SUPPRESSION OF BOSE CONDENSATE IN A SYSTEM OF INTERACTING BOSE PARTICLES

K.V. GRIGORISHIN, B.I. LEV

Bogolyubov Institute for Theoretical Physics, Nat. Acad. of Sci. of Ukraine
(14b, Metrolohichna Str., Kyiv 03143, Ukraine; e-mail: konst_dark@mail.ru)

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We propose a model of suppression of a Bose condensate in a weakly non-ideal Bose gas due to dynamic quantum fluctuations, whose existence follows from the uncertainty principle. Two approaches to the description of the mechanism of this phenomenon are considered: studying the motion of separate particles of the system in the self-consistent field approximation and the analysis of collective motions in the random phase approximation.

1. Introduction

It is well known that, at sufficiently low temperatures, the occupation number N_0 of the lowest-energy state by Bose particles or quasiparticles (in nonequilibrium systems) represents a macroscopic value $N_0 \leq N$. As a rule, this state is the one, where particles have a zero momentum $\mathbf{p} = 0$. Such a system becomes a macroscopic quantum one, which induces, in turn, a number of interesting and unique properties, such as superfluidity, quantum vortices and rings, interference of condensates (analogs of the Josephson effect), etc. The given phenomenon is observed in a system of sparse ultracold atoms in a magnetic trap [1–3], superfluid helium [4–6], exciton gas of semiconductors [9], and magnon gas [10].

From the viewpoint of statistical mechanics, the uniqueness of the Bose–Einstein condensation (BEC) phenomenon consists in that it can be considered as a phase transition in the ideal gas. The problem in the case of the ideal gas is solved exactly, because all thermodynamic functions of both phases, the condensate density, and the transition temperature are determined:

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_0}\right)^{3/2}, \qquad T_0 = \frac{2\pi\hbar^2}{m}\left(\frac{N/V}{2.612}\right)^{2/3}. \quad (1)$$

One can see that all particles are in the Bose condensate (BC) $N_0 = N$ at the temperature $T = 0$. In order to find the spectrum of quasiparticles in a Bose gas with repulsive interaction as well as the ground-state energies of such a system, M.M. Bogolyubov assumed that the Bose condensate density is not equal to the total one $N_0 < N$, i.e. the over-condensate particles exist even at the absolute zero of temperature [11]. It turns out that the number of condensate particles in this model is determined by the interaction and the mean density:

$$N_0 = N\left(1 - \frac{8}{3}\sqrt{\frac{Na^3}{\pi V}}\right), \quad (2)$$

where $a > 0$ is the scattering length. Formula (2) is valid under the condition $\frac{a^3}{V/N} \ll 1$, i.e. for a very low-density (weakly non-ideal) gas. In this case, $\frac{N_0}{N} \simeq 1$, that is why almost all particles are in the BC. The over-condensate particles are distributed according to a certain law; moreover, the maximum of the distribution function $\sim p^2 N_{\mathbf{p}}$ falls on $p/\hbar \sim \sqrt{aN/V}$. One can see that the interaction results in the spreading of the BC, and the given effect must be more pronounced in strongly interacting systems. For example, it was experimentally established for the superfluid helium phase (He II) that $\frac{N_0}{N} \approx 0.07$ [4, 5], i.e. the BC is strongly suppressed.

After the consistent application of the Bogolyubov model to the description of a weakly non-ideal Bose gas, there arose the questions concerning its generalization for denser systems, where $\frac{a^3}{V/N} \simeq 1$, the microscopic nature of the superfluid component (as its density at $T = 0$ is equal to the fluid density, but $N_0 < N$), and respectively, the mechanism of BC suppression. Another discoursive point regards the role of the BEC in the superfluidity phenomenon. The Foldy—Brueckner approach [12] generalizes the Bogolyubov one in the sense that the former partially takes the interaction of over-condensate

particles into account. In this model, all particles not being a part of the one-particle condensate with the mean value of the field operator $\langle\widehat{\psi}\rangle = \sqrt{n_0}$ are joined into an even BC that represents an analog of Cooper pairs in a semiconductor and are described by the "anomalous averages" $\langle\widehat{\psi}\widehat{\psi}\rangle \neq 0$ and $\langle\widehat{\psi}^{+}\widehat{\psi}^{+}\rangle \neq 0$. In strongly interacting systems, for example in He II, some models [12–14] allow the existence of higher even BCs (four-, six-particle, and so on). Moreover, a one-particle BC is suppressed due to the growth of the even BC due to interaction [14]. However, such approaches meet some difficulties such as, for example, the formation of a gap in the spectrum of quasiparticles that is to be eliminated, the existence of different kinds of excitations for different condensates that should be reduced to one type, *etc.*

Along with the Bogolyubov–Belyaev–Brueckner field-theoretic approach, a quantum-mechanical one initiated in [15] and [16] with the use of the Jastrow expansion [17] was developed. Later on, this approach starts to use the powerful technique of collective variables first applied in the work by M.M. Bogolyubov and D.N. Zubarev [18] and developed in [19, 20]. In contrast to the previous field-theoretic approach, this one does not require the introduction of BCs of different kinds and proceeds from the many-particle quantum-mechanical problem. Here, the number of BCs is calculated with the help of density matrices. It turns out that, in addition to a one-particle BC, there also exists an even one, but higher condensates are forbidden [21]. For example, for He II, $N_1/N = 0.061$ and $N_2/N = 0.16$, i.e. not all particles belong to the condensates. These approaches also meet a number of difficulties, such as the absence of a small parameter in the perturbation theory based on the use of the Jastrow expansion. That is why, one has to omit not small terms, which results in a low accuracy of the results obtained in this approach.

Taking into account all the complexity and diversity of the problem of quantum Bose liquids and gases, the problem of their description remains urgent till now. The aim of this work is to propose and describe a real physical model of suppression of a one-particle BC in Bose systems with repulsive short-range interaction based on the first principles of quantum mechanics, such as the principle of uncertainty and that of particle identity. As was said above, the description of strongly interacting systems meets serious mathematical difficulties. Therefore, we will apply our model to quantitative calculations for a weakly non-ideal Bose gas. For quantum liquids, the mechanism of BC suppression must have the identical nature and be the same on the qualitative level. The given problem will be considered from two basically different positions – the analysis of the motion of one particle of the system in the medium formed by other atoms and that of collective motions in the system. This gives a possibility to describe the mechanism of the same phenomenon from different positions.

2. One-particle motion

Let us consider a collection of N interacting Bose particles confined in some volume V. In the general form, the Hamiltonian of such a system can be presented as

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{1\leq i<j\leq N} \Phi(|\mathbf{r}_i - \mathbf{r}_j|), \tag{3}$$

where the first term denotes the kinetic energy of the particles, whereas the second one – the potential energy of their pairwise interaction. In the Hartree approximation, the wave function of the system is presented by the product of the one-particle wave functions

$$\Psi(\mathbf{r}_1, ...\mathbf{r}_N, t) = \prod_{i=1}^{N} \psi(\mathbf{r}_i, t), \tag{4}$$

where ψ stands for the normalized wave function of the one-particle state that determines the density of the system:

$$\int\limits_V |\psi(\mathbf{r}, t)|^2 dV = 1, \qquad n(\mathbf{r}, t)) = N|\psi(\mathbf{r}, t)|^2. \tag{5}$$

For non-interacting particles, $\psi = 1/\sqrt{V}$.

The Schrödinger equation in the mean field approximation takes the form

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m}\triangle\psi(\mathbf{r}, t) +$$

$$+\psi(\mathbf{r}, t)N\int |\psi(\tilde{\mathbf{r}}, t)|^2\Phi(\mathbf{r} - \tilde{\mathbf{r}})d\tilde{\mathbf{r}}. \tag{6}$$

The interaction potential Φ will be considered a point one

$$\Phi(\mathbf{r} - \tilde{\mathbf{r}}) = \frac{4\pi\hbar^2}{m}a\delta(|\mathbf{r} - \tilde{\mathbf{r}}|), \tag{7}$$

where a is the scattering length of the order of the interaction radius. Then Eq.(6) will take the form of the well-known Gross–Pitaevskii equation [22, 23]

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\triangle\psi + \frac{4\pi\hbar^2}{m}aN|\psi|^2\psi. \tag{8}$$

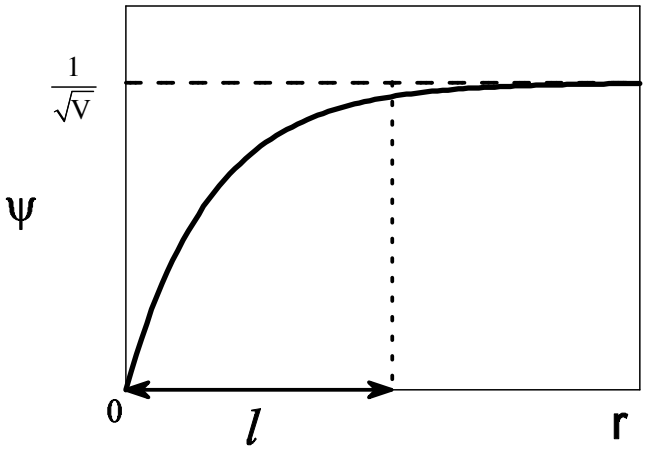

Fig. 1. Wave function of the ground state of a weakly non-ideal Bose gas. The amplitude of the state $\psi(r)$ tends to zero if particles overlap and specifies the mean density of the system if they are sufficiently far from each other. The quantity l is the radius of such a "polaron" (16) formed by the interaction of the particle with the self-consistent field of all other atoms

Let us consider such stationary solutions of this equation that

$$\psi(\mathbf{r},t)=\psi(\mathbf{r})\exp\left(-\frac{i}{\hbar}\chi t\right), \tag{9}$$

where χ is some parameter of the energy dimension. In this case, the previous equation (8) can be rewritten in the form

$$\chi\psi=-\frac{\hbar^2}{2m}\triangle\psi+\frac{4\pi\hbar^2}{m}aN|\psi|^2\psi. \tag{10}$$

The solution of this equation will be searched for, by proceeding from the following considerations. Let some particle be fixed at the point $r=0$. At infinity, the wave function $\psi(r)$ of another free particle of the system must specify the mean density in the given system, i.e. $\psi(r\to\infty)=1/\sqrt{V}$. As the potential acting between the atoms is repulsive, the probability of their location close to one another is lower than at large distances. That is why one can suppose $\psi(0)=0$ under the condition that they cannot penetrate into each other (it is well fulfilled for hard spheres). Then the wave function at large distances can be presented in the form

$$\psi(r)=\frac{1}{\sqrt{V}}(1-\varphi(r)), \tag{11}$$

where $0<\varphi(r)\ll 1$. Such an assumption allows one to linearize Eq.(10) in the region far from the origin of coordinates and to neglect the term $\frac{2}{r}\frac{\partial\varphi}{\partial r}$:

$$\frac{\partial^2\varphi}{\partial r^2}-\frac{2m}{\hbar^2}\left(\frac{3UN}{V}-\chi\right)\varphi=\frac{2m}{\hbar^2}\left(\chi-\frac{UN}{V}\right), \tag{12}$$

where $U=\frac{4\pi\hbar^2}{m}a$. In order to satisfy the boundary condition at infinity, $\varphi=0$, it is necessary to set

$$\chi=\frac{UN}{V}=\frac{4\pi\hbar^2Na}{Vm}\equiv\mu, \tag{13}$$

where μ is the chemical potential of the Bose gas with interaction (6) [24]. Then the solution of Eq.(12) takes the form

$$\psi(r)=\frac{1}{\sqrt{V}}\left[1-C\exp\left(-\sqrt{\frac{4mUN}{\hbar^2V}}r\right)\right], \tag{14}$$

where C is the integration constant. Now let us interpolate the given expression to the origin of coordinates so that the condition $\psi(0)=0$ be satisfied (for this purpose, it is necessary to set $C=1$):

$$\psi(r)=\frac{A}{\sqrt{V}}\sqrt{\frac{4mUN}{\hbar^2V}}r, \tag{15}$$

where the constant A will be determined in what follows. As the atoms forming the system are considered as hard spheres, the amplitude of the state including two overlapping particles is very small, which is reflected by the behavior of the wave function (Fig.1), i.e. its vanishing in the case of the overlapping of atoms and equiprobable positions for sufficiently remote atoms.

The obtained solution can be interpreted in the following way. Each particle of the medium polarizes its surroundings, and, as the interaction potential corresponds to repulsive forces, there arises some rarefaction around a particle. On the other hand, the particle itself interacts with the formed deformation, i.e. it appears in a potential well. The dimensions of this well can be estimated, by using function (14):

$$l\sim\sqrt{\frac{\hbar^2V}{4mUN}}. \tag{16}$$

Being in the well, the considered particle performs a finite motion with a certain energy ε. Using relation (10) and asymptotics (15), the energy of its interaction with the self-consistent field of other particles can be presented in the form

$$UN|\psi(r)|^2=A^2\frac{4mU^2N^2}{\hbar^2V^2}r^2\equiv\frac{1}{2}m\omega^2r^2. \tag{17}$$

Thus, each particle moves in a potential well formed by all the other particles of the system. In this sense, a Bose liquid is equivalent to a collection of N harmonic three-dimensional oscillators

$$-\frac{\hbar^2}{2m}\triangle\Xi(r)+\frac{1}{2}m\omega^2\Xi(r)=\varepsilon\Xi(r). \tag{18}$$

Here, the constant $A=\sqrt{2}/6$ is chosen in such a way that the energy of the ground state

$$\mu=\frac{\partial(\varepsilon N)}{\partial N}\Longrightarrow\varepsilon=\frac{3}{2}\hbar\omega=\frac{2\pi\hbar^2Na}{Vm}. \tag{19}$$

The solution of Eq.(18) is

$$\Xi(r)=C\exp\left(-\frac{r^2}{2l^2}\right), \tag{20}$$

where C is the integration constant, while l can be called the oscillatory length:

$$l^2=\frac{\hbar}{m\omega}=\frac{6V}{2\sqrt{2}Na}. \tag{21}$$

As was noted above, the interaction results in some localization of the particle in a region with the size $\Delta x\sim l$. As the non-ideality parameter $\frac{a}{V/N}$ increases, the localization region decreases. As $a\to 0$, the particle is completely delocalized, which corresponds to the conditions of the ideal gas.

According to the uncertainty principle, the localization of the particle in a region with size l results in the uncertainty of the momentum $\Delta p\sim\hbar/l$. Then, in contrast to the ideal Bose gas, the particle cannot be in the BC, as the momentum in the BC is completely determined: $p=0$. Thus, we can conclude that *interaction results in the suppression of the Bose condensate*. In the limiting case of ideal gas, particles are completely delocalized; in this case, the momentum uncertainty tends to zero $\Delta p\sim\hbar/l=0$, i.e. completely agrees with the condition of BC existence.

Let us now pass to the momentum representation according to the well-known rule

$$\Xi(k)=\frac{1}{(2\pi)^{3/2}}\int\limits_0^\infty e^{i\mathbf{kr}}\Xi(r)4\pi r^2dr=$$

$$=\frac{1}{(2\pi)^{3/2}}\frac{4\pi}{k}\int\limits_0^\infty r\Xi(r)\sin(kr)dr=Cl^3\exp\left(-\frac{l^2}{2}k^2\right), \tag{22}$$

where $k=p/\hbar$. As was expected, the momentum uncertainty (localization in the momentum space) $\Delta k\sim 1/l$. Knowing the wave function (22), we can now determine the occupation numbers for the states with momenta $k\neq 0$:

$$N_k=N|\Xi(k)|^2=NC^2l^6\exp\left(-l^2k^2\right). \tag{23}$$

The momentum distribution function of particles $\sim k^2N_k$ reaches a maximum at the momentum

$$k_m^2=\frac{2}{l^2}\sim\sqrt{\frac{Na}{V}}, \tag{24}$$

which coincides with the maximum of the distribution function obtained by Bogolyubov [25]. The integration constant C can be determined, by normalizing the wave function $\Xi(r)$ to one

$$\int\limits_0^\infty|\Xi(r)|^2 4\pi r^2dr=1\Longrightarrow C^2=\frac{1}{\pi^{3/2}l^3}. \tag{25}$$

The number of over-condensate particles can be obtained, by integrating (23) over the whole momentum space:

$$\Delta N=N\int\limits_0^\infty|\Xi(k)|^2 4\pi k^2dk=N\cdot 1\Rightarrow N_0=0. \tag{26}$$

Thus, due to the action of the uncertainty principle, the one-particle BC is completely suppressed in the presence of an interaction regardless of its intensity.

Now let us take into account the principle of identity of particles. The given principle does not give a possibility to identify atoms. This means that we cannot choose an arbitrary particle in order to consider its motion in the field of other particles, as we have done it above. The coordinate uncertainty will be equal to the linear dimension $L\to\infty$ of the whole macroscopic volume occupied by atoms, rather than to l. That is why the momentum uncertainty will be equal to zero $p\sim\hbar/L\to 0$, and all particles will be in the BC regardless of interaction: $N_0=N$ [26]. Thus, we are faced with a paradox: due to the uncertainty principle, the BC is completely suppressed, whereas due to the identity principle, all particles are in the BC regardless of the interaction intensity. In turn, the experiment performed with He II [4–6] demonstrates that He I includes a one-particle BC of the order of 10%.

In order to overcome the above-stated contradiction, we consider the application of the identity principle to

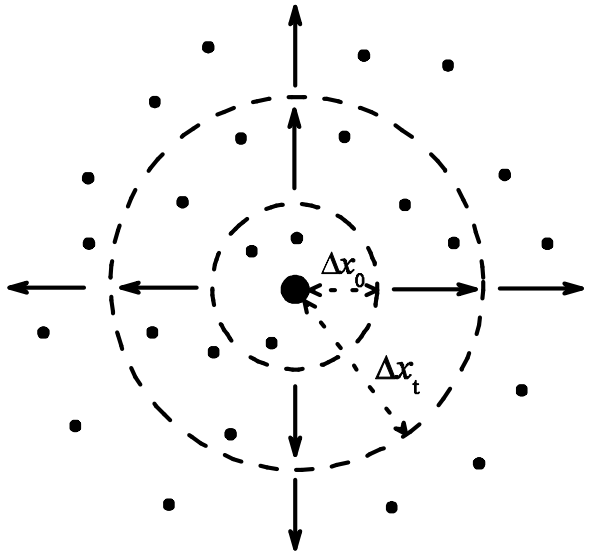

Fig. 2. Spreading of the wave packet of a particle with the initial size Δx_0 in a system of non-interacting atoms. The packet width Δx_t indefinitely increases covering all other particles of the system

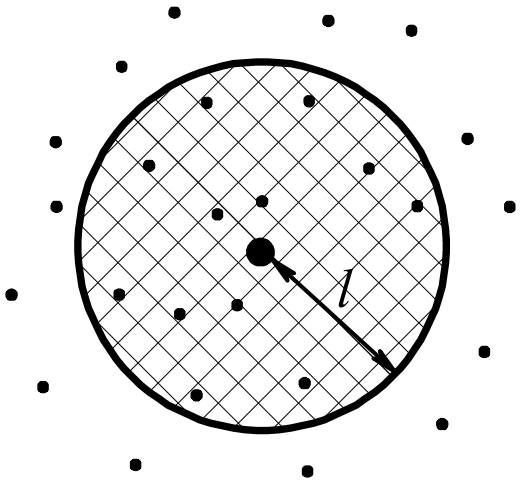

Fig. 3. Stabilization of the wave packet of a particle in a Bose liquid due to the polarization of its environment. l is the characteristic size of the packet that covers a certain share of particles $\sim \frac{l^3}{V}N < N$ in contrast to the case of an ideal gas

a system of interacting atoms in more details. Let us examine a system of N identical particles. In classical mechanics, we can trace each of them, as they move along their trajectories and therefore do not lose their identities. In quantum mechanics, the situation is different. Each particle is presented by a wave packet as a superposition of de Broglie waves [26]:

$$\psi(x,t) = \int\limits_{-\infty}^{+\infty} dk e^{-(k-k_0)^2\langle(\Delta x_0)^2\rangle} e^{ik_0x - i\hbar k^2 t/2m}. \qquad (27)$$

In this case, the wave packet width at any time moment t amounts to

$$\langle(\Delta x)^2\rangle = \langle(\Delta x)^2\rangle_0 + \frac{\hbar^2 t^2}{4m^2\langle(\Delta x)^2\rangle_0}. \qquad (28)$$

Thus, the packet indefinitely spreads in the course of time. If we number each particle at the initial time moment, their wave packets will overlap at the following one, and the numbering of particles will mix up. That is, localizing one of them, we are not able to identify it in some time. Therefore, we have no possibility to distinguish identical particles.

The mechanism of the BC formation can be understood from the following considerations. The wave packet of each particle (27) covers $\simeq \frac{\langle\Delta x\rangle_t^3}{V/N}$ other atoms of the system; here, $\langle\Delta x\rangle_t^3$ is the volume of the wave packet, V/N is the volume per one particle. Then probability (25) is equally shared between all particles due to their identity:

$$\int\limits_0^\infty |\Xi(r)|^2 4\pi r^2 dr = \frac{1}{\frac{\langle\Delta x\rangle_t^3}{V/N}} \Longrightarrow C^2 = 0, \qquad (29)$$

as the wave packets of non-interacting particles indefinitely spread $\langle\Delta x\rangle^3 \to \infty$ at $t \to \infty$ (Fig. 2). Then we obtain from (23) that $N_k = 0$, i.e. all particles of the ideal Bose gas are in the BC.

For a system of interacting particles, the situation somewhat changes. The wave packet of each particle is described by the oscillatory function (20) corresponding to the packet width $\langle(\Delta x)\rangle \sim l$ (21). That is, the spreading of the wave packets of particles is stopped by interaction (Fig. 3). Then probability (25) is shared between the particles covered by the wave packet (20), which means that the normalizing condition can be presented in the following way:

$$\int\limits_0^\infty |\Xi(r)|^2 4\pi r^2 dr = 1/\frac{4\pi l^3/3}{V/N} \Rightarrow C^2 = \frac{3V}{4\pi^{5/2}Nl^6}. \qquad (30)$$

From here, we obtain the occupation numbers for the states with the momenta $k \neq 0$:

$$N_k = N|\Xi_k|^2 = N\frac{3V}{4\pi^{5/2}N}\exp\left(-l^2k^2\right). \qquad (31)$$

The number of over-condensate particles can be found integrating (31) over the whole momentum space

$$\Delta N = N \int\limits_0^\infty |\Xi(k)|^2 4\pi k^2 dk = \frac{3}{4\pi}\frac{V}{l^3}. \tag{32}$$

As $\Delta N = N - N_0$, the number of particles in the BC can be found in the following way:

$$N_0 = N\left(1 - \frac{3}{4\pi}\sqrt{\frac{3}{\sqrt{2}}\frac{Na^3}{V}}\right), \tag{33}$$

that is we obtain a completely identical functional dependence on the density of the system and the interaction constants as in the Bogolyubov formula (2). The difference in the coefficients is of the order of one and appears due to the estimating character of our calculations. For the superfluid phase of helium, $V/N \simeq l^3$, and the BC is strongly suppressed. That is why our approximations cannot be applied to this case, though the qualitative picture is the same. Thus, one can state that the number of BCs in the ground state of a Bose system is determined by the balance between the uncertainty principle, whose suppressing action on the BC intensifies with increasing the density and the interaction, and the identity principle that leads to the macroscopic occupation of the level with $k = 0$.

It is worth noting that the distribution function of over-condensate particles has a sense of the square of the wave function. That is, before the measuring process, a particle has no certain value of the momentum; it appears only during this process. Thus, to our mind, each particle occupies a superposition of states with non-zero momentum $k \neq 0$ and the state with zero momentum $k = 0$

$$\Psi = C_1\varphi_{\mathbf{k}\neq 0} + C_2\varphi_{\mathbf{k}=0}$$

$$C_1^2 = \frac{3}{4\pi}\frac{V/N}{l^3}, \qquad C_2^2 = 1 - \frac{3}{4\pi}\frac{V/N}{l^3}, \tag{34}$$

where the coefficients C_1 and C_2 specify the probabilities of these states and the condition $l^3 \gg V/N$ is realized. That is, the BC density is determined by the probability of each particle of the system to occupy the state with zero momentum. In the measuring process, there takes place a collapse (reduction) of the wave function Ψ to the state $\varphi_{\mathbf{k}=0}$ (condensate particle) or $\varphi_{\mathbf{k}\neq 0}$ (over-condensate particle).

3. Collective Motion

Now let us proceed to another approach to the description of the same phenomenon in terms of collective variables. In this approach, the criterion of BC suppression can be directly obtained from the solution of a many-particle problem. Let us consider a stationary Schrödinger equation for Hamiltonian (3). We deal with the many-particle quantum-mechanical problem consisting in obtaining the solutions of the given equation in the form of wave functions symmetric with respect to the permutation of an arbitrary pair of N particles. The variables describing the system will be the collective coordinates

$$\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{-i\mathbf{k}\mathbf{r}_j}, \qquad \rho_{\mathbf{k}}^* = \rho_{-\mathbf{k}}, \tag{35}$$

that represent the Fourier coefficient of the fluctuation of the particle density

$$\Delta n(\mathbf{r}) = \sum_{j=1}^{N}\delta(\mathbf{r} - \mathbf{r}_j) - \frac{1}{V}. \tag{36}$$

The quantities $\rho_{\mathbf{k}}$ are symmetric with respect to permutations of the particle coordinates $(\mathbf{r}_1, ..., \mathbf{r}_N)$, therefore the wave functions of these particles in the collective variable space also will be symmetric. Thus, the identity principle is fulfilled automatically, and the solutions of the Schrödinger equation require no additional symmetrization. The potential energy of the many-particle system in terms of these variables has a form

$$\Phi(\mathbf{r}_1 \dots \mathbf{r}_N) \equiv \sum_{1\leq i<j\leq N}\Phi(|\mathbf{r}_i - \mathbf{r}_j|) =$$

$$= \frac{N(N-1)}{2V}\nu_0 + \frac{N}{2V}\sum_{\mathbf{k}\neq 0}\nu_{\mathbf{k}}(\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - 1). \tag{37}$$

Here, $\nu_{\mathbf{k}}$ stands for the Fourier transform of the interaction potential presented as follows:

$$\nu_{\mathbf{k}} = \int e^{-i\mathbf{k}\mathbf{r}}\Phi(r)d\mathbf{r} = \frac{4\pi\hbar^2}{m}a. \tag{38}$$

Then, after the Hermitian procedure, Hamiltonian (3) in the random-phase approximation (RPA) can be written down in terms of the collective variables (35) [26] as

$$\widehat{H} = \sum_{\mathbf{k}\neq 0}\frac{\hbar^2 k^2}{2m}\left[-\frac{\partial^2}{\partial\rho_{\mathbf{k}}\partial\rho_{-\mathbf{k}}} + \frac{1}{4}\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - \frac{1}{2}\right] +$$

$$+\frac{N(N-1)}{2V}\nu_0+\frac{N}{2V}\sum_{\mathbf{k}\neq 0}\nu_{\mathbf{k}}(\rho_{\mathbf{k}}\rho_{-\mathbf{k}}-1). \quad (39)$$

It represents the Hamiltonian of a collection of independent harmonic oscillators, i.e. a Bose liquid can be presented in the form of such a collection. The excitation of an oscillator of this system corresponds to the appearance of one quasiparticle. The motion of each oscillator in the ground or excited state corresponds to collective motions of all particles of the system and is interpreted by an observer as a perturbation of the density (fluctuations, first and second sounds, *etc.*)

The wave function of the ground state describes zero oscillations of a Bose liquid. That is why, in the harmonic approximation, it is a Gaussian function of collective coordinates. Then the wave function of the ground state can be presented in the form [19]

$$\psi=e^U, \qquad U=\sum_{\mathbf{k}} f(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}. \quad (40)$$

This expression means that our system represents a collection of independent harmonic oscillators, and the energy of the ground state can be presented as a sum of the energies of oscillators

$$E_0=\sum_{\mathbf{k}} E_0^{\mathbf{k}}+\frac{N(N-1)}{2V}\nu_0. \quad (41)$$

The Schrödinger equation in terms of collective variables for the ground state of an oscillator of the Bose liquid can be presented as follows:

$$\varepsilon(k)\left[-\frac{\partial^2 U}{\partial\rho_{\mathbf{k}}\partial\rho_{-\mathbf{k}}}-\frac{\partial U}{\partial\rho_{\mathbf{k}}}\frac{\partial U}{\partial\rho_{-\mathbf{k}}}+\frac{1}{4}\rho_{\mathbf{k}}\rho_{-\mathbf{k}}-\frac{1}{2}\right]+$$

$$+\frac{N}{2V}\nu_k(\rho_{\mathbf{k}}\rho_{-\mathbf{k}}-1)=E_0^k, \quad (42)$$

where $\varepsilon(k)=\hbar^2k^2/2m$. Then we can write the equations for the coefficients $f(k)$ and the energy as

$$\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\left[-\varepsilon(k)f(k)^2+\frac{1}{4}\varepsilon(k)+\frac{N}{2V}\nu_k\right]-$$

$$-\varepsilon(k)f(k)-\frac{1}{2}\varepsilon(k)-\frac{N}{2V}\nu_k-E_0^k=0. \quad (43)$$

This yields

$$f(k)=-\frac{1}{2}\sqrt{1+\frac{2N}{V}\frac{\nu(k)}{\varepsilon(k)}},$$

$$E_0^k=\frac{1}{2}\hbar\omega-\frac{1}{2}\varepsilon(k)-\frac{N}{2V}\nu_k, \quad (44)$$

where the oscillator energy quantum

$$\hbar\omega=\sqrt{\varepsilon(k)^2+\frac{2N}{V}\nu(k)\varepsilon(k)}. \quad (45)$$

On the other hand, Eq.(42) can be rewritten in the following way:

$$-\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial\rho_{\mathbf{k}}\partial\rho_{-\mathbf{k}}}+\frac{1}{2}M\omega^2\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\psi=E_0^*\psi, \quad (46)$$

where the "mass" and the "energy" are given by

$$M=\frac{m}{k^2}, \qquad E_0^*=-\varepsilon(k)f(k). \quad (47)$$

Based on the virial theorem, we obtain that

$$\frac{M\omega^2}{2}\langle\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\rangle=\frac{E_0^*}{2}\Rightarrow S_2(k)\equiv\langle\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\rangle=-\frac{1}{2f(k)}, \quad (48)$$

where $S_2(k)$ denotes the structural factor of the quantum liquid.

According to the uncertainty principle, the oscillator energy in the ground state cannot be equal to zero, whereas, according to the virial theorem, the kinetic and potential energies are equally shared. This zero energy is that of the density fluctuations of the quantum liquid. These fluctuations exist in the ground state of the medium as well, which means, in turn, that the collective motion of the liquid exists even in this state. On the microscopic level, the given collective motion corresponds to the self-consistent motion of particles of the system. This implies that not all particles can be in the BC (or, according to our interpretation (34), occupy the pure state $\varphi_{\mathbf{k}=0}$), i.e. the one-particle BC is spread due to dynamic fluctuations.

Using Eq.(43), the ground-state energy of the system can be written down in the following form:

$$\sum_{\mathbf{k}\neq 0}\varepsilon(k)\left[-f(k)^2\rho_{\mathbf{k}}\rho_{-\mathbf{k}}-f(k)+\frac{1}{4}\rho_{\mathbf{k}}\rho_{-\mathbf{k}}-\frac{1}{2}\right]+$$

$$+\frac{N(N-1)}{2V}\nu_0+\sum_{\mathbf{k}\neq 0}\frac{N}{2V}\nu_k(\rho_{\mathbf{k}}\rho_{-\mathbf{k}}-1)=E_0. \quad (49)$$

Averaging this expression over the ground state according to the rule $\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\to\langle\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\rangle$ with regard for the expression for the potential energy of the system (37) and the evident equality $E_0=\langle T\rangle+\langle\Phi\rangle$, we obtain the

mean values of the kinetic and potential energies of the system

$$\langle T\rangle = \sum_{\mathbf{k}\neq 0}\varepsilon(k)\left[\left(-f(k)^2+\frac{1}{4}\right)\langle\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\rangle - f(k) - \frac{1}{2}\right], \tag{50}$$

$$\langle\Phi\rangle = \frac{N(N-1)}{2V}\nu_0 + \sum_{\mathbf{k}\neq 0}\frac{N}{2V}\nu_k(\langle\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\rangle - 1). \tag{51}$$

As $\varepsilon(k) = \hbar^2k^2/2m$ is the kinetic energy of one particle, the expression in brackets in (50) can be considered as the occupation numbers of over-condensate particles $N_{\mathbf{k}}$. Using relation (48), the kinetic energy and the corresponding occupation numbers can be presented in terms of the function $f(k)$ or the structural factor $S_2(k)$:

$$\langle T\rangle = \sum_{\mathbf{k}}\frac{\hbar^2k^2}{2m}\left[\frac{(2f(k)+1)^2}{-8f(k)}\right], \tag{52}$$

$$N_{\mathbf{k}} = \frac{(2f(k)+1)^2}{-8f(k)} = \frac{(S_2(k)-1)^2}{4S_2(k)}. \tag{53}$$

In the limiting case of non-interacting particles, we have $f(k)\to -1/2$. Therefore, $N_{\mathbf{k}} = 0$, i.e. all particles are in the BC. In the case of a weakly non-ideal Bose gas with interaction (38), the amount of the BC is determined in the following way:

$$N_0 = N - \sum_{\mathbf{k}\neq 0}N_{\mathbf{k}} = N - \frac{V}{(2\pi)^3}\int\limits_0^\infty \frac{(2f+1)^2}{-8f}4\pi k^2dk =$$

$$= N - N\frac{8}{3}\sqrt{\frac{Na^3}{\pi V}}, \tag{54}$$

That is, we again obtain the Bogolyubov formula (2). This result can be considered from another viewpoint, by rewriting (53) in terms of the fluctuation energy (45):

$$\hbar\omega = -\varepsilon(k)f(k) \Rightarrow \langle T\rangle = \sum_{\mathbf{k}}\hbar\omega(k)\left[\frac{(2f+1)^2}{8f^2}\right]. \tag{55}$$

Then the expression in brackets can be interpreted as the distribution of virtual quasiparticles [27]. Thus, one can state that, due to the uncertainty principle, there exist the dynamic fluctuations with energy quanta $\hbar\omega(k)$ in the ground state of the system that provide the non-zero kinetic energy (55). These fluctuations spread the BC, which is observed as the presence of over-condensate particles with distribution (53). Such an interpretation is confirmed by the following experimental fact.

In [4, 5], the distribution function of over-condensate particles in He II was measured. The given function decreases with increase in the momentum (energy) of particles and is rather close to zero already at $k\sim 2$ Å^{-1}, which is just the region of wave vectors of elementary excitations. In experiments on deeply inelastic scattering of neutrons in He II, a distribution function with characteristic condensate peak was obtained. This function allows one to determine the BC density that amounts to 6-8% of the total mass at the absolute zero of temperature. However, the kinetic energy transferred to helium atoms by neutrons (momentum ≈ 20 Å^{-1}) exceeds the elementary excitation energy. Due to this reason, such neutrons are scattered by liquid helium as by a system of non-interacting particles. In this case, each atom plays a role of density fluctuations and has no time to interact with its environment during the scattering. Thus, it looks as if the scattering takes place on particles of an ideal gas. Such a situation occurs in the so-called momentum approximation, where the transferred momentum $k\to\infty$ [7,8]. The above-mentioned condensate peak vanishes at lower energies of incident neutrons, which represents the scattering on dynamic density fluctuations of the Bose system. That is, at finite transferred momenta, the non-zero kinetic energy of the ground state $\langle T\rangle$ can be understood as expression (55), whereas, in the momentum approximation, the same kinetic energy can be presented by expression (53).

In addition to dynamic fluctuations, the BC is also suppressed by kinematic (thermal) ones caused by the chaotic motion of particles of the system at non-zero temperature. The structural factor at $T\neq 0$ can be found, by generalizing Eq.(48) to the excited states

$$\frac{M\omega^2}{2}\langle\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\rangle = \hbar\omega\left(\frac{1}{2}+n_{\mathbf{k}}\right) \Rightarrow S_2 = S_2^0(1+2n_{\mathbf{k}}), \tag{56}$$

where S_2^0 is the structural factor at $T=0$, $n_{\mathbf{k}}$ is the number of quanta of the oscillator that we understand as the number of quasiparticles. To a high accuracy, they can be considered distributed according to the Bose–Einstein statistics

$$\langle n_{\mathbf{k}}\rangle = \frac{1}{\exp(\hbar\omega/T)-1}. \tag{57}$$

Substituting the obtained structural factor in the formula for the number of over-condensate particles (53),

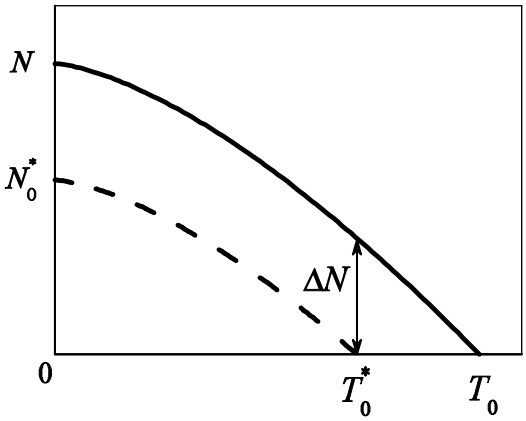

Fig. 4. Effect of dynamic quantum fluctuations on the Bose condensation temperature. T_0 and T_0^* are the above-mentioned temperatures for the ideal and weakly non-ideal gases, respectively. ΔN is the number of over-condensate particles existing at $T = 0$ as a measure of the intensity of dynamic fluctuations

we obtain that

$$N_{\mathbf{k}} = \frac{(S_2^0(k)-1)^2}{4S_2^0(k)} + \frac{1}{2}\left(S_2^0 + \frac{1}{S_2^0}\right)\langle n_{\mathbf{k}}\rangle, \tag{58}$$

where the system is considered weakly excited, $n_{\mathbf{k}} \ll 1$. Thus, it is easy to see that the kinematic fluctuations caused by thermal motion suppress the BC along with dynamic ones.

The BC spreading due to dynamic fluctuations must result in a decrease of the temperature of its appearance. In the ideal gas, this temperature is determined with the help of formula (1). It can be understood as the limit, where kinematic fluctuations already have no possibility to spread the BC and which appears, for the first time, with decrease in the temperature. In the presence of an interaction, the BC is additionally spread by dynamic fluctuations. That is why we can write

$$N_0(T) = N - N\left(\frac{T}{T_0}\right)^{3/2} - \Delta N, \tag{59}$$

where ΔN is the number of over-condensate particles at $T = 0$. That is, at $T = T_0$, the BC should already be formed, but it must become intense enough due to the action of fluctuations to exceed the dispersion ΔN (Fig. 4). Hence, the temperature of the BC formation $N_0(T_0^*) = 0$ can be given by the expression

$$T_0^* = T_0\left(1 - \frac{\Delta N}{N}\right)^{2/3} = T_0\left(1 - \frac{8}{3}\sqrt{\frac{Na^3}{\pi V}}\right)^{2/3}. \tag{60}$$

Thus, as the non-ideality parameter $\frac{a}{V/N}$ increases, the BC formation temperature decreases. For example, this temperature for helium exactly coincides with the temperature of the λ-transition [4] and amounts to 2.17 K, whereas the corresponding temperature of the Bose-condensation of the ideal gas at the same density is equal to 3.13 K.

4. Conclusions

The given work considers a model of suppression of the one-particle BC in Bose systems with repulsive short-range interaction. The analysis of the motion of separate particles with the help of the Gross–Pitaevskii equation has demonstrated that, at the absolute zero of temperature, the BC is suppressed due to the action of the uncertainty principle. Each particle polarizes its environment due to the interaction with it and thus appears in a potential well. In this well (that can be approximately considered oscillatory), the particle performs a finite motion at the lowest energy level. Due to the finiteness of this motion, the momentum has an uncertainty which is the higher, the stronger is the interaction between particles of the system. Thus, the BC is completely spread in the presence of the interaction. In its absence (ideal gas), the oscillatory length becomes infinite, and all particles get back to the BC. The allowance for the principle of identity of particles changes the situation. The wave packets of the particles indefinitely expand and will intersect, which results in their indistinguishability. That is why we cannot fix a separate particle in its well, as the probability of its location there is equally shared between all particles of the system due to their identity. Then all atoms of the system appear in the BC. The interaction restricts the packet spreading, while the oscillatory length plays a role of the wave packet width. Therefore, the wave packets of particles being at a sufficiently large distance do not intersect. This means that the probability to find a particle in the well is shared only between the particles appearing in its wave packet, which gives a possibility to estimate the number of BCs in a weakly non-ideal gas. The estimation results in the well-known Bogolyubov formula (1). That is, we can state that, at $T = 0$, BCs are suppressed by dynamic quantum fluctuations resulting from the uncertainty principle. It does not restrict the range of phenomena that cause such fluctuations, for example, they can induce quantum phase transitions in various systems [28].

The above-described process can be considered from the viewpoint of collective motions of particles. The analysis demonstrates that the BC is suppressed due to kinematic and dynamic fluctuations. The former are

caused by thermal motion of particles and exist at non-zero temperatures. These fluctuations spread the BC the stronger, the higher is the temperature, and finally result in its complete destruction. Dynamic fluctuations are induced by an interaction. In the RPA-approximation, a Bose system can be represented as a collection of independent harmonic oscillators. The physical meaning of an oscillator is density oscillations propagating in the system. Due to the uncertainty principle, the oscillation energy in the ground state is also non-zero. These vacuum oscillations represent the above-mentioned dynamic fluctuations that spread the BC, as they provide a non-zero kinetic energy in the system in the ground state. This energy would be zero if the BC density were equal to that of the system (as it is in the ideal gas). The given energy can be represented as the kinetic energy of over-condensate particles. On the other hand, the same energy can be presented as the energy of virtual quasiparticles. Such a dualism is related to the fact that, as it was demonstrated in the previous approach, a particle has no certain momentum due to a polarization of its environment and the uncertainty principle. The Schrödinger equation in the space of collective variables gives a possibility to calculate the above-mentioned vacuum energy and the number of BCs. The obtained formula coincides with the Bogolyubov one (1). In addition, it is shown that dynamic fluctuations result in a decrease of the BEC temperature. We also obtained an expression for the number of BCs in weakly excited states of a Bose system, where an important role is also played by kinematic fluctuations that represent excited states of the above-mentioned oscillators and additionally suppress the BC.

These two approaches represent different patterns of the same mechanism of BC suppression. In the both cases, the reason for this phenomenon consists in the uncertainty principle, whose action is the stronger, the more intense is the interaction between particles, and is partially balanced by the action of the principle of particle identity. This balance causes a finite number of BCs with a lower density than that of the system. A particle in a non-ideal Bose gas has no certain momentum, and its distribution function represents a squared wave function in the momentum space. One can consider that each particle occupies a superposition of condensate and over-condensate states. The measurement of its momentum results in a reduction of the wave function to one of these states. The weight of each state determines the fraction of condensate and over-condensate particles observed experimentally.

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ПОДАВЛЕННЯ БОЗЕ-КОНДЕНСАТУ В СИСТЕМІ ВЗАЄМОДІЮЧИХ БОЗЕ-ЧАСТИНОК

К.В. Григоришин, Б.І. Лев

Р е з ю м е

Запропоновано модель подавлення бозе-конденсату у слабоневзаємодіючому бозе-газі за рахунок динамічних квантових флуктуацій, існування яких зумовлено принципом невизначеності. Розглянуто два підходи до описання механізму даного явища: вивчення руху окремих частинок системи у наближенні самоузгодженого поля та вивчення колективних рухів у наближенні випадкових фаз.