac{\sin (k_{2j-1} x)}{2j-1} \frac{4}{y_{2j-1}^2 + 4},$$

where $L$ is the size of the system, $k_j = \frac{\pi j}{L}$, $\varphi_2(x) = \sqrt{\frac{2}{L}} \cdot \sin (k_j x)$, $y_j = \frac{j}{\sqrt{\Gamma}}$, $\Gamma = \frac{n N N_0}{n_0}$, $\tilde{T} = \frac{k_B T}{n_0}$, and $n_0 = \frac{N_0}{L}$. The solution is written for the point interatomic interaction $[U(|x_j - x_l|) = 2 c \delta(x_j - x_l), \gamma = \frac{2 m c}{R_n}, n = \frac{N}{L}]$ and is valid for $0 < \gamma \ll 1$, $\Gamma \gg 1$, $N_0 \approx N \gtrsim 10^3$.

The point approximation is justified for the description of states with $k_j \ll \pi / r_0$, since the transition to a potential with nonzero radius $r_0$ changes such solutions slightly.

It is seen from (41) and (42) that the expansion of the function $\bar{F}_1(x, x')$ is nondiagonal, but the sum $\sum_l \chi_l \varphi_2^*(x') \varphi_2(x)$ has a diagonal form. In this case, $\bar{F}_1(x, x')$ is orthogonal (in each of the arguments $x$ and $x'$) to any term of the sum $\sum_l \chi_l \varphi_2^*(x') \varphi_2(x)$, and the functions $\varphi_2(x)$ are orthonormalized. Therefore, it is clear that $\sum_l \chi_l \varphi_2^*(x') \varphi_2(x)$ is the sum $\sum_l \lambda_l \varphi_2^*(x') \varphi_2(x)$ from the diagonal expansion (41). To represent the function $F_1(x, x')$ in the form (41), we need to find a diagonal expansion

$$\bar{F}_1(x, x') = \sum_{j=1,2,\ldots,\infty} \lambda_{2j-1} \varphi_{2j-1}^*(x') \varphi_{2j-1}(x).$$

It is convenient to pass from (45) to the equivalent system of equations

$$\int_0^L dx' \varphi_{2j-1}^*(x') \tilde{F}_1(x, x') = \lambda_{2j-1} \varphi_{2j-1}(x), \quad j = 1, 2, \ldots, \infty.$$
We seek the functions $\varphi_{2j-1}(x)$ in the form

$$
\varphi_{2j-1}(x) = \sum_{l=1,2,\ldots,\infty} A_{2l-1}^{(2j-1)} \sqrt{\frac{2}{L}} \sin (k_{2l-1} x),
$$

which ensures the orthogonality of $\varphi_{2j-1}(x)$ to the functions $\varphi_2(x)$. Let us substitute (47) in (46) and take formulae (42), (44) into account. We obtain the system of equations

$$
\sum_{l=1,2,\ldots,\infty} A_{2l-1}^{(2j-1)} (\chi_{2l-1} - \lambda_{2j-1}) \sin (k_{2l-1} x) + \frac{8N_0}{\pi^2} \sum_{p,l=1,2,\ldots,\infty} \frac{A_{2p-1}^{(2j-1)} \sin (k_{2p-1} x)}{2p-1} \frac{4}{2l-1} \frac{4 + y_{2p-1}^2}{4 + y_{2l-1}^2} = 0,
$$

where $j = 1, 2, \ldots, \infty$. By equating the coefficients of the functions $\sin (k_{2l-1} x)$ to zero, we get

$$
A_{2l-1}^{(2j-1)} = -\frac{8N_0}{\pi^2} \frac{1}{2l-1} \frac{4}{4 + y_{2l-1}^2} \frac{S_{2j-1}}{\chi_{2l-1} - \lambda_{2j-1}}, \quad j, l = 1, 2, \ldots, \infty,
$$

$$
S_{2j-1} = \sum_{l=1,2,\ldots,\infty} \frac{A_{2l-1}^{(2j-1)}}{2l-1} \frac{4}{4 + y_{2l-1}^2}.
$$

Substituting $A_{2l-1}^{(2j-1)}$ in (50), we obtain the secular equation for the numbers $\lambda_{2j-1}$:

$$
1 + \sum_{l=1,2,\ldots,\infty} \frac{f_{2l-1}}{\chi_{2l-1} - \lambda_{2j-1}} = 0, \quad f_{2l-1} = \frac{8N_0}{\pi^2} \frac{1}{(2l-1)^2} \frac{4}{(4 + y_{2l-1}^2)^2}.
$$

It is easy to show analytically that $\lambda_1 \approx N_0$ (for $\gamma \ll 1$) and $\lambda_{2j-1} \approx |\chi_{2j-1}, \chi_{2j-3}|$ for $j \geq 2$.

We note that, for the interacting system, the genuine condensate is determined by the diagonal expansion (1), where the number $\lambda_j/N$ is the probability of the location of an atom in the single-particle state $\phi_j(r)$. The average $\langle \hat{\psi}(x,t) \rangle$ is also often called a condensate. Usually, $\langle \hat{\psi}(x,t) \rangle$ coincides with the condensate determined with the help of (1). But such a coincidence is not always the case (see below). Therefore, we will call the quantity $\langle \hat{\psi}(x,t) \rangle$ the effective condensate.

The density matrix $F_1(x, x + x')$ (41) at $T = 0$ decreases, as $|x'|$ increases, by a power law $|x'|^{-s}$ with $s = \sqrt{7}/2\pi$ [49]. In this case, it is accepted to talk about a quasicondensate instead of a condensate (fragmented or not). The Bogoliubov method works at $|s| \ll 1$.

Therefore, for a finite system, $F_1(x, x + x') \approx const$ for all points $x'$ not too close to boundaries (see details in [49]). In this case, the quasicondensate can be considered as a true condensate. For the infinite system, $F_1(x, x + x')|_{x' \to \infty} = const \cdot |x'|^{-s} \to 0$ even for very small nonzero $|s|$. We arrive at Hohenberg’s conclusion that the condensate is absent [55]. Thus, the true condensate can exist in a $1D$ Bose system, if this system is finite.

### 4.1 The case of $T = 0$

We now present the solutions $\lambda_j$ for $\Gamma = 10^7$, $N = 10^5$, see Table 1. We have checked this solution. It satisfies the normalization $\lambda_1 + \lambda_2 + \ldots + \lambda_{50001} = 0.999N$, and the functions...
are orthogonal to each other. Since \( F_1(x, x') = F_1^*(x', x) \), the eigenvalues \( \lambda_l \) in (1) are real, and the collection \( \{ \lambda_l \} \) is unique \[56\]. In addition, if all \( \lambda_l \) are different, the natural basis \( \{ \phi_l(x) \} \) is unique \[56\]. In our case, all \( \lambda_l \) are different. Therefore, the above solution is unique. Note that the functions \( \varphi_{2j+1}(x) \) are roughly close to \( -\sqrt{2/L} \cdot \cos k_{2j} x \).

At different \( \Gamma, N \), we have \( \lambda_{2j+1} < \lambda_{2j} \) provided that \( j \geq 1 \). Thus, we have found the diagonal expansion (1).

The above solution has two significant properties. (I) The quasicondensate can be fragmented. Indeed, for a finite system we may consider the state \( \varphi_j(x) \) to be macroscopically occupied at \( \lambda_j \gtrsim N/\Theta \). Here, the choice of the value of \( \Theta \) is somewhat arbitrary. Whether \( \lambda_j = 0.03N \) is macroscopic? Probably not if \( N \lesssim 100 \). Probably yes if \( N \gtrsim 10^4 \). In our opinion, it is reasonable to set \( \Theta = (\ln N)^2 \). According to such criterion, states 2 and 3 from the above solution (for \( \tilde{T} = 0, \Gamma = 10^7, N = 10^5 \)) are occupied macroscopically. (II) The structure of a fragmented quasicondensate depends on the boundaries. Indeed, it is easy to obtain from the Bogoliubov formulae \[2\] that, for a periodic system,

\[
F_1(x, x') = \sum_{j=1,2,\ldots} \chi_{-2j} \phi_{-2j}^p(x') \phi_{-2j}^p(x) + N_0 \phi_{0}^p(x') \phi_{0}^p(x) \\
+ \sum_{j=1,2,\ldots} \chi_{2j} \phi_{2j}^p(x') \phi_{2j}^p(x),
\]

where \( \phi_{2j}^p(x) = e^{ik_{2j} x} / \sqrt{L} \), and \( \chi_{-2j} = \chi_{2j} \) is set by formula \[13\]. We remark that for a periodic system \( F_1(x, x') = F_1(x - x') \), and the Fourier transform of the function \( F_1(x - x') \) coincides with \( \chi_{2j} \phi_{2j}^p(x') \phi_{2j}^p(x) \).

The solution \( F_1(x, x') \) obtained above under zero BCs can be written in a similar way:

\[
F_1(x, x') = \sum_{j=1,2,\ldots} \lambda_{2j+1} \phi_{2j+1}^*(x') \phi_{2j+1}(x) + \lambda_1 \phi_1^*(x') \phi_1(x) \\
+ \sum_{j=1,2,\ldots} \lambda_{2j} \phi_{2j}^*(x') \phi_{2j}(x).
\]

Here, \( \lambda_1 \approx N \) and \( \lambda_{2j} = \chi_{2j} \neq \lambda_{2j+1} \). Thus, under periodic BCs we have \( \lambda_{-2j} = \lambda_{2j} \). However, under zero BCs the analogous symmetry is absent: \( \lambda_{2j+1} \neq \lambda_{2j} \). The difference between \( \lambda_{2j+1} \) and \( \lambda_{2j} \) is essential for small \( j \) and decreases, as \( j \) increases. The property \( \lambda_{-2j} = \lambda_{2j} \) is related to the cyclic symmetry of the system. The boundaries break this symmetry; therefore, the equality \( \lambda_{2j+1} = \lambda_{2j} \) is also violated. Thus, a change in the numbers \( \lambda_j \) at the transition from periodic BCs to the zero ones is related to a change in the topology of the system.

For the system under zero BCs we now clarify the conditions, under which the quasicondensate is fragmented. At small \( l \) we have \( \lambda_{2l} = \chi_{2l} \approx \frac{1}{2\delta_{2l}} = \frac{\sqrt{7}}{4} \approx \frac{N_0}{4\pi l} \) (here, we have used that \( N_0 \approx N \) at the weak coupling \[49\]). In this case, \( \lambda_{2l+1} = \lambda_{2l} - |\delta_{2l}| \), where \( \delta_{2l} \) is small. The criterion \( \lambda_{2l} \gtrsim \frac{N}{(\ln N)^2} \) requires \( \sqrt{7} \gtrsim \frac{4\pi l}{(\ln N)^2} \). These formulae imply that the states \( 2, 3, 4, \ldots, 2l + 1 \) are macroscopically occupied, if

\[
\sqrt{7} \gtrsim \frac{4\pi l}{(\ln N)^2}.
\]
Table 1: Natural occupations $\lambda_j$ for different $\Gamma$, $N$, and $\bar{T} = \frac{k_B T}{\epsilon_{n0}}$. We determined the values of $q_0$, $q_T$, $\tilde{N}_0$, $N_0$, and $\gamma$ from the formula $\Gamma = \frac{2N_0 N}{\pi^2}$ and Eqs. (78)–(83) in work [49]. Here, $\tilde{N}_0$ is the number of atoms in the effective condensate $\langle \hat{\psi}(x,t) \rangle$, and $N_0$, $q_0$, $q_T$ are auxiliary numbers [49]. The numbers $\lambda_{2j+1}$ were obtained by solving Eq. (51) numerically. For the “even” harmonics we have $\lambda_{2l} = \chi_{2l}$ [43].

| $T$    | 0    | 0.0005 | 0.001 | 0    | 0    | 0.01  | 0.02  |
|--------|------|--------|-------|------|------|-------|-------|
| $\Gamma$ | $10^7$ | $10^7$ | $10^7$ | $10^6$ | $10^6$ | $10^6$ | $10^6$ |
| $N$    | $10^5$ | $10^5$ | $10^5$ | $3.5 \cdot 10^4$ | $10^5$ | $10^5$ | $10^5$ |
| $q_0$  | 0.995492 | 0.995492 | 0.99479 | 0.99479 | 0.99479 | 0.99479 | 0.99479 |
| $q_T$  | 0.34422 | 0.550123 | 0.791791 | 0.876522 | 0.99479 | 0.99479 | 0.99479 |
| $\tilde{N}_0/N$ | 0.87315 | 0.859037 | 0.82804 | 0.90183 | 0.965641 | 0.900714 | 0.821891 |
| $N_0/N$ | 0.87328 | 0.859166 | 0.828165 | 0.90226 | 0.966102 | 0.901145 | 0.822284 |
| $\gamma$ | 0.011302 | 0.011487 | 0.00893 | 0.001022 | 0.001095 | 0.0012  | 0.0012  |
| $\lambda_1/N$ | 0.886652 | 0.882725 | 0.871153 | 0.91402 | 0.969903 | 0.942379 | 0.905786 |
| $\lambda_2/N$ | 0.0079  | 0.009269 | 0.014119 | 0.00713 | 0.002495 | 0.012661 | 0.025078 |
| $\lambda_3/N$ | 0.0066  | 0.008741 | 0.013613 | 0.00596 | 0.00209 | 0.01231 | 0.023645 |
| $\lambda_4/N$ | 0.00395 | 0.003998 | 0.004632 | 0.00356 | 0.001245 | 0.003285 | 0.006328 |
| $\lambda_5/N$ | 0.00354 | 0.003752 | 0.0045  | 0.00318 | 0.001155 | 0.003256 | 0.006228 |
| $\lambda_6/N$ | 0.00263 | 0.002633 | 0.002751 | 0.00237 | 0.000828 | 0.001547 | 0.002856 |
| $\lambda_7/N$ | 0.00242 | 0.002487 | 0.002666 | 0.00218 | 0.000764 | 0.001537 | 0.002833 |
| $\lambda_8/N$ | 0.00197 | 0.001972 | 0.001967 | 0.00177 | 0.00062 | 0.000936 | 0.00164 |
| $\lambda_9/N$ | 0.00185 | 0.001877 | 0.001935 | 0.00166 | 0.000581 | 0.00093 | 0.001632 |
| $\lambda_{10}/N$ | 0.00158 | 0.001576 | 0.001582 | 0.00141 | 0.000469 | 0.000647 | 0.001073 |
| $\lambda_{11}/N$ | 0.00149 | 0.00151 | 0.001535 | 0.00134 | 0.000469 | 0.000647 | 0.001073 |
| $\lambda_{50}/N$ | 0.000311 | 0.000311 | 0.000311 | 0.000095 | 0.000095 | 0.000096 |
| $\lambda_{51}/N$ | 0.000295 | 0.000307 | 0.000308 | 0.00009 | 0.000094 | 0.000095 |
| $\lambda_{100}/N$ | 0.000153 | 0.000153 | 0.000153 | 0.000045 | 0.000045 | 0.000045 |
| $\lambda_{101}/N$ | 0.000149 | 0.000148 | 0.000152 | 0.000044 | 0.000045 | 0.000045 |
On the other hand, the criterion of applicability of the Bogoliubov method, $N - \tilde{N}_0 \lesssim 0.1N$, and the formulae $N_0 \approx \tilde{N}_0$, $1 - \frac{\tilde{N}_0}{N} \approx \frac{\sqrt{T}}{4N} \ln \Gamma$ \cite{49} yield the inequality

$$\sqrt{\gamma} \lesssim \frac{0.4\pi}{\ln (\gamma^2N^2/\pi^2)}.$$  \hspace{1cm} (55)

Inequalities (54) and (55) are compatible only for definite values of $\gamma$ and $N$. In particular, for $N \lesssim 10^3$ inequalities (54) and (55) are not compatible. For $N = 10^4$ they are compatible, if $\gamma \approx 0.015$, $l = 1$ (in this case, the states 1, 2, 3 are macroscopically occupied). For $N = 10^5$ we find $\gamma \approx 0.01$, $l = 1$ and for $\gamma \approx 2 \cdot 10^{-3}$, $l = 2$ (in the last case, the states 1, 2, 3, 4, 5 are macroscopically filled). We do not consider the values $N > 10^{10}$, since they are not experimentally realizable.

The diagonal representation (52) for a periodic 1D Bose system at $T = 0$ was found previously by a different method \cite{32}. Instead of $\chi_{2l}$ (43), close occupation numbers were obtained:

$$\lambda_{2l} = \sqrt{\gamma} N_0 \frac{4|l|}{\pi}, \quad l = \pm 1, \pm 2, \ldots$$  \hspace{1cm} (56)

This formula holds for $l \ll \sqrt{\Gamma}$. At the replacement $N_0 \rightarrow \sqrt{N\tilde{N}_0}$ formula (56) passes to $\lambda_{2l} = \frac{\sqrt{T}}{4|l|}$, which coincides with $\chi_{2l}$ (43) at $T = 0$, $l \ll \sqrt{\Gamma}$. The difference between $N_0$ and $\sqrt{N\tilde{N}_0}$ is insignificant, since the methods in \cite{32,49} require $N_0 \approx N$. Note that the density matrix was found in \cite{32} directly from the ground-state wave function without any assumptions about the condensate. At $\gamma \lesssim 0.01$ the solution in \cite{32} is close to the exact one.

It is clear that, as $\gamma$ increases, the atoms from the lowest single-particle states transit in higher ones. Therefore, we may expect that the number of lowest macroscopically populated states increases with $\gamma$. At $\gamma \gg 1$ the atoms are apparently distributed over the very large number of states, and there are no macroscopically occupied states. However, we cannot verify these assumptions, since the methods in \cite{2,32,49} are valid only at small $\gamma$.

As we noted above, the condensate exists only in a finite 1D system. Bogoliubov’s method is also applicable only to a finite (1D) system (condition (55)). The quasicondensate (condensate) is fragmented, if condition (54) with $l \geq 1$ is satisfied. Inequality (54) follows from the criterion $\lambda_{2l} = \chi_{2l} \gtrsim \frac{N}{(\ln N)^2}$ and formula (43) for the quantity $\chi_{2l} \equiv N_{k_2l}$ \cite{49}. Since the occupation numbers $N_{k_j}$ at $T = 0$ should correspond to the smallest energy of the system, inequality (54) is, in fact, the condition for the fragmentation of a condensate to be energy-gained.

4.2 The case of $T > 0$

The thermal equilibrium in a system is possible, if the number of quasiparticles is large. This requires \cite{49} that $E(k_1) \ll k_BT$, which yields $\tilde{T} \gg y_1 = \Gamma^{-1/2} \approx \frac{\pi}{\sqrt{\gamma}N}$ (here, $E(k)$ is the dispersion law of quasiparticles). On the other hand, the criterion of applicability of the Bogoliubov method $0 < \frac{\sqrt{T}}{2\pi} \ln \frac{N\sqrt{\gamma}}{\pi} + 0.08\gamma N\tilde{T} \ll 1$ \cite{49} requires $\tilde{T} \ll \frac{\pi^2}{\gamma N}$. In this case, for
\sqrt{\Gamma} \gg 1 \text{ and small } j, \text{ relation (43) yields}
\chi_j \approx \frac{1}{2y_j} \left(1 + \frac{2}{e^{\frac{2y_j}{\gamma}} - 1}\right) \approx \frac{1}{2y_j} \left(1 + \frac{\tilde{T}}{y_j}\right).

(57)

If \( j < 10 \), then \( \tilde{T} \gg y_j \). Therefore, the main contribution to \( \chi_j \) is given by the temperature term \( \tilde{T}/y_j \). Thus, at \( y_1 \ll \tilde{T} \ll \frac{12}{\gamma N} \) the temperature affects the density matrix significantly.

In Table 1 we present the solutions with the above-considered parameters \( \Gamma = 10^7, N = 10^5 \) for \( \tilde{T} = 0.0005; 0.001 \). At both temperatures, the states 1, 2, 3 are filled macroscopically.

Let us consider the case \( \Gamma = 10^6, N = 10^5 \) for \( \tilde{T} = 0; 0.01; 0.02 \). As is seen from Table 1, at \( \tilde{T} = 0 \) only the state 1 is macroscopically occupied. At \( \tilde{T} = 0.01 \), the states 1, 2, 3 are macroscopically populated. At last, for \( \tilde{T} = 0.02 \) the states 1, 2, 3, 4, 5 are macroscopically occupied.

We see that, as \( \tilde{T} \) increases, the atoms transit from the state 1 to the states 2, 3 and to higher ones. It cannot be excluded that, at sufficiently high temperatures, the state 1 is occupied microscopically, but the states 2 and 3 are occupied macroscopically.

Interestingly, for a finite system the order parameter \( \langle \hat{\psi}(x,t) \rangle \) does not generally coincide with the genuine condensate defined with the help of criterion (1). Under periodic BCs, the function \( F_1(x,x') \) is set by formula (52), and the number \( \tilde{N}_0 \) of atoms in the effective condensate \( \langle \hat{\psi}(x,t) \rangle \) is equal to \( N_0 \). If the genuine condensate is not fragmented, it coincides with \( \langle \hat{\psi}(x,t) \rangle \). But if the genuine condensate is fragmented, there is no coincidence, since the states \( \phi_{p \pm 2}(x), \phi_{p \pm 4}(x), \ldots \) do not enter the average \( \langle \hat{\psi}(x,t) \rangle = \text{const} \cdot e^{-i\omega t/\hbar} \). Under zero BCs, the effective condensate \( \langle \hat{\psi}(x,t) \rangle \) does not coincide with the genuine one, since \( \tilde{N}_0 \neq \lambda_1 \), even if the genuine condensate is not fragmented. For example, for \( \Gamma = 10^6, N = 3.5 \cdot 10^4, T = 0 \) we get \( \lambda_1 \approx 0.914N, \lambda_2 \approx 0.00713N, \lambda_3 \approx 0.00596N \) (see Table 1). According to the criterion \( \lambda_j \gtrsim N/(\ln N)^2 \), only the state 1 is macroscopically occupied. In this case, \( \tilde{N}_0 \neq \lambda_1 \). This noncoincidence is related to the anomalous averages and the difference of the natural occupations \( \lambda_j \) under the zero and periodic BCs. For periodic BCs, \( \tilde{N}_0 = \lambda_1 = N_0 \) (the states \( -2, -4, \ldots \) under periodic BCs correspond to the states 3, 5, \ldots under zero BCs; at the transition from the periodic to zero BCs, a part of atoms passes from the states \( -2, -4, \ldots \) to the state 1 for zero BCs). However, even if the effective condensate does not coincide with the genuine one, the former is close to the latter, at least for the weak coupling. For the applicability of the Bogoliubov method to a 1D Bose system, namely the effective condensate \( \langle \hat{\psi}(x,t) \rangle \) is significant: The number of atoms \( \tilde{N}_0 \) in this condensate should be close to \( N \).

5 Conclusion

We have shown in two ways that the fragmentation of the condensate in a uniform Bose system is possible. Within the quasi-single-particle approach, we have found approximate one-dimensional crystal-like solutions with a fragmented condensate. Such solutions are pos-
sible for 1D, 2D, and 3D high-density system. However, they apparently correspond to highly excited states of the system. With the help of the more accurate collective approach, we obtained that the ground state of a uniform 1D Bose system with repulsive interatomic potential contains a fragmented quasicondensate at low $T$ and at definite values of the parameters of the system. In this case, the number of quasicondensates forming a fragmented quasicondensate can be equal to 3 or 5. The occupation numbers of a fragmented quasicondensate depend on the boundary conditions, though the energy of the ground state $E_0$ and the dispersion law $E(k)$ are independent of BCs [36, 49, 51, 53]. In recent years, the experiments with a uniform gas in a trap became possible [10]. Therefore, we hope for that the above obtained solutions will be verified experimentally.

*Note added in proof.* Recently, we became aware of works [57, 58], in which crystal-like solutions with a condensate of atoms were also considered.

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