Abstract: The comparative behaviour of normal and anomalous averages as functions of momentum or energy, at different temperatures, is analysed for systems with Bose-Einstein condensate. Three qualitatively distinct temperature regions are revealed: The critical region, where the absolute value of the anomalous average, for the main energy range, is much smaller than the normal average. The region of intermediate temperatures, where the absolute values of the anomalous and normal averages are of the same order. And the region of low temperatures, where the absolute value of the anomalous average, for practically all energies, becomes much larger than the normal average. This shows the importance of the anomalous averages for the intermediate and, especially, for low temperatures, where these anomalous averages cannot be neglected.

Normal and anomalous averages for systems with Bose-Einstein condensate

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1. Introduction

In the last years, the physics of dilute Bose gases has received much consideration both in theoretical and experimental aspects. An exhaustive list of references can be found in the recent review articles [1–4] and books [5,6]. The theoretical description of dilute systems with Bose-Einstein condensate is, to a large extent, based on the ideas of the Bogolubov theory, advanced in the papers [7,8] and thoroughly expounded in books [9,10]. This is because the present-day experiments deal in the majority of cases exactly with such dilute Bose gases.

The starting idea of the Bogolubov theory is the breaking of gauge symmetry by means of the so-called Bogolubov shift for the field operator

\[ \psi(r) = \eta(r) + \psi_1(r), \]

where \( \eta(r) \) is the condensate wave function, related to a coherent state [11,12] and defining the condensate density \( \rho_0(r) = |\eta(r)|^2 \). As soon as the gauge symmetry is broken, in addition to the normal averages \( \langle \psi^+(r)\psi(r') \rangle \) or \( \langle a_\ell^+ a_k \rangle \), depending on whether the real or momentum space is considered, the anomalous averages \( \langle \psi(r)\psi(r') \rangle \) or \( \langle a_k a_{-k} \rangle \) arise in the theory.

The physical meaning and general features of the normal averages, which are directly connected with the reduced density matrices [13], seem to be familiar and clear

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to everyone. Contrary to this, the role and general behaviour of the anomalous averages are not always properly understood. There exists a very widespread delusion that the anomalous averages can be omitted at all, even at low temperatures. One often ascribes this unjustified trick to Popov, calling it the "Popov approximation". However, as is easy to infer from the original works by Popov [14–17], he has never done anything like that. He considered the temperatures in the close vicinity of the critical temperature $T_c$. When the temperature $T$ tends to $T_c$, then the condensate density $\rho_0$ tends to zero. The anomalous averages are proportional to $\rho_0$, hence, also tend to zero together with $\rho_0$. Contrary to this, the normal averages are proportional to the density of noncondensed particles $\rho_1$, which is close to the total density $\rho$, when $T \approx T_c$. That is why in a narrow neighbourhood of $T_c$ the anomalous averages automatically become much smaller than the normal averages, without any additional assumptions. However, for a dilute gas at low temperatures $T \ll T_c$, the condensate density can become comparable with the total density, $\rho_0 \approx \rho$, while, vice versa, the density of noncondensed particles can be much smaller than $\rho$. Then anomalous averages can be much larger than the normal ones, and there is no any grounds for omitting the former. Popov [14–17] has never neglected the anomalous averages at low temperatures $T \ll T_c$.

It is the aim of the present paper to analyse the behaviour of the anomalous averages at different temperatures and to illustrate the properties of the anomalous averages as compared to those of the normal averages. Such a comparison reveals the role of the anomalous averages emphasizing the importance of their contribution, especially at low temperatures, where the anomalous averages can never be neglected.

Throughout the paper, the system of units is employed, where the Planck constant $\hbar = 1$ and the Boltzmann constant $k_B = 1$ are set to unity.

2. Normal and anomalous averages

The behaviour of the averages can be rather different at varying temperature. It is possible to distinguish three principally different regions. For this purpose, the temperature $T$ should be compared with the characteristic value $\rho_0$, where $\rho \equiv N/V$ is the particle density for $N$ particles in volume $V$ and

$$\Phi_0 \equiv \int \Phi(r) \, dr \tag{1}$$

is the integral of the interaction potential $\Phi(r)$, assumed to be integrable. The value $\rho \Phi_0$ characterizes the average strength of particle interactions. Another typical quantity is the critical temperature $T_c$, which for a weakly interacting gas is close to the critical temperature for an ideal gas

$$T_c = \frac{2\pi}{m} \left[ \frac{\rho}{\zeta(3/2)} \right]^{2/3}, \tag{2}$$

where $m$ is particle mass and $\zeta(3/2) = 2.612$. The relation between $\rho \Phi_0$ and $T_c$ can be obtained by introducing the scattering length $a_s$ through the equation

$$\Phi_0 \equiv 4\pi \frac{a_s}{m}. \tag{3}$$

For the repulsive interactions, the scattering length is positive, which is assumed in what follows. Then we find

$$\frac{\rho \Phi_0}{T_c} = 2 \left[ \frac{\zeta}{\sqrt{3}} \right]^{2/3} \rho^{1/3} a_s. \tag{7}$$

Keeping in mind a dilute gas, for which by definition

$$\rho a_s^3 \ll 1, \tag{4}$$

we obtain

$$\frac{\rho \Phi_0}{T_c} \ll 1. \tag{5}$$

In this way, we can distinguish the following temperature regions. The interval of low temperatures is

$$0 \leq T \leq \rho \Phi_0. \tag{6}$$

Intermediate temperatures correspond to the inequalities

$$\rho \Phi_0 < T \ll T_c. \tag{7}$$

And the temperatures $T \sim T_c$ close to the critical point pertain to the critical temperature region.

The critical region of temperatures in the close vicinity of the condensation temperature $T_c$ was analysed by Popov [14–16]. In this region, the anomalous averages turned out to be small as compared to the normal ones. This fact is very simple to understand, since when temperature tends to $T_c$, the anomalous averages are proportional to the density of condensed particles $\rho_0$, which tends to zero as $T \to T_c$. But the normal averages are proportional to the density of noncondensed particles $\rho_1$, which tends, as $T \to T_c$, to the finite value $\rho$ of the total particle density. This is why in the close neighbourhood of $T_c$ the contribution of the anomalous averages is small as compared to that of the normal averages.

However at the temperatures outside the critical region, the situation can be drastically different. And we have to study these lower temperatures more attentively. We shall consider a uniform dilute gas, for which the inequality (4) is valid.

In a dilute gas, for $T \ll T_c$, almost all particles are condensed. Then the Bogolubov theory [7–10] is applicable. Following this theory, one makes the Bogolubov shift of the field operators and retains quadratic fluctuations of the noncondensed particles, which results in the Hamiltonian

$$H = \frac{1}{2} N_0 \rho_0 \Phi_0 - \mu N_0 + \sum_{k \neq 0} \omega_k a_k^\dagger a_k +$$

$$\frac{1}{2} \sum_{k \neq 0} \sum_{h \neq 0} \Delta_k \left[ a_k^\dagger a_h^\dagger + a_{-h} a_k \right] , \tag{8}$$

where $\Delta_k$ is the scattering length and $\omega_k$ is the energy of the scattering.
in which $N_0$ is the number of condensed particles, $\rho_0 \equiv N_0/V$ is their density,

$$\omega_k \equiv \frac{k^2}{2m} + \rho_0(\Phi_0 + \Phi_k) - \mu ,$$

(9)

$\mu$ is chemical potential, and

$$\Delta_k \equiv \rho_0 \Phi_k ,$$

(10)

with $\Phi_k$ being the Fourier transform of the interaction potential,

$$\Phi_k = \int \Phi(r)e^{-ikr} \, dr .$$

Under the considered conditions, $N_0 \approx N$ is close to the total number of particles $N$.

The Hamiltonian (8) is diagonalized by means of the Bogolubov canonical transformation

$$a_k = u_k b_k + v^*_k b^+_k ,$$

in which the coefficient functions can be chosen to be symmetric and real, such that $u^*_k = u_{-k} = u_k$ and $v^*_k = v_{-k} = v_k$. They are defined by the relations

$$u^2_k - v^2_k = 1 , \quad u_k v_k = -\frac{\Delta_k}{2\epsilon_k} ,$$

$$u^2_k = \frac{\sqrt{\epsilon_k^2 + \Delta^2_k} + \epsilon_k}{2\epsilon_k} = \frac{\omega_k + \epsilon_k}{2\epsilon_k} ,$$

$$v^2_k = \frac{\sqrt{\epsilon_k^2 + \Delta^2_k} - \epsilon_k}{2\epsilon_k} = \frac{\omega_k - \epsilon_k}{2\epsilon_k} ,$$

where the Bogolubov spectrum is

$$\epsilon_k = \sqrt{\omega^2_k - \Delta^2_k} .$$

(11)

Under this transformation, Hamiltonian (8) is recast to the diagonal form

$$H_B = E_0 + \sum_{k \neq 0} \epsilon_k b^+_k b_k - \mu N_0 ,$$

(12)

with the ground-state energy

$$E_0 = \frac{1}{2} \rho_0 \Phi_0 + \frac{1}{2} \sum_{k \neq 0} (\epsilon_k - \omega_k) .$$

The separation of the condensate contribution, as is well known, is meaningful only when the momentum distribution of particles becomes singular at the point $k = 0$, which is associated with the particle spectrum touching zero at $k = 0$. Only then there is a reason of separating the zero-momentum terms [18], which is equivalent to the Bogolubov shift of the field operators [9,10]. At the same time, this guarantees a gapless spectrum, in agreement with the theorems by Hugenholtz and Pines [19] and Bogolubov [9,10]. These requirements can be simply formulated as the condition

$$\lim_{k \to 0} \epsilon_k = 0 , \quad \epsilon_k \geq 0 .$$

(13)

Then from spectrum (11), we get the chemical potential

$$\mu = \rho_0 \Phi_0 .$$

(14)

Another way of defining the chemical potential is by minimizing the thermodynamic potential

$$\Omega = -T \ln \text{Tr} \ e^{-\beta H}$$

with respect to $N_0$. Then from the equation

$$\frac{\partial \Omega}{\partial N_0} = \langle \frac{\partial H}{\partial N_0} \rangle = 0 ,$$

in the frame of the Bogolubov approximation, one obtains the same chemical potential (14). Respectively, Eq. (11) acquires the known form of the Bogolubov spectrum

$$\epsilon_k = \sqrt{\omega^2_k - \Delta^2_k} .$$

(15)

The diagonal Hamiltonian (12) makes it possible to find explicit expressions for different averages [20–22]. Our concern here is the normal average

$$n_k \equiv \langle a^+_k a_k \rangle$$

(16)

and the anomalous average

$$\sigma_k \equiv \langle a_k a_{-k} \rangle ,$$

(17)

whose absolute values are to be compared.

First of all, we can derive a general relation between averages (16) and (17), following from the Bogolubov inequality

$$\left| \langle \hat{A} \hat{B} \rangle \right|^2 \leq \left( \langle \hat{A} \hat{A}^+ \rangle \langle \hat{B}^+ \hat{B} \rangle \right) ,$$

valid for the averages involving any two operators. Setting here $\hat{A} = a_k$ and $\hat{B} = a_{-k}$, we find

$$|\langle a_k a_{-k} \rangle|^2 \leq \left| \langle a_k a_k \rangle \langle a_{-k} a_{-k} \rangle \right| .$$

This yields

$$\sigma_k^2 \leq n_k (1 + n_k) .$$

(18)

Calculating expressions (16) and (17), we have the normal average

$$n_k = \frac{\sqrt{\epsilon_k^2 + \Delta^2_k}}{2\epsilon_k} \coth \left( \frac{\epsilon_k}{2T} \right) - \frac{1}{2}$$

(19)

and the anomalous average

$$\sigma_k = -\frac{\Delta_k}{2\epsilon_k} \coth \left( \frac{\epsilon_k}{2T} \right) .$$

(20)
Inequality (18) holds true, since
\[ n_k (1 + n_k) - \sigma_k^2 = \left[ 2 \sinh \left( \frac{\varepsilon_k}{2T} \right) \right]^{-2}. \]

The spectrum (15) possesses the asymptotic properties
\[ \varepsilon_k \approx c k \quad (k \to 0), \quad \varepsilon_k \approx \frac{k^2}{2m} \quad (k \to \infty), \]
where \( c \equiv \sqrt{\rho_0 \Phi_0 / m} \) is the sound velocity, which tells us that \( \varepsilon_k \) varies in the range
\[ 0 \leq \varepsilon_k < \infty. \]

It is, therefore, convenient to analyse the behaviour of Eqs. (19) and (20) with respect to the variable \( \varepsilon_k \).

At small excitation energy, such that
\[ \varepsilon_k \ll \Delta_k, \quad \varepsilon_k \ll T, \]
the normal average (19) has the asymptotic behaviour
\[ n_k \approx \frac{T \Delta_k}{\varepsilon_k^2} + \frac{\Delta_k}{2 \Delta_k} + \frac{T}{2 \Delta_k} - \frac{1}{2}, \]
and the anomalous average (20) is
\[ \sigma_k \approx - \frac{T \Delta_k}{\varepsilon_k^2} - \frac{\Delta_k}{2 \Delta_k} + \frac{\Delta_k \varepsilon_k}{720 T^3}. \]

Hence at low energies \( \varepsilon_k \), or low momenta \( k \), the values \( n_k \) and \( |\sigma_k| \) asymptotically coincide for all temperatures. The region of small momenta \( k \) usually gives the largest contribution to the integrals representing the observable quantities. Consequently, the anomalous average plays an important role.

At large excitation energy, such that
\[ \varepsilon_k \gg \Delta_k, \quad \varepsilon_k \gg T, \]
the normal average behaves as
\[ n_k \approx \left( \frac{\Delta_k}{2 \varepsilon_k} \right)^2 - \left( \frac{\Delta_k}{2 \varepsilon_k} \right)^4 + e^{-\beta \varepsilon_k}, \]
while the anomalous average, as
\[ \sigma_k \approx - \frac{\Delta_k}{2 \varepsilon_k} (1 + 2 e^{-\beta \varepsilon_k}). \]

This shows that for \( k \to \infty \), the absolute value of the anomalous average is always much larger than \( n_k \ll |\sigma_k| \).

From Eqs. (22) and (23), we have
\[ \lim_{k \to 0} \left| \sigma_k \right| - n_k = \frac{1}{2} \left( 1 - \frac{T}{\rho \Phi_0} \right), \]
where we take into account that for the considered dilute gas \( \rho_0 \approx \rho \). Equality (26) demonstrates that, when \( T > \rho \Phi_0 \), then the value \( |\sigma_k| \) is smaller than \( n_k \) at \( k = 0 \), though becomes larger than the latter for \( k \to \infty \), according to Eqs. (24) and (25). This defines the region of intermediate temperatures (7), where \( |\sigma_k| \) is comparable with \( n_k \), being below \( n_k \) for small \( k \) and surpassing \( n_k \) for large \( k \). And for low temperatures from the interval (6), the absolute value of the anomalous average \( |\sigma_k| \) is larger than \( n_k \) in the whole range of the momenta \( k \geq 0 \).

To illustrate pictorially the relative behaviour of the normal and anomalous averages, we calculate Eqs. (19) and (20) numerically. It is convenient to measure the temperature \( T \) in units of \( \rho \Phi_0 \) and to treat \( n_k \) and \( \sigma_k \) as the functions of the dimensionless variable
\[ E \equiv \frac{\varepsilon_k}{\Delta_k}. \]

Then Eq. (19) can be rewritten as
\[ n(E) = \sqrt{1 + \frac{E}{2E}} \coth \left( \frac{E}{2T} \right) - \frac{1}{2}, \]
and Eq. (20) takes the form
\[ \sigma(E) = - \frac{1}{2E} \coth \left( \frac{E}{2T} \right). \]

The normal average (28) is non-negative for all \( E \geq 0 \), while the anomalous average (29) is always negative. To compare their absolute values, it is useful to introduce the notation
\[ A(E) \equiv |\sigma(E)|, \]
for the absolute value of the anomalous average (29).

Fig. 1 shows the typical behaviour of the anomalous value (30) and the normal average (28) for the low-temperature region (6), where \( A(E) \) is always larger than

\[ \frac{E}{\Delta_k}. \]
1. Conclusion

In the theory with broken gauge symmetry, anomalous averages play an important role. Although in the critical region, close to the condensate temperature, they become much smaller by the absolute value, as compared to the normal averages, however at lower temperatures, the situation turns to be essentially different. At temperatures \( \rho \varphi_0 < T \ll T_c \) in the dilute Bose gas, the absolute value of the anomalous average is of the same order as the normal average. For very low temperatures \( T \leq \rho \varphi_0 \), the anomalous average surpasses by its absolute value the normal average and can even be much larger than the latter. This analysis shows that, as soon as the gauge symmetry is broken, the anomalous averages come into play, being at low temperatures as important as the normal ones. It is,
Figure 6 The ratio $n(E)/A(E)$ for the intermediate temperature $T/\rho \phi_0 = 10$

therefore, principally incorrect to omit the anomalous averages for $T \ll T_c$. 

Note also the fundamental importance of the anomalous averages in the calculations of the particle fluctuations [23–25]. In the frame of the Bogolubov theory [7–10], the dispersion of the number-of-particle operator $N$ is

$$\Delta^2(N) = N[1 + 2 \lim_{k \to 0} (n_k + \sigma_k)].$$

The long-wave limits of $n_k$ and $\sigma_k$ separately are divergent, as follows from Eqs. (22) and (23). However, their singularities are the same in the absolute values while opposite in signs, because of which they cancel each other, yielding the finite limit

$$\lim_{k \to 0} (n_k + \sigma_k) = \frac{1}{2} \left( \frac{T}{m c^2} - 1 \right).$$

As a result, the dispersion of $\hat{N}$ becomes

$$\Delta^2(\hat{N}) = \frac{T N}{m c^2},$$

describing normal particle fluctuations. If one would omit $\sigma_k$ in $\Delta^2(\hat{N})$, this would lead to a divergent dispersion, hence, to a divergent isothermal compressibility $\kappa_T = \Delta^2(\hat{N})/\rho T N$, which would mean the system instability [23–25]. Thus, neglecting the anomalous averages not merely can drastically distort quantitative values of observables, but also provokes qualitatively wrong unphysical consequences.

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