

Degenerate Bose gas without anomalous averages

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Abstract. Theory of a weakly non-ideal Bose gas in the canonical ensemble is developed without assumption of the C-number representation of the creation and annihilation operators with zero momentum. Instead of this assumption, we use the assumption on the C-number nature of the density operator $N_0 = a_0^\dagger a_0$ with zero momentum. It is shown that the pole of the “density–density” Green function (DDGF), as well as the pole of the single-particle Green function (SPGF), exactly coincide with the Bogoliubov phonon–roton spectrum of excitations for both assumptions. This spectrum, as is known confirmed by many neutron and x-ray experimental measurements of the dynamic structure factor in He II, is straightly related to the DDGF. At the same time, we show that in the other case under consideration, when neither N_0 nor $a_0^\dagger$ and a_0 are C-numbers, a gap can exist in SPGF. This gap in SPGF excitations is straightly related to the density of particles in the “condensate”. Therefore, the spectra of excitations for the DDGF and SPGF in the last case under consideration are different, in contrast to the Bogoliubov-type theory where these spectra are identical.

1. Introduction and historical remarks

Starting with Bogoliubov’s paper [1], the microscopic theory of the degenerate Bose gas was based on the special assumption that the creation $a_0^\dagger$ and annihilation a_0 operators of particles with zero momentum can be replaced by the C-number,

$$a_0^\dagger = a_0 = \langle N_0 \rangle^{1/2}, \quad (1)$$

where $\langle N_0 \rangle$ is the average number of particles in the state with $\mathbf{p} = 0$ (“condensate”).

This assumption leads to the necessity of introducing the *anomalous averages* (“quasi-averages”) into the theory. This is a strong assumption for the homogeneous and isotropic system under consideration. Let us pay attention that statement (1) in Bogoliubov’s papers is directly related to the requirement of the weak interparticle interaction in the degenerated Bose gas. The Bogoliubov theory gives rise to many important and widely recognized results, such as the expression for the spectrum of excitations, explanation of the experimental data and agreement with the Landau superfluidity condition. However, there are some doubts on the necessity of relation (1), as well as on the validity and agreement of the Hamiltonian corresponding to the assumption (1) with the original Hamiltonian of the system under consideration.

In this work, we propose a self-consistent and non-contradictory description of the degenerate Bose gas in which we do not use the assumption (1).



In section 2, we establish the equivalence of two Hamiltonians with and without the term containing the Fourier-component of the interaction potential $u(q = 0)$ for describing the averages of the non-ideal Bose gas in the canonical ensemble.

In section 3, the explicit (at low temperatures) equations for the auxiliary functions $F(\mathbf{p}, \mathbf{q}, z)$ defining the retarded density–density Green function $\chi^R(\mathbf{q}, z)$ are formulated. In this way, we can find the dynamic structure factor for strongly degenerate Bose gas $S(\mathbf{q}, \omega)$, observed by neutron and x-ray scattering.

In section 4, the equations formulated in section 3 are solved under the assumption that the operator $N_0 = a_0^\dagger a_0$ is a C-number (instead of the assumption that $a_0^\dagger$ and a_0 are C-numbers). On this basis, the density–density Green function is found. The collective excitation spectrum in the “density–density” Green function (DDGF) is exactly identical to that in the Bogoliubov theory of the approximate Hamiltonian diagonalization.

In section 5, within the equations formulated in section 3, we demonstrate the version of the perturbation theory, which permits to find the single-particle Green function (SPGF) with the same poles as in the DDGF. To obtain this result, the introduction of the anomalous Green’s function and the assumption on C-number behavior of the operators $a_0^\dagger$ and a_0 are not necessary. At the same time, we show that the use of these assumptions in general equations leads to the same result for the spectrum as for the consideration of anomalous averages. Therefore, we conclude that anomalous averages in the problem under consideration are not necessary, and all results of the theory based on anomalous averages can be reproduced based on the proposed theory without anomalous averages.

Finally, in section 6, we analyze the other approximation for solving explicit equations obtained in section 3. This approach does not use the assumptions on C-number behavior of operators at all. At the same time, the higher-order terms on the interaction potential are omitted. This approximation seems valid for a weakly non-ideal Bose system. In particular, in this way we show that the gap in the spectrum of single-particle excitations exists. The statement that the spectrum of single-particle excitations can have a gap along with the usual phonon–roton branch of collective excitations in the degenerate Bose gas was formulated in [2].

It should be noted that the gap in the spectrum of the weakly non-ideal Bose gas was examined by Bogoliubov in [1], by Landau for superfluid He in [3], and in some other papers. However, this opportunity was omitted by the reason of the necessity to obtain the sound excitations observed in He II.

At the same time, the opportunity to find different excitations in the density–density Green function (DDGF, directly measured by neutron and x-ray scattering) and in the single-particle Green function (SPGF, which cannot be directly measured experimentally) was recognized later, but it could not be implemented within the theory with anomalous averages due to the Goldstone theorem. However, the Goldstone theorem itself is valid only in the framework of the theory with anomalous averages (see [4] for more details). This means that when constructing the theory without anomalous averages, as is done below, one should consider the possibility of obtaining different poles in DDGF and SPGF. The necessary condition associated with experimental observations is only the existence of Bogoliubov-type phonon–roton excitations in the DDGF. However, the approach including both spectra, with and without a gap, has not yet been found. The coexistence of these two excitation branches is justified in this paper.

As we mentioned, the existence of the gap was suggested in [2]. The spectra, thermodynamics, and dynamic structure factor for weakly non-ideal Bose gas below the condensation temperature $T < T_0$ were considered in [5–7], in terms of the dielectric formalism, similar to that in plasma-like systems. The dielectric formalism based on the Bogoliubov assumption (1) for the operators $a_0^\dagger$ and a_0 was developed (see, e.g. [4]).

Recently, the gap-existence problem for the weakly non-ideal Bose gas was considered by different methods [8–10].

In fact, the paper [8] confirmed (independently) and developed not only the statement of [2] about the existence of the gap in the SPGF for the weakly non-ideal Bose gas below the condensation temperature, but also the results of the papers [5–7] on the possibility of considering the superfluid system without symmetry breaking. Surely, the existence of the gap disagrees with the conventional opinion that the gap is missing. We do believe that the conclusion about a missing gap is related to the Bogoliubov simplifying assumption (1), and is not obliged to persist in the theory. At the same time, we also constructed a version of the theory without anomalous averages, in which the DDGF and SPGF are identical [10]. The results of this paper are close to the theory with anomalous averages and to the theory by Belyayev [11]. In fact, in our approach, these two versions appear as a result of a different kind of summation in the series of the perturbation theory. The final choice between these two theories can be done based on theoretical self-consistence, as well as by qualitative and quantitative comparisons of theoretical calculations of thermodynamic functions of He II, followed by a comparison of these calculations with experiments in a wide temperature range, including the vicinity of the superfluid-to-normal transition temperature.

In the present work, we suggest that all particles tend to occupy the zero-momentum state in the limit of strong degeneracy $T \rightarrow 0$, where T is the system temperature, which means that

$$\lim_{T \rightarrow 0} \langle N_0 \rangle = \langle N \rangle, \quad (2)$$

where $\langle N \rangle$ is the average number of particles in the system. This statement is confirmed in the paper by the self-consistent consideration. Below we use the canonical ensemble, where N can be considered as a given C-number for calculating all physical quantities described by Hermitian operators.

2. Statistical sum and averages in the canonical ensemble

Let us consider the Hamiltonian of the non-ideal Bose gas of particles with zero spin and mass m in volume V

$$H = \sum_p \varepsilon_p a_p^\dagger a_p + \frac{1}{2V} \sum_{\mathbf{q}, \mathbf{p}_1, \mathbf{p}_2} u(\mathbf{q}) a_{\mathbf{p}_1 - \mathbf{q}/2}^\dagger a_{\mathbf{p}_2 + \mathbf{q}/2}^\dagger a_{\mathbf{p}_2 - \mathbf{q}/2} a_{\mathbf{p}_1 + \mathbf{q}/2}, \quad (3)$$

where $a_p^\dagger$ and a_p are the creation and annihilation operators of particles with momentum $\hbar \mathbf{p}$,

$$[a_{\mathbf{p}_2}, a_{\mathbf{p}_1}^\dagger] = a_{\mathbf{p}_2} a_{\mathbf{p}_1}^\dagger - a_{\mathbf{p}_1}^\dagger a_{\mathbf{p}_2} = \delta_{\mathbf{p}_1, \mathbf{p}_2}. \quad (4)$$

$\varepsilon_p = \hbar^2 \mathbf{p}^2 / 2m$ is the energy spectrum of a free particle and $u(\mathbf{q})$ is the Fourier component of the inter-particle interaction potential.

It is convenient to extract the particular term U_0 with $\mathbf{q} = 0$ from the sum over $\mathbf{q}$ in the Hamiltonian (3). This term can be written as

$$U_0 = u(0) \frac{N(N-1)}{2V}, \quad \hat{N} = \sum_p a_p^\dagger a_p, \quad u(0) = u(\mathbf{q} = 0). \quad (5)$$

Here we use the possibility of replacing the operator $\hat{N}$ of the total number of particles by the C-number $N = \langle \hat{N} \rangle$ in the canonical ensemble everywhere, where the physical variables are considered. These variables are described by Hermitian operators. Hereafter, the brackets $\langle \dots \rangle$ mean the canonical-ensemble averaging over the equilibrium state. Since, therefore, U_0 is the C-number, one can write the statistical sum of the system under consideration in the form

$$Z = \text{Tr} \exp(-H/T) = \exp \left(-u(0) \frac{N(N-1)}{2VT} \right) \text{Tr} \exp(-H_0/T), \quad (6)$$

where

$$H_0 = H - U_0 = \sum_p \varepsilon_p a_p^\dagger a_p + \frac{1}{2V} \sum_{\mathbf{q} \neq 0, \mathbf{p}_1, \mathbf{p}_2} u(\mathbf{q}) a_{\mathbf{p}_1 - \mathbf{q}/2}^\dagger a_{\mathbf{p}_2 + \mathbf{q}/2}^\dagger a_{\mathbf{p}_2 - \mathbf{q}/2} a_{\mathbf{p}_1 + \mathbf{q}/2}. \quad (7)$$

Therefore, to provide convergence of the statistical sum (7) in the thermodynamic limit $V \rightarrow \infty$, $N \rightarrow \infty$, $n = N/V = \text{const}$, the known condition $u(0) > 0$ has to be fulfilled. Since U_0 is a C-number, it does not affect any averaging at all; hence, the Hamiltonian $\hat{H}$ is equivalent to $\hat{H}_0$ for calculating average values. For an arbitrary operator $\langle A \rangle$, we get

$$\langle A \rangle = Z^{-1} \text{Tr}\{\exp(-H/T)A\} = Z_0^{-1} \text{Tr}\{\exp(-H_0/T)A\} \equiv \langle A \rangle_0, \quad Z_0 = \text{Tr} \exp(-H_0/T). \quad (8)$$

Let us now consider a more complicated situation associated with calculations of time-dependent correlation functions $f(t)$ such as

$$f(t) = \langle [A(t), B(0)] \rangle, \quad A(t) = \exp(iHt/\hbar)A \exp(-iHt/\hbar). \quad (9)$$

The time dependence of the operators $a_p^\dagger(t)$ and $a_p(t)$ can be represented in the form

$$a_p^\dagger(t) = \exp(iH_0t/\hbar) a_p^\dagger \exp(-iH_0t/\hbar) \exp(iNu(0)t/V\hbar), \quad (10)$$

$$a_p(t) = \exp(-iNu(0)t/V\hbar) \exp(iH_0t/\hbar) a_p \exp(-iH_0t/\hbar). \quad (11)$$

Therefore, if the numbers of creation and annihilation operators coincide in each of the operators A and B (which is typical of the operators of the physical variables), the time-dependent correlation function can be written as

$$f(t) = \langle [A(t), B(0)] \rangle_0, \quad A(t) = \exp(iH_0t/\hbar)A \exp(-iH_0t/\hbar), \quad (12)$$

where $\langle \dots \rangle_0$ hereafter means averaging over the canonical equilibrium ensemble defined by the Hamiltonian $\hat{H}_0$. On this basis, in what follows, we consider the average values with the Hamiltonian $\hat{H}_0$ (7) within the canonical ensemble. The free energy of the initial system with the Hamiltonian H (3), according to (5)–(7), reads

$$F = -T \ln Z = U_0 + F_0, \quad F_0 = -T \ln Z_0. \quad (13)$$

3. Equations for “density–density” Green function

Experimentally, the collective excitation spectrum is usually found from data on the well observed maxima in the dynamic structure factor $S(\mathbf{q}, \omega)$ for $\mathbf{q} \neq 0$,

$$S(\mathbf{q}, \omega) = \frac{1}{V} \int_{-\infty}^{\infty} \exp(i\omega t) \langle \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) \rangle_0 dt, \quad (14)$$

$$\rho_{\mathbf{q}}(t) = \sum_p a_{\mathbf{p}-\mathbf{q}/2}^\dagger(t) a_{\mathbf{p}+\mathbf{q}/2}(t), \quad (15)$$

where $\rho_{\mathbf{q}}(t)$ is the Fourier component of the density operator in the Heisenberg representation. The dynamic structure factor $S(\mathbf{q}, \omega)$ (14) is directly related to imaginary part of the retarded density–density Green function $\chi^R(\mathbf{q}, z)$ which is analytical in the upper semi-plane of the complex variable z ($\text{Im}z > 0$),

$$S(\mathbf{q}, \omega) = -\frac{2\hbar}{1 - \exp(-\hbar\omega/T)} \text{Im} \chi^R(\mathbf{q}, \omega + i0), \quad (16)$$

$$\chi^R(\mathbf{q}, z) = -\frac{i}{\hbar V} \int_0^\infty dt \exp(izt) \langle [\rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0)] \rangle_0 \equiv \frac{1}{V} \langle \langle \rho_{\mathbf{q}} | \rho_{-\mathbf{q}} \rangle \rangle_z, \quad (17)$$

where square brackets $[AB]$ mean the commutator of the corresponding operators $[AB] = AB - BA$, while brackets $\langle\langle \dots \rangle\rangle$ mean a convenient notation for the integral in (17), which simplifies further calculations. The definitions (16), (17) have to be taken in the thermodynamic limit, where

$$\lim_{T \rightarrow 0} \langle N_0 \rangle_0 = \langle N \rangle_0 = N. \quad (18)$$

According to equation (14), the retarded function $\chi^R(\mathbf{q}, z)$ can be represented in the form

$$\chi^R(\mathbf{q}, z) = \frac{1}{V} \sum_p F(\mathbf{p}, \mathbf{q}, z), \quad F(\mathbf{p}, \mathbf{q}, z) = \langle\langle a_{\mathbf{p}-\mathbf{q}/2}^\dagger a_{\mathbf{p}+\mathbf{q}/2} | \rho_{-q} \rangle\rangle_z. \quad (19)$$

The equation of motion for the function $F(\mathbf{p}, \mathbf{q}, z)$ with the Hamiltonian H_0 , determined by equation (7), can be written in the form

$$\begin{aligned} (\hbar z + \varepsilon_{\mathbf{p}-\mathbf{q}/2} - \varepsilon_{\mathbf{p}+\mathbf{q}/2}) F(\mathbf{p}, \mathbf{q}, z) &= f_{\mathbf{p}-\mathbf{q}/2} - f_{\mathbf{p}+\mathbf{q}/2} \\ &- \frac{1}{V} \sum_k u(k) \sum_{p_1} \langle\langle (a_{\mathbf{p}+\mathbf{k}-\mathbf{q}/2}^\dagger a_{\mathbf{p}_1-\mathbf{k}/2}^\dagger a_{\mathbf{p}_1+\mathbf{k}/2} a_{\mathbf{p}+\mathbf{q}/2} \\ &- a_{\mathbf{p}-\mathbf{q}/2}^\dagger a_{\mathbf{p}_1-\mathbf{k}/2}^\dagger a_{\mathbf{p}_1+\mathbf{k}/2} a_{\mathbf{p}-\mathbf{k}+\mathbf{q}/2}) | \rho_{-q} \rangle\rangle_z. \end{aligned} \quad (20)$$

Here $f_{\mathbf{p}}$ is the single-particle distribution function over the momenta $\hbar \mathbf{p}$

$$f_{\mathbf{p}} = \langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \rangle_0. \quad (21)$$

For temperatures $T < T_0$, where T_0 is the condensation temperature, the single-particle distribution function $f_{\mathbf{p}}$ can be represented as

$$f_{\mathbf{p}} = \langle N_0 \rangle_0 \delta_{\mathbf{p},0} + f_{\mathbf{p}}^T (1 - \delta_{\mathbf{p},0}), \quad (22)$$

where $\hat{N}_0 = a_0^\dagger a_0$ is the operator of the number of particles with zero momentum (“condensate”), $f_{\mathbf{p}}^T = \langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \rangle_0$ is the single-particle distribution function with non-zero momenta (the “overcondensate” states). Therefore,

$$n = n_0 + \frac{1}{V} \sum_{p \neq 0} f_{\mathbf{p}}^T = n_0 + \int \frac{d^3 p}{(2\pi)^3} f_{\mathbf{p}}^T, \quad (23)$$

where $n_0 = \langle N_0 \rangle_0 / V$ is the average density of particles in the condensate. From (20) and (22), we find that the function $F(\mathbf{p}, \mathbf{q}, z)$ has singularities at $\mathbf{p} = \pm \mathbf{q}/2$. Therefore, the density-density function $\chi^R(q, z)$ (19) can be written as

$$\chi^R(q, z) = \frac{1}{V} F(\mathbf{q}/2, \mathbf{q}, z) + \frac{1}{V} F(-\mathbf{q}/2, \mathbf{q}, z) + \frac{1}{V} \sum_{p \neq \pm q/2} F^T(\mathbf{p}, \mathbf{q}, z). \quad (24)$$

The index T means that the respective function describes the “overcondensate” particles. The singularities (conditioned by the condensate) in this function are absent. Then, in the last term in equation (24), we can replace summation by integration over momenta. The functions

$F(\pm \mathbf{q}/2, \mathbf{q}, z)$ extracted above satisfy, according to equations (20) and (22), the exact equations of motion

$$(\hbar z - \varepsilon_q) F(\mathbf{q}/2, \mathbf{q}, z) = [\langle N_0 \rangle_0 - f_{\mathbf{q}}^T] - \frac{1}{V} \sum_{k \neq 0} u(k) \sum_{p_1} \langle \langle (a_{\mathbf{k}}^\dagger a_{\mathbf{p}_1 - \mathbf{k}/2}^\dagger a_{\mathbf{p}_1 + \mathbf{k}/2} a_{\mathbf{q}} - a_0^\dagger a_{\mathbf{p}_1 - \mathbf{k}/2}^\dagger a_{\mathbf{p}_1 + \mathbf{k}/2} a_{\mathbf{q} - \mathbf{k}}) | \rho_{-q} \rangle \rangle_z, \quad (25)$$

$$(\hbar z + \varepsilon_q) F(-\mathbf{q}/2, \mathbf{q}, z) = -[\langle N_0 \rangle_0 - f_{\mathbf{q}}^T] - \frac{1}{V} \sum_{k \neq 0} u(k) \sum_{p_1} \langle \langle (a_{\mathbf{k} - \mathbf{q}}^\dagger a_{\mathbf{p}_1 - \mathbf{k}/2}^\dagger a_{\mathbf{p}_1 + \mathbf{k}/2} a_0 - a_{-\mathbf{q}}^\dagger a_{\mathbf{p}_1 - \mathbf{k}/2}^\dagger a_{\mathbf{p}_1 + \mathbf{k}/2} a_{-\mathbf{k}}) | \rho_{-q} \rangle \rangle_z. \quad (26)$$

Let us further consider the case of strongly degenerate gas, where $T \rightarrow 0$. To find the main terms, according to the Bogoliubov procedure applied to this case, let us extract the terms on the right-hand sides of equations (25) and (26), which are determined by the maximum number of the operators $a_0^\dagger$ and a_0 . In the limit of strong degeneracy, taking into account (18), we can omit the other terms in calculating F . Then, since $f_{\mathbf{q}}^T = f_{-\mathbf{q}}^T$ ($\mathbf{q} \neq 0$), equations (25), (26) take the form

$$(\hbar z \mp \varepsilon_q) F^{(0)}(\pm \mathbf{q}/2, \mathbf{q}, z) = \pm[\langle N_0 \rangle_0 - f_{\mathbf{q}}^T] \pm \frac{1}{V} u(q) \langle \langle (a_0^\dagger a_0^\dagger a_{\mathbf{q}} a_0 + a_0^\dagger a_{-\mathbf{q}}^\dagger a_0 a_0) | \rho_{-q} \rangle \rangle_z. \quad (27)$$

Equations (27) are exact at low temperature, since they define the functions $F^{(0)}(\pm \mathbf{q}/2, \mathbf{q}, z)$. To calculate the Green functions on the right-hand side of equations (27), some approximations can be introduced.

4. Determination of collective excitations

It should be emphasized that the Bogoliubov approach, in which the operators $a_0^\dagger$ and a_0 are considered as C-numbers, leads to violation of the exact relations (25) and (26). In this approach (1), the main term $F^{(0)}$ of the function F has the form

$$F^{(0)}(\pm \mathbf{q}/2, \mathbf{q}, z) = \langle N_0 \rangle_0 \langle \langle a_{\pm \mathbf{q}} | a_{\pm \mathbf{q}}^\dagger \rangle \rangle_z. \quad (28)$$

Accordingly, instead of the exact equations for two-particle Green functions (25) and (26), we obtain the equation of motion for the single-particle Green functions form (28). As is shown below, the equations of motion for the two-particle Green functions without the approximation of the C-number representation of the operators $a_0^\dagger$ and a_0 are essentially different from the equations for the single-particle distribution functions. Therefore, the assumption (1) cannot be used to calculate the Green functions on the right-hand side of (27). At the same time, the idea itself of the C-number approximation seems very attractive for some operators. Below we apply this idea to the version alternative to the Bogoliubov assumption. According to (18), it is natural to accept that to calculate the Green functions in the limit of strong degeneracy $T \rightarrow 0$, the C-number approximation has to be applied not to the operators $a_0^\dagger$ a_0 , but to the physical quantity, i.e., the operator of the number of particles in the “condensate” $\hat{N}_0$

$$N_0 = \langle \hat{N}_0 \rangle_0. \quad (29)$$

For low temperatures T , the operator $\hat{N}_0$ in the averages (under the angle brackets) can be replaced by the operator of the total number of particles $\hat{N}$ (equal to $\rho_{q=0}$), which is the C-number (in the sense mentioned in section 2) in the canonical ensemble. Therefore, in the case at hand, it can be removed from brackets. Therefore, for low temperatures, the proposed approximation seems asymptotically exact.

In this approximation, it directly follows from (27) that

$$(\hbar z - \varepsilon_q) F^{(0)}(\mathbf{q}/2, \mathbf{q}, z) = [\langle N_0 \rangle_0 - f_{\mathbf{q}}^T] + \frac{\langle N_0 \rangle_0}{V} u(q) \{F^{(0)}(\mathbf{q}/2, \mathbf{q}, z) + F^{(0)}(-\mathbf{q}/2, \mathbf{q}, z)\}, \quad (30)$$

$$(\hbar z + \varepsilon_q) F^{(0)}(-\mathbf{q}/2, \mathbf{q}, z) = -[\langle N_0 \rangle_0 - f_{\mathbf{q}}^T] - \frac{\langle N_0 \rangle_0}{V} u(q) \{F^{(0)}(\mathbf{q}/2, \mathbf{q}, z) + F^{(0)}(-\mathbf{q}/2, \mathbf{q}, z)\}. \quad (31)$$

From equations (30), (31), one can find the solutions to the functions $F(\pm q/2, q, z)$

$$F(\mathbf{q}/2, \mathbf{q}, \hbar z) = \frac{[\langle N_0 \rangle_0 - f_{\mathbf{q}}^T](\hbar z + \varepsilon_q)}{(\hbar z)^2 - (\hbar \omega(q))^2}; \quad F(-\mathbf{q}/2, \mathbf{q}, z) = -\frac{[\langle N_0 \rangle_0 - f_{\mathbf{q}}^T](\hbar z - \varepsilon_q)}{(\hbar z)^2 - (\hbar \omega(q))^2}, \quad (32)$$

$$\hbar \omega(q) \equiv \sqrt{\varepsilon_q^2 + 2n_0 u(q) \varepsilon_q}, \quad (33)$$

where $n_0 = N_0/V$. The relation (33) for the spectrum $\hbar \omega(q)$ corresponds exactly to the known Bogoliubov expression [1]. By substituting to (19), and taking into account that the contribution of the functions $F^T(\mathbf{p}, \mathbf{q}, z)$ is negligible in the case of strong degeneracy, we obtain the expression for the main term $\chi^{(0)}(q, z)$ of the “density–density” Green function $\chi(q, z)$

$$\chi^{(0)}(q, z) = \frac{2n_0 \varepsilon_q}{(\hbar z)^2 - (\hbar \omega(q))^2} \left\{ 1 - \frac{f_{\mathbf{q}}^T}{\langle N_0 \rangle_0} \right\}. \quad (34)$$

As is well known, the singularities of the function $\chi^R(q, z)$ determine the collective excitation spectrum in the system. Therefore, under the assumption about C-number behavior of the operator $\hat{N}_0$, we obtain the Bogoliubov result for the collective excitation spectrum in the degenerate and weakly interacting Bose gas. However, the question on the braced term $f_{\mathbf{q}}^T / \langle N_0 \rangle_0$ in (34) remains open. The problem is in the behavior of the function $f_{\mathbf{q}}^{\text{id}}$ for the ideal Bose gas

$$f_{\mathbf{q}}^{\text{id}} = \left\{ \exp \left(\frac{\varepsilon(q)}{T} \right) - 1 \right\}^{-1}. \quad (35)$$

In the limit of small wave vectors q the function $f_{\mathbf{q}}^{\text{id}}$ diverges at non-zero temperatures (hereafter, $1/q^2$ —divergence). Moreover,

$$\lim_{T \rightarrow 0} \lim_{q \rightarrow 0} f_{\mathbf{q}}^{\text{id}} \neq \lim_{q \rightarrow 0} \lim_{T \rightarrow 0} f_{\mathbf{q}}^{\text{id}}. \quad (36)$$

The similar problem arises when (22) is used.

5. Single-particle excitations

To calculate the distribution function $f_{\mathbf{q}}^T$ for “overcondensate” particles in the Bose gas, let us consider the single-particle Green function $g^R(q, z)$

$$g^R(q, z) = \langle \langle a_{\mathbf{q}} | a_{\mathbf{q}}^\dagger \rangle \rangle_z, \quad \mathbf{q} \neq 0. \quad (37)$$

This function is directly related to the distribution function $f_{\mathbf{q}}^T$ as

$$f_{\mathbf{q}}^T = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g^<(q, \omega), \quad g^<(q, \omega) = -2\hbar \left\{ \exp \left(\frac{\hbar \omega}{T} \right) - 1 \right\}^{-1} \text{Im } g^R(q, \omega + i0). \quad (38)$$

The equation of motion for the Green function $g^R(q, z)$ for $q \neq 0$ reads

$$(\hbar z - \varepsilon_q) g^R(q, z) = 1 + \frac{1}{V} \sum_{k \neq 0} u(k) \sum_p \langle \langle a_{\mathbf{p}+\mathbf{k}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}+\mathbf{k}} | a_{\mathbf{q}}^\dagger \rangle \rangle_z. \quad (39)$$

As for the “density–density” Green function, we consider the case of strong degeneracy and extract the terms with the maximum number of operators $a_0^\dagger$ and a_0 on the right-hand side of equation (39). Then from equation (39), we find

$$(\hbar z - \varepsilon_q) g^R(q, z) = 1 + \frac{1}{V} u(q) \left\{ \langle \langle a_0^\dagger a_{\mathbf{q}} a_0 | a_{\mathbf{q}}^\dagger \rangle \rangle_z + \langle \langle a_{-\mathbf{q}}^\dagger a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle \rangle_z \right\} (1 - \delta_{q,0}). \quad (40)$$

In this case, it is assumed that the separated main term on the right-hand side of (40) corresponds to the case of the weak interaction. In the general case, when the interparticle interaction potential $u(q)$ is not small, in separating the terms with a maximum number of the operators $a_0^\dagger$ and a_0 on the right-hand side of (40), it is necessary to write an infinite series of the perturbation theory on the interaction $u(q)$. It is clear that a similar situation occurs when using (27) instead of (26). Thereby, strictly speaking, the question whether the terms separated on the right-hand side of (40) are main from the viewpoint of the passage to the limit of the weak interaction remains open.

If we now apply the assumption (1) about the C-number representation of particle creation $a_0^\dagger$ and annihilation a_0 operators at a zero momentum to the calculation of Green functions on the right-hand side of (40), we come to the necessity of introducing the so-called “anomalous” Green functions

$$g_{\text{anom}}^R(q, z) = \langle \langle a_{-\mathbf{q}}^\dagger | a_{\mathbf{q}}^\dagger \rangle \rangle_z, \quad \mathbf{q} \neq 0. \quad (41)$$

Let us pay attention that the nonzero value of the anomalous function g_{anom}^R , strictly speaking, requires the influence of an external field of special form on the system under consideration.

We stress that, to provide a non-zero value of anomalous averages, this external field should include nonphysical combinations of the creation and annihilation operators, or other words to be nonphysical. As a result, taking into account (1) and (41), relation (40) takes the form

$$(\hbar z - \varepsilon_q) g^R(q, z) = 1 + n_0 u(q) \{ g^R(q, z) + g_{\text{anom}}^R(q, z) \}. \quad (42)$$

Then we use the equation of motion for the anomalous function $g_{\text{anom}}^R(q, z)$ at $q \neq 0$ with Hamiltonian (7),

$$(\hbar z + \varepsilon_q) g_{\text{anom}}^R(q, z) = -\frac{1}{V} \sum_{k \neq 0} \sum_p u(k) \langle \langle a_{\mathbf{q}-\mathbf{k}}^\dagger a_{\mathbf{p}-\mathbf{k}}^\dagger a_{\mathbf{p}} | a_{\mathbf{q}}^\dagger \rangle \rangle_z. \quad (43)$$

Now, as in the above consideration, we separate terms with a maximum number of the operators $a_0^\dagger$ and a_0 on the right-hand side of (43). Then, from (43), we obtain

$$(\hbar z + \varepsilon_q) g_{\text{anom}}^R(q, z) = -\frac{u(\mathbf{q})}{V} \left\{ \langle \langle a_0^\dagger a_{-\mathbf{q}}^\dagger a_0 | a_{\mathbf{q}}^\dagger \rangle \rangle_z + \langle \langle a_0^\dagger a_0^\dagger a_{\mathbf{q}} | a_{\mathbf{q}}^\dagger \rangle \rangle_z \right\}. \quad (44)$$

Using the assumption (1) on the C-number representation of the particle creation $a_0^\dagger$ and annihilation a_0 operators at a zero momentum in the calculation of Green functions on the right-hand side of (44), we find

$$(\hbar z + \varepsilon_q) g_{\text{anom}}^R(q, z) = -n_0 u(q) \{ g^R(q, z) + g_{\text{anom}}^R(q, z) \}. \quad (45)$$

It is evident that relations (42) and (45) form a set of algebraic equations in the functions $g^R(q, z)$ and $g_{\text{anom}}^R(q, z)$, from which it immediately follows that

$$g^R(q, z) = \frac{\hbar z + \varepsilon_q + n_0 u(q)}{(\hbar z)^2 - (\hbar \omega(q))^2}, \quad (46)$$

where the spectrum $\omega(q)$ is defined by relation (33). Thus, the poles of the single-particle Green function $g^R(q, z)$ when using the assumption (1) about the C-number representation of the particle creation $a_0^\dagger$ and annihilation a_0 operators at a zero momentum coincide with the poles of the DDGF $\chi^R(q, z)$, see (34).

The above consideration is based on the assumption that it is sufficient to consider the terms with a maximum number of the operators $a_0^\dagger$ and a_0 in the calculation of Green functions at the temperature close to zero. In this case, it is supposed that the interparticle interaction is weak.

Let us now show that the result (46) can be obtained based on the consideration of the terms with a maximum number of the operators $a_0^\dagger$ and a_0 without the use of anomalous Green functions $g_{\text{anom}}^R(q, z)$. To this end, we write the equation of motion for the function $\langle\langle a_{-\mathbf{q}}^\dagger a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle\rangle_z$, see (40),

$$\begin{aligned} (\hbar z + \varepsilon_q) \langle\langle a_{-\mathbf{q}}^\dagger a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle\rangle_z = & -\frac{1}{V} \sum_{k \neq 0} \sum_p u(k) \langle\langle \{ a_{\mathbf{k}-\mathbf{q}}^\dagger a_{\mathbf{p}-\mathbf{k}}^\dagger a_p a_0 a_0 \\ & - a_{-\mathbf{q}}^\dagger a_{\mathbf{p}-\mathbf{k}}^\dagger a_p a_{-\mathbf{k}} a_0 - a_{\mathbf{k}-\mathbf{q}}^\dagger a_0 a_{\mathbf{p}-\mathbf{k}}^\dagger a_p a_{-\mathbf{k}} \} | a_{\mathbf{q}}^\dagger \rangle\rangle_z. \end{aligned} \quad (47)$$

Then, on the right-hand side of (47), we separate the terms with a maximum number of the operators $a_0^\dagger$ and a_0 ,

$$(\hbar z + \varepsilon_q) \langle\langle a_{-\mathbf{q}}^\dagger a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle\rangle_z = -\frac{u(q)}{V} \left\{ \langle\langle a_0^\dagger a_0^\dagger a_q a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle\rangle_z + a_0^\dagger a_{-\mathbf{q}}^\dagger a_0 a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle\rangle_z \right\}. \quad (48)$$

We now use the previously advanced assumption (29) that the operator of the number of “condensate” particles $\hat{N}_0 = a_0^\dagger a_0$ is the C-number, rather than the operators $a_0^\dagger$ and a_0 . Then, from (48), it immediately follows that

$$(\hbar z + \varepsilon_q) \langle\langle a_{-\mathbf{q}}^\dagger a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle\rangle_z = -n_0 u(q) \left\{ \langle N_0 \rangle_0 g^R(q, z) + \langle\langle a_{-\mathbf{q}}^\dagger a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle\rangle_z \right\}, \quad (49)$$

or

$$\langle\langle a_{-\mathbf{q}}^\dagger a_0 a_0 | a_{\mathbf{q}}^\dagger \rangle\rangle_z = -\frac{n_0 u(q)}{(\hbar z)^2 + \varepsilon(q) + n_0 u(q)} \langle N_0 \rangle_0 g^R(q, z). \quad (50)$$

If we substitute relation (50) into (40), we again obtain the expression for the single-particle Green function $g^R(q, z)$.

Thus, to obtain the known results for the spectra of excitations in the degenerate Bose gas, there is no need for the assumption (1) about the C-number representation of the particle creation $a_0^\dagger$ and annihilation a_0 operators at a zero momentum and no need for putting into consideration anomalous Green functions (41).

Let us now return to relation (34) for the “density–density” Green function $\chi^R(q, z)$, from which it follows the necessity of calculating the single-particle distribution function f_q^T for “overcondensate” states. Substituting the obtained expression (46) for the single-particle Green function into (38), we find

$$f_q^T = \frac{\varepsilon(q) + n_0 u(q)}{2\hbar \omega(q)} \coth \left(\frac{\hbar \omega(q)}{2T} \right) - \frac{1}{2}. \quad (51)$$

Let us pay attention that the dependence of the single-particle distribution function f_q^T for “overcondensate” states on the order of limit transitions $T \rightarrow 0$ and $q \rightarrow 0$, see (36), again follows from (51). At the same time, to solve the problem of the braced term $f_q^T / \langle N_0 \rangle_0$ in relation (34), we can reason as follows. The minimum nonzero wave vector q in a specified large but finite volume V is proportional to $V^{-1/3}$. Therefore, in the thermodynamic limit $V \rightarrow \infty$, $N \rightarrow \infty$, $N/V = \text{const}$, the term $f_q^T / \langle N_0 \rangle_0$ can be considered to be zero provided that $n_0 = \langle N_0 \rangle_0 / V \neq 0$, independently of the order of the limit transitions $T \rightarrow 0$ and $q \rightarrow 0$.

At first sight, the above results in the limit of the weak interaction completely solve the problem of the description of the weakly non-ideal degenerate Bose gas. However, it should be taken into account that, as follows from (23), (50), the number of particles in “overcondensate” states

$$\langle N_T \rangle_0 = N - \langle N_0 \rangle_0 = V \int d^3q f_q^T \quad (52)$$

is nonzero even at zero temperature. Thus, in the limit $T \rightarrow 0$, the number of particles in the condensate $\langle N_0 \rangle_0 \neq N$. Hence, the assumption about C-number behavior of the operator $\hat{N}_0 = a_0^\dagger a_0$, and even more so the operators $a_0^\dagger$ and a_0 separately cannot be considered as grounded even in the limit of the weak interaction.

6. Gap and the self-consistent distribution function

In this regard, let us return to the consideration of equation (40) under the assumption that we correctly considered the effects of the weak interparticle interaction. Then, taking into account the above consideration, we will not assume C-number behavior of the operator $\hat{N}_0 = a_0^\dagger a_0$ as well as the operators $a_0^\dagger$ and a_0 separately. Then, from the viewpoint of the perturbation theory on the interparticle interaction, the second braced term on the right-hand side of (40) is the higher-order term in comparison with the first term; therefore, it can be neglected in the assumption of our interest. This approach seems necessary since the SPGF (37) is the average of the non-Hermitian operator structure; in this case, the C-number representation is, strictly speaking, unacceptable even for the operator N , see (10), (11). Let us pay attention that, from this point of view, the result (34) for the DDGF remains valid.

Then, in the limit of the weak interparticle interaction, from equation (40) we obtain

$$g^R(q, z) = \frac{1}{\hbar z - E_q}. \quad (53)$$

The expression for the spectrum of single-particle excitations E_q is given by

$$E_q = \varepsilon_q + n_0 u(q). \quad (54)$$

From equations (38), (52), (53), for the limit of strong degeneracy $T \ll T_0$, for the distribution function of the overcondensate particles, we obtain

$$f_q^T = \frac{1}{\exp(E_q/T) - 1}. \quad (55)$$

Therefore, the function f_q^T is finite for $q \rightarrow 0$. Moreover, in the limit of strong degeneracy $T \rightarrow 0$

$$f_q^T \rightarrow 0 \quad (56)$$

for arbitrary values of q , in contrast to the case of the ideal Bose gas. Therefore, the representation (22) for the single-particle distribution function f_p is valid, the initial suggestions

(2), (18) are satisfied, and the used procedure for extracting the main terms is self-consistent. As is easily seen from (42), (43) for $T \rightarrow 0$, all particles in the considered approximation are placed in the “condensate” with the momentum $p = 0$, in contrast to the Bogoliubov theory of the weakly non-ideal homogeneous Bose gas (the effects of inhomogeneity will be considered in further publication). According to the accepted theory, the interaction between particles leads to the quantum depletion of the condensate, which means the appearance of the particles with $p \neq 0$ at $T = 0$. However, this statement is based on the assumption about the identity of the excitation spectra for the single-particle Green function and dynamic structure factor. Only in this case, the condensate density $n_0(T)$ can be calculated based on the experimental data for $S(q, \omega)$ and the corresponding collective excitations. This coincidence takes place in the standard theory of weakly non-ideal Bose gas, which is constructed on the assumption about anomalous averages. This assumption is extended to liquid He II, where the approximate scheme for calculating n_0 is used. Therefore, the depletion of the Bose condensate is not an experimental fact, but is the consequence of applying the theoretical concept of the identity of single-particle and collective spectra, obtained in the anomalous averages approach for weakly non-ideal Bose gas. It was shown above that the theories based on C-number approximations for operators in the state with zero momentum are not self-consistent.

In the theory developed for SPGF in the approximation considered in this Section, depletion is absent and, according to the above argumentation, there is no contradiction between this result and the existing experiments for the dynamic structure factor, since the latter cannot be applied to calculate the particle momentum distribution. In general, in a more elaborated theoretical approach taking into account the higher-order terms on the interaction potential, the depletion for $T \rightarrow 0$ can appear in the theory without anomalous averages. In this case, the above-condensate can appear even at $T = 0$ as a result of the strong interaction. However, even for such an approach, the identity of the SPGF and DDGF poles seems an exceptional occasion. Therefore, the Bose particle momentum distribution should be found theoretically using the corresponding approximation for the SPGF. In our opinion, based on the above theoretical results, the experimental determination of depletion requires a further deep analysis which will be performed in the separate paper.

For the approach under consideration, the gap appears in the spectrum of single-particle excitations (in the pole of the SPGF), which is given by

$$\Delta_{\text{int}} \equiv \Delta^{(h)} = E_{q \rightarrow 0} = n_0 u(0). \quad (57)$$

The value of the gap is completely defined by the density of particles in the “condensate” (see figure 1). The existence of the gap permits to extend essentially the applicability of the results obtained for $T \rightarrow 0$. It is obvious that the condition $T \rightarrow 0$ is equivalent to the condition $T \ll \Delta^{(h)}$ in many applications.

Taking into account (44) we can rewrite equation (56) for the function $\chi^{(0)}(q, z)$ in the form

$$\chi^{(0)}(q, z) = \frac{2n_0 \varepsilon_q}{(\hbar z)^2 - (\hbar \omega(q))^2}. \quad (58)$$

Based on (58), almost all known results for the thermodynamic functions of the degenerate Bose gas can be reproduced as in [5–7].

Therefore, in contrast to the approach based on the C-number approximation for the operators $a_0^\dagger$ and a_0 (or on the C-number approximation for the operator $\hat{N}_0$ in the direct perturbation theory in the presence of the condensate), in the case of the perturbation theory without C-number approximation, we find that the spectra of collective and single-particle excitations are different. Both spectra, as is easily seen, satisfy the Landau condition for superfluidity. For the single-particle spectrum, the Landau condition is satisfied for the

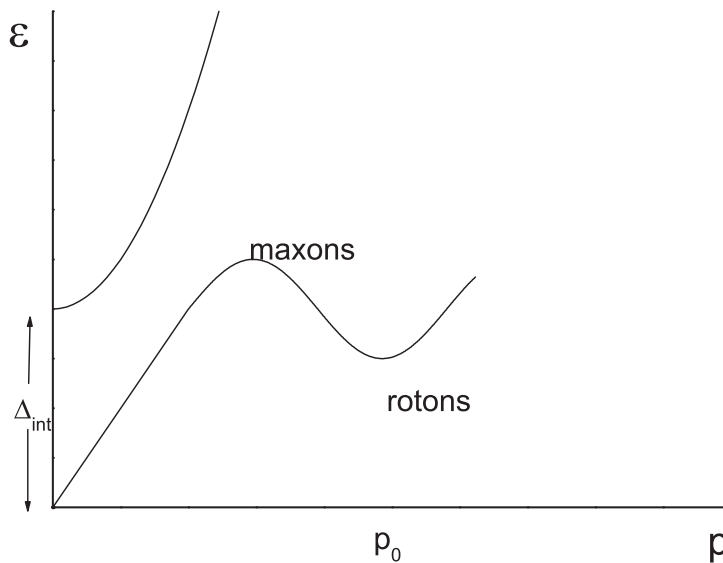


Figure 1. Phonon–roton spectrum and the expected spectrum of single-particle excitations (“helons”) with the gap $\Delta_{\text{int}} \equiv \Delta^{(h)}(T)$ depending on interaction and temperature.

transitions between the “condensate” and the “overcondensate” state. The Landau condition is, naturally, violated for transitions between the “overcondensate” states.

7. Conclusions

Summarizing the above consideration, we can assert that the calculation of the Green functions for the highly degenerate Bose gas on the basis of the C-number approximation for the operator N_0 and the straightforward perturbation theory allows the following conclusions.

- (i) The problem of the $1/q^2$ divergence, arising for the ideal Bose gas, can be solved.
- (ii) The system has two different branches of excitations, i.e., the single-particle and collective ones, both satisfying the Landau condition of superfluidity. The former and latter appear as SPGF and DDGF poles, respectively.
- (iii) The single-particle excitation spectrum contains the gap in the region of small wave vectors, associated with the existence of the “condensate”.
- (iv) The collective excitation spectrum corresponds to “phonon–roton” excitations observed in the experiments on inelastic neutron scattering. This spectrum is the gapless mode which unrelated to the Goldstone theorem.
- (v) There is no need for anomalous averages (quasi-averages) to describe the degenerate Bose gas.

In this connection, we emphasize that the Goldstone theorem which justifies the gapless branch of excitations is in itself the result of the breaking symmetry assumption. Therefore, it cannot be applied to the theory considered above, which is constructed without breaking symmetry assumption (e.g., without anomalous averages). In our paper, we showed that the breaking symmetry is not necessary.

At the same time, the Bogoliubov result for the collective phonon–roton mode is completely reproduced in our approach as the branch of excitations for the DDGF.

It should also be mentioned that Hugenholtz and Pines, constructing the diagram technique for the degenerated Bose gas, reformulated the problem at the beginning, by changing, according

to Bogoliubov, the operators $a_0^\dagger$ and a_0 by C-numbers. In this way, they could apply almost automatically the quantum field theory methods to the study of the Bose gas with “condensate”. In particular, it was shown that, for the C-number representation of the operators $a_0^\dagger$ and a_0 , the gap in excitations associated with the single-particle Green function cannot exist.

We note that the DDGF and SPGF poles coincide, according to existed theories associated with the anomalous averages assumption. However, recently, Kita [12] first paid attention that the dielectric formalism is based on the analysis of the structure of the perturbation theory series, performed separately (non-self-consistently) for the matrices of anomalous single- and two-particle Green functions. This means that coincidence of the DDGF and SPGF is absent even in the extended description on the basis of anomalous averages. Thus, such an analysis can be inadequate due to the ambiguity how to determine self-energy and vertex functions inherent to Bose-Einstein condensate, using the relation with two-particle Green functions. In other words, such an analysis should be performed within the formalism allowing unified consideration of both single- and two-particle Green functions.

In the case at hand, it should be noted that the assumption about anomalous averages has no any fundamental basis, is inapplicable to the ideal Bose gas and, as we showed above, can be avoided for the non-ideal Bose gas. Historically, the assumption of breaking symmetry in the Bose gas theory played a crucial role and was very useful, but in fact it is not necessary.

The proposed theory does not contradict the fundamental physical laws; the known experiments on the collective mode can be qualitatively described since this mode is the same as that in the existing theory based on the breaking symmetry assumption. The Landau criterion of superfluidity breakdown is also fulfilled for both excitation branches (DDGF and SPGF). The respective limitation for the superfluid velocity following from the phonon–roton gap existence is, naturally, the same as in the breaking symmetry approach. The limitation following from the SPGF depends on the gap parameters.

Therefore, the interparticle interaction in Bose systems leads not only to the drastic difference (in comparison with the ideal Bose gas) in the structure of collective excitations, which are described by the DDFG, but also to the crucial change in the distribution function of single-particle excitations and in the single-particle excitation spectrum of “overcondensate” particles.

Based on the results obtained, the special diagram technique similar to that in [11] can be developed, but with the use of the C-number approximation for the operator $\hat{N}_0$.

The principal difference between the results of this study and the results of the “traditional” C-number approximation for the operators $a_0^\dagger$ and a_0 (as well as for the operator N_0) is the existence of the gap in the spectrum of single-particle excitations. The above analysis shows that this gap cannot manifest itself in the experiments on inelastic neutron scattering in superfluid helium. However, such possibility cannot be excluded in the experiments on Raman light scattering.

Probably, the gap for single-particle excitations can manifest itself in the experiments on the density profile in trapped Bose gases [13]. However, this question cannot be considered within the present paper and has to be studied separately.

Acknowledgments

The authors would like to thank M V Fedorov, G J F van Heijst, A M Ignatov, A G Khrapak, Yu A Kukharevko[†], A A Rukhadze and A G Zagorodny for the helpful discussions. This study was supported by the Russian Science Foundation (project No. 14-19-01492).

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