

CALCULATION OF NONEQUILIBRIUM THERMODYNAMIC POTENTIAL OF BOSE SYSTEM NEAR THE CONDENSATION POINT

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Bose system of zero spin particles is considered in the presence of the Bose–Einstein condensate in the vicinity of the phase transition point. The system is investigated in the framework of the Bogolyubov model with the separated condensate. In this model an effective Hamiltonian of the system is introduced by replacing condensate creation and annihilation operators in system Hamiltonian by $n_0^{1/2}$ where n_0 is occupation number of the condensate state. According to Bogolyubov, the grand canonical thermodynamic potential related to the effective Hamiltonian is considered as nonequilibrium thermodynamic potential. In the present paper this potential is investigated as a function of the small variable n_0 . With the help of the thermodynamic perturbation theory it is shown that it is expanded in a series over integer powers of n_0 . This corresponds to the basic idea of the Landau theory of the phase transitions of the second kind. Coefficients at terms of the first and second orders in n_0 in the expansion are calculated for Bose gas in the main approximation in small interaction. Calculation of the coefficients at terms of the third and fourth orders needs accounting contributions of the thermodynamic perturbation theory at least of the 4th order and will be done elsewhere. It is established that the results obtained for Bose gas do not fit into the Landau theory of phase transitions of the second kind. Some comments that discuss the situation are given.

Keywords: Bose–Einstein condensation, model with the separated condensate, nonequilibrium thermodynamic potential, phase transitions of the second kind.

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1. Introduction

The concept of nonequilibrium thermodynamic (TD) potentials was formed as a means of studying the formation of structures in macroscopic systems by methods of thermodynamics [1]. In particular, this applies to the theory of phase transitions of the second kind developed by Landau. In the applications of nonequilibrium TD potentials in the Boltzmann formula they are also called effective Hamiltonians of the system [2]. Parameters that describe the emerging structure are called order parameters. The use of this or that nonequilibrium TD potential is not significant. If the temperature T and pressure p of the system are controlled, the nonequilibrium Gibbs TD potential $\Phi(T, p, \eta)$ is used ($\eta \equiv \{\eta_a\}$; in a general case η_a is a many-component order parameter). The most important property of a nonequilibrium TD potential is the presence of an extremum in equilibrium (in particular, $\Phi(T, p, \eta)$ has a minimum). In fact, nonequilibrium TD potentials are characteristics of the state of incomplete equilibrium of the system. In this case one subsystem is in equilibrium with the parameters T , p and another subsystem, which is not necessarily allocated in space, is nonequilibrium one and is described by the order parameter η_a as a parameter of the reduced description.

A number of approaches to the definition of nonequilibrium TD potentials are known in the literature. In the Landau–Leontovich approach [3, 4] (see also [5]) it is said that the nonequilibrium TD potential $\Phi(T, p, \eta)$ is obtained by the Legendre transformation of equilibrium TD potential in the presence of an external field $\Phi(T, p, h)$ ($h \equiv \{h_a\}$, in the general case h_a is a many-component external field whose contribution to the Hamiltonian of the system has the form $\sum_a h_a \hat{\eta}_a$ where $\hat{\eta}_a$ is the microscopic value of the order parameter η_a). Another definition, which also belongs to Landau [2], is introduced using the Boltzmann

formula, which gives the distribution of the values of the order parameter in equilibrium and is considered to be accurate. The realization of these definitions in the microscopic theory is developed in our papers [6, 7] for states in the vicinity of equilibrium. In this case the smallness of the deviation from equilibrium is the only small parameter of the theory.

Another approach to the problem of constructing a nonequilibrium TD potential belongs to Bogolyubov [8] (see also [9]) and it is based on the fact that in the TD limit one can substitute the microscopic values of the order parameter $\hat{\eta}_a$ by its mean values in the system Hamiltonian. It introduces an effective Hamiltonian and an appropriate TD potential that plays the role of a nonequilibrium TD potential. Note that this corresponds to Landau's idea that the quantum nature of the order parameter is not important in the theory (see [2]). The realization of this definition in a microscopic theory in the vicinity of equilibrium, as the construction of a nonequilibrium TD potential in general, is an actual task (see, for example, [10, 11]).

In this paper, we discuss the implementation of the Bogolyubov definition for the Bose system in the presence of condensate (in the literature there is an increase of interest to the study of Bose condensation (see, for example, [11, 12])). In such a system, the order parameter is the occupation number of the one-particle state with the momentum $\mathbf{p} = 0$. At a temperature T below the condensation temperature T_0 , the equilibrium value n_0^o of the occupation number is macroscopic, that is n_0^o / \mathbf{V} is a finite value (\mathbf{V} is the system volume). Bogolyubov's approach to the theory of the Bose system in the presence of condensate is called the model with the separated condensate. In the framework of this approach, the Hamiltonian of the system \hat{H} is replaced by an effective one $\hat{H}(n_0)$, the grand canonical TD potential $\Omega(T, \mu)$ is replaced by the function $\Omega(T, \mu, n_0)$ that has its minimum in equilibrium [8] (see also [9]) and gives potential $\Omega(T, \mu)$. The task of our work is to calculate the TD potential $\Omega(T, \mu, n_0)$ in the case of a small occupation number n_0 , that is, in the vicinity of the transition point.

The paper is constructed as it follows. The section 2 describes the Bogolyubov approach to the theory of Bose systems in the presence of condensate. The section 3 is devoted to the construction of the thermodynamic perturbation theory for calculating the nonequilibrium grand canonical potential near the phase transition point.

2. The Bogolyubov model with the separated condensate

Bose system of zero spin particles in the presence of condensation is considered. The Hamilton operator of the system is chosen in the usual form

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{H}_1, \quad \hat{H}_0 = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a_{\mathbf{p}}^+ a_{\mathbf{p}}, \\ \hat{V} &= \frac{1}{2\mathbf{V}} \sum_{\mathbf{p}_1 \dots \mathbf{p}_4} v(\mathbf{p}_1 - \mathbf{p}_3) \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{p}_3 + \mathbf{p}_4} a_{\mathbf{p}_1}^+ a_{\mathbf{p}_2}^+ a_{\mathbf{p}_3} a_{\mathbf{p}_4} \end{aligned} \quad (1)$$

where

$$\varepsilon_{\mathbf{p}} = p^2 / 2m, \quad v(\mathbf{p}) = \int d\mathbf{x} \Phi(|\mathbf{x}|) e^{i\mathbf{p}\mathbf{x}},$$

$\Phi(r)$ is the potential of interaction between particles, \mathbf{V} is the volume of the system (we put that $\hbar = 1$).

The grand canonical statistical operator of the system in the absence of condensate has the form

$$w = e^{\beta\{\Omega - \hat{H} + \mu\hat{N}\}}, \quad \text{Sp } w = 1; \quad \hat{N} = \sum_{\mathbf{p}} a_{\mathbf{p}}^+ a_{\mathbf{p}} \quad (2)$$

where β is an inverse temperature, μ is a chemical potential, \hat{N} is the operator of the number of particles. The thermodynamic potential Ω is determined by the normalization condition (2), and the average value \bar{A} of an arbitrary physical quantity A with the corresponding operator \hat{A} is calculated by the formula

$$\bar{A} = \text{Sp } w \hat{A}. \quad (3)$$

In the presence of the condensate, one-particle state with the momentum $\mathbf{p} = 0$ contains the macroscopic number of particles $n_0 \sim \mathbf{V}$. In this case, condensate operators a_0, a_0^+ can be considered as real c-numbers for which $a_0^+ a_0 = n_0$. In the approach developed by Bogolyubov (the model with the separated condensate) [8], the statistical operator $w(n_0)$ is introduced by replacing $a_0, a_0^+ \rightarrow n_0^{1/2}$

$$w(n_0) = e^{\beta\{\Omega(n_0) - \hat{H}(n_0) + \mu\hat{N}(n_0)\}}, \quad \tilde{\text{Sp}} w(n_0) = 1 \quad (4)$$

where

$$\begin{aligned} \hat{N}(n_0) &\equiv \hat{N}|_{a_0, a_0^+ \rightarrow n_0^{1/2}} = \hat{N}_1 + n_0, & \hat{H}(n_0) &\equiv \hat{H}|_{a_0, a_0^+ \rightarrow n_0^{1/2}} = \hat{H}_0 + \hat{V}(n_0); \\ \hat{V}(n_0) &\equiv \hat{V}|_{a_0, a_0^+ \rightarrow n_0^{1/2}} = v_0 \frac{n_0^2}{2\mathbf{V}} + v_0 \frac{n_0}{\mathbf{V}} \hat{N}_1 + n_0 \hat{V}_2 + n_0^{1/2} \hat{V}_3 + \hat{V}_4 \end{aligned} \quad (5)$$

($v(\mathbf{p} = 0) \equiv v_0$) and the notations

$$\begin{aligned} \hat{N}_1 &= \sum_{\mathbf{p} \neq 0} a_{\mathbf{p}}^+ a_{\mathbf{p}}, & \hat{V}_2 &= \frac{1}{2\mathbf{V}} \sum_{\mathbf{p} \neq 0} v(\mathbf{p})(a_{\mathbf{p}}^+ a_{\mathbf{p}} + a_{\mathbf{p}}^+ a_{-\mathbf{p}}) + h.c., \\ \hat{V}_3 &= \frac{1}{\mathbf{V}} \sum_{\mathbf{p}_1, \dots, \mathbf{p}_3 \neq 0} v(\mathbf{p}_2) \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{p}_3} a_{\mathbf{p}_1}^+ a_{\mathbf{p}_2}^+ a_{\mathbf{p}_3}^+ + h.c., \\ \hat{V}_4 &= \frac{1}{2\mathbf{V}} \sum_{1234 \neq 0} v(\mathbf{p}_1 - \mathbf{p}_3) \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{p}_3 + \mathbf{p}_4} a_{\mathbf{p}_1}^+ a_{\mathbf{p}_2}^+ a_{\mathbf{p}_3} a_{\mathbf{p}_4} \end{aligned} \quad (6)$$

are introduced. Here and thereafter the trace $\tilde{\text{Sp}}$ is taken over the non-condensate states. The normalization condition (4) determines the TD potential $\Omega(n_0)$. Bogolyubov proved [8] (see also [9]) that the equilibrium value n_0^o of the occupation number n_0 can be found from the condition of the extremum of this potential

$$\left. \frac{\partial \Omega(n_0)}{\partial n_0} \right|_{n_0 = n_0^o} = 0. \quad (7)$$

This suggests that one can consider $\Omega(n_0)$ as nonequilibrium TD potential of the Bose system in the presence of condensate. At the same time, the operator $\hat{H}(n_0)$, which is defined by formula (6), can be considered as an effective Hamiltonian of the system. In addition, it can be proved [9] that formula (7) is equivalent to such expression for the chemical potential of the system

$$\mu = \tilde{\text{Sp}} w(n_0) \frac{\partial \hat{V}(n_0)}{\partial n_0} \Big|_{n_0=n_0^o} . \quad (8)$$

Equilibrium TD potential is given by the formula [8, 9]

$$\Omega = \Omega(n_0^o) . \quad (9)$$

The average value \bar{A} of an arbitrary physical quantity A with an operator \hat{A} should be calculated according to the formula [8, 9]

$$\bar{A} = \tilde{\text{Sp}} w(n_0^o) \hat{A}(n_0^o), \quad \hat{A}(n_0) \equiv \hat{A} \Big|_{a_0, a_0^+ \rightarrow n_0^{1/2}} . \quad (10)$$

The purpose of this work is to calculate the function $\Omega(n_0)$ near the condensation point when the value n_0 / \mathbf{V} is small. The obtained expression for nonequilibrium thermodynamic potential can be compared with the Landau theory of phase transition of the second kind.

3. Construction of the thermodynamic perturbation theory

The statistical operator $w(n_0)$ can be written in the form

$$w(n_0) = e^{\beta\{F - (\hat{\mathbf{H}}_0 + \hat{\mathbf{U}})\}}, \quad \hat{\mathbf{U}} = \hat{U}_1 + \hat{U}_2 \quad (11)$$

where it is denoted

$$\begin{aligned} F &= \Omega(n_0) - \frac{v_0}{2} \frac{n_0^2}{\mathbf{V}} + \mu n_0, & \hat{\mathbf{H}}_0 &= \hat{H}_0 - \mu \hat{N}_1 + \hat{V}_4, \\ \hat{U}_1 &= n_0^{1/2} \hat{V}_3, & \hat{U}_2 &= n_0 (\hat{V}_2 + \frac{v_0}{\mathbf{V}} \hat{N}_1). \end{aligned} \quad (12)$$

In the main approximation in the small occupation number n_0 the statistical operator $w(n_0)$ takes the form

$$w_0 = e^{\beta\{F_0 - \hat{\mathbf{H}}_0\}}, \quad \tilde{\text{Sp}} w_0 = 1. \quad (13)$$

In accordance with the TD perturbation theory, the potential F is given by the formula (see, for example, [9, 13])

$$\beta F = \beta F_0 - \ln[1 + \tilde{\text{Sp}} w_0 (\hat{S}_1 + \hat{S}_2 + \dots)] \quad (14)$$

where

$$\hat{S}_n = (-1)^n \int_0^\beta d\beta_1 \dots \int_0^{\beta_{n-1}} d\beta_n \hat{\mathbf{U}}(\beta_1) \dots \hat{\mathbf{U}}(\beta_n), \quad \hat{\mathbf{U}}(\beta) = e^{\beta \hat{\mathbf{H}}_0} \hat{\mathbf{U}} e^{-\beta \hat{\mathbf{H}}_0}. \quad (15)$$

The structure of operators \hat{S}_n is determined by the formulas

$$\begin{aligned} \hat{S}_1 &= \hat{S}_1^1 + \hat{S}_1^2, \\ \hat{S}_2 &= \hat{S}_2^{11} + (\hat{S}_2^{12} + \dots) + \hat{S}_2^{22}, \\ \hat{S}_3 &= \hat{S}_3^{111} + (\hat{S}_3^{112} + \dots) + (\hat{S}_3^{122} + \dots) + \hat{S}_3^{222}, \\ \hat{S}_4 &= \hat{S}_4^{1111} + (\hat{S}_4^{2111} + \dots) + (\hat{S}_4^{2211} + \dots) + (\hat{S}_4^{2221} + \dots) + \hat{S}_4^{2222}, \\ \hat{S}_5 &= \hat{S}_5^{11111} + (\hat{S}_5^{21111} + \dots) + (\hat{S}_5^{22111} + \dots) + (\hat{S}_5^{22211} + \dots) + (\hat{S}_5^{22221} + \dots) + \hat{S}_5^{22222}. \end{aligned} \quad (16)$$

Here the contribution $S_{n+m}^{\overbrace{2\dots 2}^n \overbrace{1\dots 1}^m}$ contains the product of the operators \hat{U}_1, \hat{U}_2 in the order $\overbrace{\hat{U}_2\dots\hat{U}_2}^n \overbrace{\hat{U}_1\dots\hat{U}_1}^m$. The three points in (16) denote the contributions that can be obtained from $S_{n+m}^{\overbrace{1\dots 1}^n \overbrace{2\dots 2}^m}$ with all the permutations of the operators \hat{U}_1, \hat{U}_2 .

The total number of creation and annihilation operators a_p^+, a_p in an operator \hat{A} , which is the product of operators a_p^+, a_p with different moments, is denoted by $\sigma(\hat{A})$. From (6) and (12) it is clear that

$$\sigma(S_{n+m}^{\overbrace{2\dots 2}^n \overbrace{1\dots 1}^m}) = 2n + 3m, \quad S_{n+m}^{\overbrace{2\dots 2}^n \overbrace{1\dots 1}^m} \sim n_0^{n+m/2}. \quad (17)$$

When calculating averages in (14), it is useful to take into account the formulas

$$[\hat{N}_1, a_p] = -a_p, \quad [\hat{N}_1, a_p^+] = a_p^+$$

which give

$$[\hat{N}_1, \hat{A}] = \hat{A}s(\hat{A}) \quad (18)$$

where \hat{A} is an arbitrary product of creation and annihilation operators a_p^+, a_p ; $s(\hat{A})$ is the difference of the quantities of the operators a_p^+ and a_p in \hat{A} . The relation (18) shows that the operators \hat{H}_0 (12) and w_0 (13) commute with the operator \hat{N}_1

$$[\hat{H}_0, \hat{N}_1] = 0, \quad [w_0, \hat{N}_1] = 0. \quad (19)$$

Hence a number of selection rules for calculating the averages with the statistical operator w_0 follow; they are the consequence of the identity

$$0 = \tilde{\text{Sp}}[w_0, \hat{N}_1]\hat{A} = \tilde{\text{Sp}} w_0[\hat{N}_1, \hat{A}] = s(\hat{A})\tilde{\text{Sp}} w_0\hat{A},$$

i.e.

$$\tilde{\text{Sp}} w_0\hat{A} = 0 \quad \text{at} \quad s(\hat{A}) \neq 0. \quad (20)$$

It is clear that for an operator \hat{A} with an odd total number $\sigma(\hat{A})$ of creation and annihilation operators the value $s(\hat{A}) \neq 0$ and its average value is zero: $\tilde{\text{Sp}} w_0\hat{A} = 0$. Therefore, it follows from (17) that in (16)

$$\tilde{\text{Sp}} w_0 S_{n+(2m+1)}^{\overbrace{2\dots 2}^n \overbrace{1\dots 1}^{2m+1}} = 0, \quad \tilde{\text{Sp}} w_0 S_{n+2m}^{\overbrace{2\dots 2}^n \overbrace{1\dots 1}^{2m}} \sim n_0^{n+m}. \quad (21)$$

Given this, we have

$$\begin{aligned} & \text{Sp} w_0 (\hat{S}_1 + \hat{S}_2 + \dots) = \\ & = \text{Sp} w_0 [\hat{S}_1^2 + \hat{S}_2^{11} + \hat{S}_2^{22} + (\hat{S}_3^{112} + \dots) + \hat{S}_4^{1111} + (\hat{S}_4^{1122} + \dots) + \hat{S}_4^{2222} + (\hat{S}_5^{11112} + \dots) + \\ & + (\hat{S}_5^{11222} + \dots) + \hat{S}_6^{111111} + (\hat{S}_6^{111122} + \dots) + (\hat{S}_6^{112222} + \dots) + \hat{S}_6^{222222} + (\hat{S}_7^{1122222} + \dots) + \\ & + (\hat{S}_7^{1111222} + \dots) + (\hat{S}_7^{1111112} + \dots) + \hat{S}_8^{22222222} + (\hat{S}_8^{11222222} + \dots) + (\hat{S}_8^{11112222} + \dots) + \\ & + (\hat{S}_8^{11111122} + \dots) + \hat{S}_8^{11111111}] + \dots \end{aligned} \quad (22)$$

where in each of the terms there is an even number of units and all terms have the integer power of n_0 . Taking into account the dependence of all terms here on n_0 given by (21), we have such an expansion in powers of n_0 for the average included in (14)

$$a \equiv \tilde{\text{Sp}} w_0 (\hat{S}_1 + \hat{S}_2 + \dots) = a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + O(n_0^7), \quad a_s \sim n_0^s \quad (23)$$

where

$$\begin{aligned} a_1 &= \tilde{\text{Sp}} w_0 [\hat{S}_1^2 + \hat{S}_2^1], & a_2 &= \tilde{\text{Sp}} w_0 [\hat{S}_2^{22} + (\hat{S}_3^{112} + \dots) + \hat{S}_4^{1111}], \\ a_3 &= \tilde{\text{Sp}} w_0 [(\hat{S}_4^{1122} + \dots) + (\hat{S}_5^{11112} + \dots) + \hat{S}_6^{111111}], \\ a_4 &= \tilde{\text{Sp}} w_0 [\hat{S}_4^{2222} + (\hat{S}_5^{11222} + \dots) + (\hat{S}_6^{111122} + \dots) + (\hat{S}_7^{1111112} + \dots) + \hat{S}_8^{11111111}], \\ a_5 &= \tilde{\text{Sp}} w_0 [\hat{S}_5^{22222} + (\hat{S}_6^{112222} + \dots) + (\hat{S}_7^{1111222} + \dots) + (\hat{S}_8^{11111122} + \dots) + \\ &\quad + (\hat{S}_9^{111111112} + \dots) + \hat{S}_{10}^{1111111111}], \\ a_6 &= \tilde{\text{Sp}} w_0 [\hat{S}_6^{222222} + (\hat{S}_7^{1122222} + \dots) + (\hat{S}_8^{11112222} + \dots) + (\hat{S}_9^{111111222} + \dots) + \\ &\quad + (\hat{S}_{10}^{1111111122} + \dots) + (\hat{S}_{11}^{11111111112} + \dots) + \hat{S}_{12}^{111111111111}]. \end{aligned} \quad (24)$$

Contributions of the sixth order are left in (23) and (24) for illustration and because such contributions are considered in generalizations of the Landau theory of phase transitions [14] (the standard theory is limited by contributions of the fourth order inclusive).

Thus, from formulas (14) and (23) it follows

$$\begin{aligned} \beta F &= \beta F_0 - \ln[1 + a_1 + a_2 + a_3 + a_4 + O(n_0^5)] = \\ &= (a_1 + a_2 + a_3 + a_4) - \frac{1}{2}(a_1^2 + a_2^2 + 2a_1a_2 + 2a_1a_3) + \\ &\quad + \frac{1}{3}(a_1^3 + 3a_1^2a_2) - \frac{1}{4}a_1^4 + O(n_0^5) \end{aligned} \quad (25)$$

because

$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + O(x^5).$$

As a result, taking into account (12), we obtain the expansion of the TD potential $\Omega(n_0)$ in powers of n_0

$$\Omega(n_0) = \Omega_0 + b_1 n_0 + b_2 n_0^2 + b_3 n_0^3 + b_4 n_0^4 + O(n_0^5) \quad (26)$$

where the coefficients b_s are expressed in terms of coefficients a_s by formulas

$$\begin{aligned} b_1 n_0 &= -a_1 / \beta - \mu n_0, & b_2 n_0^2 &= -(a_2 - \frac{1}{2} a_1^2) / \beta + \frac{V_0}{2V} n_0^2, \\ b_3 n_0^3 &= -(a_3 - a_1 a_2 + \frac{1}{3} a_1^3) / \beta, \\ b_4 n_0^4 &= -(a_4 - \frac{1}{2} a_2^2 - a_1 a_3 + a_1^2 a_2 - \frac{1}{4} a_1^4) / \beta \end{aligned} \quad (27)$$

($\Omega_0 \equiv \Omega(n_0 = 0)$). Thus, the nonequilibrium TD potential $\Omega(n_0)$ is expanded in a series with integer powers of occupation number of the condensate state n_0 .

Formulas (24), (27) are valid for an arbitrary Bose system. Let's take a closer look at the case of Bose gas in the presence of condensate. To do this, you can use the usual perturbation theory, expanding the coefficients a_1, a_2, a_3, a_4 into a series of interactions $v(\mathbf{p}) \sim \lambda$ ($\lambda \ll 1$ is a dimensionless small parameter). Note, that the developed by Bogolyubov perturbation theory for the study of Bose gas in the presence of condensate [15] considers the case when the occupation number of the condensate state n_0 is large and $n_0 / \mathbf{V} \sim \lambda^{-1}$. In our case $n_0 / \mathbf{V} \sim \lambda^0$ and according to (15) and (16) $\overbrace{S_{n+m}^{2\dots 21\dots 1}}^{n \dots m} \sim \lambda^{n+m}$. Therefore, formula (24) shows that estimates

$$a_1 \sim \lambda, \quad a_2 \sim \lambda^2, \quad a_3 \sim \lambda^4, \quad a_4 \sim \lambda^4 \quad (28)$$

are true.

We restrict ourselves to the calculation of coefficients a_1, a_2 in the main order of the perturbation theory in λ . The next coefficients require the use of the 4th order contributions of the TD perturbation theory, which is quite troublesome and will be made elsewhere. Formulas (24) give

$$\begin{aligned} a_1 n_0 &= \tilde{\text{Sp}} w_0 \hat{S}_1^2 + O(\lambda^2) = \tilde{\text{Sp}} w_0^{(0)} \hat{S}_1^{2(1)} + O(\lambda^2), \\ a_2 n_0^2 &= \tilde{\text{Sp}} w_0 \hat{S}_2^{22} + O(\lambda^3) = \tilde{\text{Sp}} w_0^{(0)} \hat{S}_2^{22(2)} + O(\lambda^3) \end{aligned} \quad (29)$$

where in accordance with (12), (13), and (15) the leading contributions to the quantities $w_0, \hat{S}_1^2, \hat{S}_2^{22}$ have the form

$$\begin{aligned} w_0^{(0)} &= e^{\beta \{F^{(0)} - \hat{H}_0 + \mu \hat{N}_1\}}; \\ \hat{S}_1^{2(1)} &= - \int_0^\beta d\beta_1 \hat{U}_2(\beta_1), \quad \hat{S}_2^{22(2)} = \int_0^\beta d\beta_1 \int_0^{\beta_1} d\beta_2 \hat{U}_2(\beta_1) \hat{U}_2(\beta_2) \end{aligned} \quad (30)$$

where

$$\hat{U}_2(\beta) \equiv e^{\beta(\hat{H}_0 - \mu \hat{N}_1)} \hat{U}_2 e^{-\beta(\hat{H}_0 - \mu \hat{N}_1)}. \quad (31)$$

(here and thereafter $a^{(s)}$ is contribution $\sim \lambda^s$ to an arbitrary quantity a). The definitions (1) and (6) give

$$e^{\beta(\hat{H}_0 - \mu \hat{N}_1)} a_{\mathbf{p}} e^{-\beta(\hat{H}_0 - \mu \hat{N}_1)} = a_{\mathbf{p}} e^{-\beta(\epsilon_{\mathbf{p}} - \mu)}, \quad e^{\beta(\hat{H}_0 - \mu \hat{N}_1)} a_{\mathbf{p}}^+ e^{-\beta(\hat{H}_0 - \mu \hat{N}_1)} = a_{\mathbf{p}}^+ e^{\beta(\epsilon_{\mathbf{p}} - \mu)}$$

and therefore, taking into account (6) and (12), we have

$$\hat{U}_2(\beta) = \frac{n_0}{\mathbf{V}} \sum_{\mathbf{p}} (v(\mathbf{p}) + v_0) a_{\mathbf{p}}^+ a_{\mathbf{p}} + \frac{n_0}{2\mathbf{V}} \sum_{\mathbf{p}} v(\mathbf{p}) [a_{\mathbf{p}} a_{-\mathbf{p}} e^{-2\beta(\epsilon_{\mathbf{p}} - \mu)} + a_{\mathbf{p}}^+ a_{-\mathbf{p}}^+ e^{2\beta(\epsilon_{\mathbf{p}} - \mu)}] \quad (32)$$

The averages with the statistical operator $w_0^{(0)}$ is calculated using the Wick–Bloch–Dominicis theorem (see, for example, [9, 13]) with elementary contractions

$$\begin{aligned} \overline{a_{\mathbf{p}}^+ a_{\mathbf{p}'}} &= n_{\mathbf{p}} \delta_{\mathbf{p}\mathbf{p}'}, \quad \overline{a_{\mathbf{p}} a_{\mathbf{p}'}} = (1 + n_{\mathbf{p}}) \delta_{\mathbf{p}\mathbf{p}'}, \quad \overline{a_{\mathbf{p}} a_{\mathbf{p}'}} = 0, \quad \overline{a_{\mathbf{p}}^+ a_{\mathbf{p}'}} = 0; \\ n_{\mathbf{p}} &\equiv \left[e^{\beta(\epsilon_{\mathbf{p}} - \mu)} - 1 \right]^{-1}. \end{aligned} \quad (33)$$

The calculations on this basis give in the leading order in interaction

$$\begin{aligned}
 a_1^{(1)} &= -\frac{\beta n_0}{\mathbf{V}} \sum_{\mathbf{p}} (v(\mathbf{p}) + v_0) n_{\mathbf{p}}, \\
 a_2^{(2)} &= \frac{\beta^2 n_0^2}{2\mathbf{V}^2} \left[\sum_{\mathbf{p}} (v(\mathbf{p}) + v_0) n_{\mathbf{p}} \right]^2 + \frac{\beta^2 n_0^2}{2\mathbf{V}^2} \sum_{\mathbf{p}} (v(\mathbf{p}) + v_0)^2 n_{\mathbf{p}} (1 + n_{\mathbf{p}}) + \\
 &\quad + \frac{n_0^2}{2\mathbf{V}^2} \sum_{\mathbf{p}} v(\mathbf{p})^2 n_{\mathbf{p}}^2 \left[\frac{e^{2\beta(\varepsilon_{\mathbf{p}} - \mu)} - 1}{4(\varepsilon_{\mathbf{p}} - \mu)^2} - \frac{\beta}{2(\varepsilon_{\mathbf{p}} - \mu)} \right].
 \end{aligned} \tag{34}$$

Hence, taking into account (27), we have the final expressions for the first coefficients of the expansion (26) of the nonequilibrium TD potential $\Omega(n_0)$ in the powers of n_0

$$\begin{aligned}
 b_1^{(1)} &= \frac{1}{\mathbf{V}} \sum_{\mathbf{p}} (v(\mathbf{p}) + v_0) n_{\mathbf{p}} - \mu, \\
 b_2^{(2)} &= -\frac{\beta}{2\mathbf{V}^2} \sum_{\mathbf{p}} (v(\mathbf{p}) + v_0)^2 n_{\mathbf{p}} (1 + n_{\mathbf{p}}) + \frac{v_0}{2\mathbf{V}} + \\
 &\quad + \frac{1}{2\mathbf{V}^2} \sum_{\mathbf{p}} v(\mathbf{p})^2 n_{\mathbf{p}}^2 \left[1 - \frac{e^{2\beta(\varepsilon_{\mathbf{p}} - \mu)} - 1}{2\beta(\varepsilon_{\mathbf{p}} - \mu)} \right] / 2(\varepsilon_{\mathbf{p}} - \mu).
 \end{aligned} \tag{35}$$

Let us make some remarks regarding the connection of this result with the Landau theory of phase transitions of the second kind. We have found that the expansion (26) of the potential occurs in integer powers of the order parameter n_0 . This corresponds to Landau's basic idea of the structure of the nonequilibrium TD potential [2, 3]. The violation of the effective Hamiltonian $\hat{H}(n_0)$ symmetry with respect to phase transformations $a_{\mathbf{p}} \rightarrow a_{\mathbf{p}} e^{i\alpha}$, $a_{\mathbf{p}}^+ \rightarrow a_{\mathbf{p}}^+ e^{-i\alpha}$ (see (5)) is the reason for the presence of odd powers of the occupation number in the expansion (26), that does not contradict to the Landau theory. In the standard approximation of the Landau theory, the condition of the potential $\Omega(n_0)$ minimum in equilibrium, according to (26), has the form

$$b_1 + b_2 n_0^o + b_3 n_0^{o2} + b_4 n_0^{o3} = 0, \quad b_2 + 2b_3 n_0^o + 3b_4 n_0^{o2} > 0. \tag{36}$$

In the absence of condensate $n_0^o = 0$, i.e. the relations

$$b_1(T, \mu) = 0, \quad b_2(T, \mu) > 0 \quad \text{at} \quad T > T_0 \tag{37}$$

must be true (T_0 is the condensation temperature). There is no reason to believe that conditions (37) are fulfilled for the functions (35), which give the main contribution to b_1 and b_2 in the small interaction approximation.

Thus, the resulting expression (26) with (35) can not serve as the basis for describing the Bose condensation in the vicinity of the transition point. One can give some comments that explain the situation. The occupation number of the non-condensate states $n_{\mathbf{p}}$ in (33) and further must be positive, therefore, the chemical potential μ must be negative

$$n_{\mathbf{p}} \geq 0 \Rightarrow \mu \leq 0. \tag{38}$$

In this case, after the TD boundary transition, the integral in (35) has no singularity and converges. Further, in the literature there is an opinion on the inapplicability of chemical potential as an independent variable in the Bose condensation theory (see, for example, [9, 12]). Moreover, in the literature, the applicability of the Gibbs grand canonical distribution to the study of Bose condensation is considered controversial (see a review in [11]). Our investigation of the Bose system will be continued elsewhere.

For a more detailed consideration of the connection of the developed theory with the Landau theory, one should calculate the coefficients b_3 , b_4 in expansion (26) of the TD potential $\Omega(n_0)$ in the TD perturbation theory. In accordance with (24), this requires considering the contributions of the 4th order of the TD perturbation theory. This will be done in another work, but note that the calculation of the coefficients b_3 , b_4 can be optimized. For this, the contribution of the perturbation theory \hat{S}_n in (15) should be used in the form

$$\hat{S}_n = \frac{(-1)^n}{n!} \int_0^\beta d\beta_1 \dots \int_0^\beta d\beta_n T \{ \hat{U}(\beta_1) \dots \hat{U}(\beta_n) \} \quad (39)$$

where the operator $T\{\dots\}$ of the ordering of products on the inverse temperature β was introduced. Since operators are commutative under the sign of this operator, all terms indicated in (24) with three dots give the contribution equal to the contribution of the first term in the corresponding bracket.

Next, it is expedient to use the standard technique of TD theory of perturbation using T - contractions [13]. It should also be taken into account that formula (14) allows further simplification

$$\beta F = \beta F_0 - \tilde{\text{Sp}}_c w_0 (\hat{S}_1 + \hat{S}_2 + \dots) \quad (40)$$

where the trace $\tilde{\text{Sp}}_c$ is taken only over conjuncted contraction systems. Even when using such considerations, the calculation of the coefficients b_3 , b_4 is rather troublesome, since it requires taking into account the contributions of the 4th order of the TD perturbation theory.

4. Conclusion

The nonequilibrium TD potential of the Bose system $\Omega(n_0)$ is calculated in the presence of the condensate near the phase transition point, when the occupation number of the condensate state n_0 is small. With the help of the TD perturbation theory the calculation of contributions up to the order n_0^6 inclusive is conducted, that is enough to analyze the generalizations of the Landau theory of phase transitions of the second kind [14]. The calculation of the proportional to n_0^3 and n_0^4 contributions to $\Omega(n_0)$, that are discussed in the standard Landau theory, requires considering the terms of the 4th order of the TD perturbation theory and will be discussed elsewhere. Coefficients at contributions to $\Omega(n_0)$ of the orders n_0^1 and n_0^2 are calculated for a Bose gas in the leading order of the small interaction approximation. It is established that the results obtained for Bose gas do not fit into the Landau theory of phase transitions of the second kind. In this regard it is noted that the literature suggests the inapplicability of the chemical potential as an independent TD variable and of the Gibbs grand canonical distribution for the consideration of the Bose condensation in general (see [9, 12] and review [11]).

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