

## A SELF-CONSISTENT THEORY OF LIQUID $^4\text{He}$

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A new method is proposed for the calculation of full density matrix and thermodynamic functions of a many-boson system. Explicit expressions are obtained in the pair correlations approximation for an arbitrary temperature. The theory is self-consistent in the sense that the calculated properties at low temperatures coincide with that of Bogoliubov theory and in the high-temperature limit lead to the results for classical non-ideal gas in the random phase approximation. The phase transition is also revealed as a consequence of Bose–Einstein condensation deformed by interatomic interactions. All the final formulae are written solely via the liquid structure factor taken as a source information instead of the interatomic potential and, therefore, interconnect only observable quantities. This gives also a possibility to study such a strongly non-ideal system as liquid  $^4\text{He}$ .

**Key words:** liquid  $^4\text{He}$ , density matrix, partition function, structure factor, effective mass, energy,  $\lambda$ -transition, Bose–Einstein condensation.

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### INTRODUCTION

The properties of liquid helium are known to have brought about ample literature. Yet due to its unique characteristics this quantum fluid keeps attracting the attention of specialists in the field of theoretical and experimental physics alike. The first principle microscopic description of thermodynamic and structure functions as well as the phenomenon of Bose–Einstein condensation at a considerable distance from the absolute zero, in particular in the vicinity of the  $\lambda$ -transition, is still a problem which cannot be taken as solved to the very end. The latter statement can be supported by a fairly instructive study of heat capacity in the vicinity of the  $\lambda$ -transition. The  $\lambda$ -like form of the heat capacity in the vicinity of the phase transition of liquid helium into the superfluid state has been taken for a logarithmic divergence with the critical exponent  $\alpha \rightarrow 0$ . This view found its way into both text-books and monographs [1–6]. Precise experiments helped to find out that in fact there is no divergence in the heat capacity [7, 8] even though the exponent  $\alpha$  is indeed a small but negative number,  $\alpha = -0.01056$  [8]. The studies of the  $\lambda$ -transition based on the renormalization group method [9] provide us with a possibility to carry out a correct calculus for the so-called universal characteristics solely, i. e., the critical characteristics of the thermodynamic functions and the relations of the amplitudes of their leading asymptotics at the temperature on either side tending to the phase transition point. Even though the thermodynamic potential functional from the two-component order parameter for liquid  $^4\text{He}$  was calculated precisely owing to the coherent states depiction [10, 11], yet its subsequent simplifications necessary for the implementation of the renormalized group approach make it impossible to describe the system's characteristics outside the closest vicinity of the phase transition point using the same method. Notwithstanding tangible efforts of the researchers the renormalization group method did

not yield the logarithmic divergence of the heat capacity (the  $\alpha$  exponent was received as a small but still finite positive number, the power divergence having been obtained). Only in the subsequent studies which made use of the summation procedure of the Borel perturbation theory divergent series established the negative value of the exponent:  $\alpha = -0.01294$  [12],  $\alpha = -0.0150$  [13],  $\alpha = -0.01126$  [14].

The fact that heat capacity at the  $\lambda$ -point acquires a finite value finds itself in agreement with London [15] in the sense that the  $\lambda$ -transition in liquid  $^4\text{He}$  is a Bose-condensation deformed by the interatomic interaction inherent of the ideal Bose-gas bringing about the steepness of the heat capacity curve in the vicinity of the Bose-condensation point. It is not easy to reveal the connection between superfluidity and Bose-condensation unequivocally. This connection is a lot more complex than a simple correspondence. For instance, at the temperature equaling absolute zero all the atoms of the ideal Bose-gas find themselves in the states with a zero momentum thus forming the one-hundred per cent Bose-condensate (BC). However, such a system is not superfluid. Conversely, liquid  $^4\text{He}$  at the absolute temperature zero is superfluid even though the number of atoms in the BC, as showed both by theoretical and experimental studies, is but a small part of the entire number of atoms. It is also well-known that one- and two-dimensional systems tend to reveal superfluid characteristics with the BC being absent. Here we are concerned with the rise of the so-called non-diagonal long-range order when the one-particle density matrix in the coordinates description dwindles in compliance with the power law rather than the exponent law, at the matrix arguments being disentangled over infinity. On the other hand a mere assumption that the BC exists in the weakly imperfect Bose-gas made it possible for Bogoliubov [16] to obtain from the first principles the energy spectrum whose properties are close to those of the liquid  $^4\text{He}$ .

One other fairly complex task lies in according Bogoliubov's theory [16] well-suited for the low temperatures

with the random phase approximation in the theory of classical systems. It may be possible to find expressions for the thermodynamic and structure functions of the Bose-liquid which would yield the results of Bogoliubov's theory for the temperatures  $T \rightarrow 0$  K. For high temperatures in the quasi-classical  $\hbar \rightarrow 0$  limit this expression would bring closer to the random phase approximation of the classical non-ideal gas theory. It might be supposed that such an expression would also give good results in the intermediate temperature area where the transition point of liquid  ${}^4\text{He}$  into the superfluid state is located. It is clear that we are referring not to the general formulae at the level of definitions which just cannot "be brought to a certain number", but to the discovery of such a first principles method of calculating the thermodynamic properties of the many-boson system which starts from the  $N$  particles Hamiltonian and makes it possible to put forward a regular perturbation theory with a consistent consideration of many-particle correlations starting with the two-particle correlations.

In the present paper we mean to dwell upon one of the possibilities of solving these problems. Some of the results to be presented here were briefly summarized in [17] just as an illustration of certain tricks applicable to the wave functions and the statistical operator [18]. However, the full scope of these findings has never been published. We shall calculate explicitly the complete density matrix taking into account the two-particle interatomic correlations as well as the Helmholtz free energy, the energy and also a pair liquid structure factor which will abide by the above requirements.

## I. INITIAL EQUATIONS

Let us consider the  $N$  set of spinless Bose-particles with the mass  $m$  with the Hamiltonian

$$\hat{H} = \sum_{j=1}^N \frac{\hat{\mathbf{p}}_j^2}{2m} + \sum_{1 \leq i < j \leq N} \Phi(|\mathbf{r}_i - \mathbf{r}_j|), \quad (1.1)$$

where the first term is the operator of the kinetic energy,  $\hat{\mathbf{p}}_j$  is the operator of the momentum of the  $j$ -th particle. The second term presents the potential energy of the two-particle interaction between the particles with the coordinates  $x = (\mathbf{r}_1, \dots, \mathbf{r}_N)$ . The particles movement is limited within a volume of  $V$ .

Let  $\psi_n(x)$  be taken for a system of eigenfunctions of the Hamiltonian  $\hat{H}$  and  $E_n$  are its eigenvalues. Let us consider such an equation for the statistical operator:

$$e^{-\beta \hat{H}} \psi_n(x) = e^{-\beta E_n} \psi_n(x), \quad (1.2)$$

where  $\beta = 1/T$ ,  $T$  is the temperature of the considered system of particles. Let us introduce a certain arbitrary function  $\varphi = \varphi(x)$  and let us multiply the left-hand side of equation (1.2) by  $\varphi(x)$ . We will integrate it over all coordinates  $x$ :

$$\int \varphi(x) e^{-\beta \hat{H}} \psi_n(x) dx = e^{-\beta E_n} \int \varphi(x) \psi_n(x) dx, \quad (1.3)$$

where

$$\int dx = \int d\mathbf{r}_1 \dots \int d\mathbf{r}_N.$$

We will impose the following condition for the function  $\varphi(x)$ :

$$\int \varphi(x) \psi_n(x) dx \neq 0. \quad (1.4)$$

Then making use of the self-conjugation of the operator  $\hat{H}$  we shall transfer it in equation (1.3) from the function  $\psi_n(x)$  to  $\varphi(x)$  multiplying the l.h.s. side of this equation by  $\psi_n^*(x')$  and summing it by all the indices of the  $n$  states:

$$\begin{aligned} & \sum_n \int \psi_n^*(x') \psi_n(x) e^{-\beta \hat{H}} \varphi(x) dx \\ &= \int \varphi(x) \sum_n \psi_n^*(x') e^{-\beta E_n} \psi_n(x) dx. \end{aligned}$$

We make use of the completeness condition

$$\sum_n \psi_n^*(x') \psi_n(x) = \delta(x' - x),$$

and also proceeding from the previous equation we will obtain the following equation with the permutation of the variables  $x$  for  $x'$  and inversely:

$$e^{-\beta \hat{H}} \varphi(x) = \int \varphi(x') R_N(x'|x) dx', \quad (1.5)$$

where

$$R_N(x'|x) = \sum_n \psi_n^*(x) e^{-\beta E_n} \psi_n(x') \quad (1.6)$$

is the density matrix in the coordinate representation.

In true fact equation (1.5) is self-evident and could have been written out at once as a matrix presentation of the statistical operator action over any function  $\varphi(x)$ . In the Dirac notations this equation can be written as follows

$$\langle x | e^{-\beta \hat{H}} \varphi \rangle = \int \langle x | e^{-\beta \hat{H}} | x' \rangle \langle x' | \varphi \rangle dx', \quad (1.7)$$

$$\langle x | e^{-\beta \hat{H}} | x' \rangle = R_N(x'|x), \quad \langle x' | \varphi \rangle = \phi(x').$$

It is clear that formula (1.5) or (1.7) is applicable both to one-particle and two-particles problems. Notwithstanding the fact that it is obvious, this formula makes it possible to fully restore the density matrix (1.6). Here most significant heuristically is an arbitrary choice of the function  $\varphi(x)$  on condition that it is non-orthogonal to the eigen-functions of the  $\hat{H}$  operator and the existence of the integral (1.4).

The present article is concerned with the calculus of the  $R_N(x'|x)$  density matrix for the studied many-boson system from the initial equation (1.5).

Should the interparticle interaction be switched off, the density matrix will transfer into that of the ideal Bose-particles  $N$  system. That is why we will try to construct the density matrix of the  $N$  system of interacting particles as a product of the density matrix of the ideal Bose-gas  $R_N^0(x'|x)$  and the  $P_N(x'|x)$  factor taking into account the interparticle interaction:

$$R_N(x'|x) = R_N^0(x'|x)P_N(x'|x), \quad (1.8)$$

where at temperature  $T \neq 0$

$$R_N^0(x'|x) = \frac{1}{N!} \left( \frac{m^*}{2\pi\beta\hbar^2} \right)^{3N/2} \times \sum_Q \exp \left[ -\frac{m^*}{2\beta\hbar^2} \sum_{j=1}^N (\mathbf{r}'_j - \mathbf{r}_{Qj})^2 \right], \quad (1.9)$$

the summation over  $Q$  is at the same time the summation over all the permutation  $N!$  numbering the particles coordinates; at  $T = 0$ , when all the particles have zero momenta, the matrix  $R_N^0(x|x') = 1/V^N$ . The mass of the particle in (1.9) is understood as a certain effective mass  $m^*$  which equals the initial mass  $m$  unless the interaction takes place. Thus a part of the contribution from the interparticle interactions is taken into account by renormalizing the particle mass, the remainder being left in the  $P_N(x'|x)$  factor. Postulating this for the density matrix (1.8) is justified also by the fact that it was obtained under certain assumptions by a different method in [19] by a direct calculus from (1.6). The expression for the effective mass was found to be in agreement with the formula for the effective mass of the impurity atom moving in the Bose-liquid if the initial impurity mass coincides with the mass of the atom of liquid. Yet for the  $R_N(x'|x)$  matrix in [19] an expression was found which is correct only at  $T \rightarrow 0$  K. Here we will try to find a formula for  $P_N(x'|x)$  which will be capable of working in the entire temperature interval. We will also postpone the discussion of the issue of determining the effective mass contained in expression (1.9).

Falling back on the phenomenological consideration concerning the insignificance of the atoms permutation which are located at the distances smaller than their own sizes quite some time ago Feynman [6,20] constructed the  $N$ -particle distribution function of the liquid  ${}^4\text{He}$ , i. e., the diagonal elements of the density matrix as a product

of the ideal Bose-gas distribution function multiplied by the factor accounting for the atom impenetrability. We would like to base our analysis on the precise equation (1.5) and suggest a consistent method for the calculus of the  $P_N(x'|x)$  function computing the latter explicitly accounting for the two-particle correlations. We will choose the  $P_N(x'|x)$  matrix which takes into account the interparticle correlations as follows:

$$P_N(x'|x) = \exp \left\{ c_0 + \sum_{\mathbf{q} \neq 0} c_1(q) \rho'_{\mathbf{q}} \rho_{-\mathbf{q}} - \frac{1}{2} \sum_{\mathbf{q} \neq 0} c_2(q) \left[ \rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}} \right] \right\}, \quad (1.10)$$

where the Fourier coefficients of the particles density fluctuations

$$\rho_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}_j}, \quad (1.11)$$

$$\rho'_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}'_j}, \quad (1.12)$$

at  $\mathbf{q} \neq 0$ . The components of the wave vector  $\mathbf{q}$  cover the integer values divisible by  $2\pi/V^{1/D}$  where  $D$  is dimensionality of the cubic box which contains the system of particles studied. We will determine the coefficient functions  $c_0$ ,  $c_1(q)$ ,  $c_2(q)$  from equation (1.5).

We have confined ourselves to the consideration of two-particle interparticle correlations in expression (1.10). Accounting of the three-particle and higher correlations is accomplishable by adding the members with a product of three or more  $\rho_{\mathbf{q}}$  in the exponent in (1.10). In our work we will not take them into account explicitly, yet we will return to them when discussing the issue of the effective mass  $m^*$ . The exponent form of the  $P_N(x'|x)$  matrix is caused by the classical boundary of its diagonal elements when  $P_N(x|x)$  turns into the usual Boltzmann factor  $\exp(-\beta\Phi)$ , where  $\Phi$  is the potential energy of the interparticle interaction thus equaling the second term in the Hamiltonian (1.1).

Finally, we must also choose the appropriate  $\varphi$  function which is contained in equation (1.5) and meets requirement (1.4). In our case we will adjust it from the class of such functions:

$$\varphi(x) = \exp \left[ \sum_{\mathbf{q} \neq 0} \lambda(q) \rho_{\mathbf{q}} \right], \quad (1.13)$$

where the arbitrary coefficient function  $\lambda(q)$  is a real function from the wave vector module  $q = |\mathbf{q}|$  with all the necessary properties.

**II. THE LEFT-HAND SIDE OF EQUATION (1.5)**

Let us represent the action of the statistical operator on the  $\varphi$  function in (1.5) in the form of the exponent function:

$$e^U = e^{-\beta\hat{H}}\varphi. \quad (2.1)$$

Here again when fixing the exponent form of this function we proceed from the assumption that in the quasi-classical limit when  $\hbar \rightarrow 0$  the statistical operator comes up to the Boltzman factor which just as the  $\varphi$  function has an exponent form. Differentiating either sides of the equation with respect to inverse temperature  $\beta$  we will find the equation for the unknown function  $U$ :

$$-\frac{\partial U}{\partial\beta} = e^{-U}\hat{H}e^U,$$

or explicitly

$$-\frac{\partial U}{\partial\beta} = -\frac{\hbar^2}{2m}\sum_{j=1}^N[\nabla_j^2 U + (\nabla_j U)^2] + \Phi, \quad (2.2)$$

where from (2.1) and (1.13) it is apparent that

$$U = \sum_{\mathbf{q}\neq 0}\lambda(q)\rho_{\mathbf{q}}, \text{ when } \beta = 0. \quad (2.3)$$

To solve equation (2.2) we will choose the function  $U$  in the form of the series "by the degrees" of the  $\rho_{\mathbf{q}}$  quantities:

$$U = a_0 + \sum_{\mathbf{q}\neq 0}a_1(q)\rho_{\mathbf{q}} + \frac{1}{2}\sum_{\mathbf{q}\neq 0}a_2(q)\rho_{\mathbf{q}}\rho_{-\mathbf{q}} + \dots \quad (2.4)$$

We have agreed to take into account the two-particle interparticle correlation only that is why the series is truncated at the second degree of  $\rho_{\mathbf{q}}$ . Higher correlations denoted as dots in (2.4) can be taken into account by summing higher degrees of  $\rho_{\mathbf{q}}$ . It is convenient to work with our equation in terms of the  $\rho_{\mathbf{q}}$  quantity rather than the individual coordinates  $x$ . That is why we will show the potential energy  $\Phi$  through the quantities of  $\rho_{\mathbf{q}}$ :

$$\Phi = \frac{N(N-1)}{2V}\nu_0 + \frac{N}{2V}\sum_{\mathbf{q}\neq 0}\nu_q(\rho_{\mathbf{q}}\rho_{-\mathbf{q}} - 1), \quad (2.5)$$

where the Fourier coefficients of the two particles potential energy

$$\nu_q = \int e^{-i\mathbf{q}\mathbf{R}}\Phi(R) d\mathbf{R}. \quad (2.6)$$

Equation (2.2) will now look as follows

$$\begin{aligned} -\frac{\partial U}{\partial\beta} &= \sum_{\mathbf{k}\neq 0}\frac{\hbar^2 k^2}{2m}\left(\rho_{\mathbf{k}}\frac{\partial U}{\partial\rho_{\mathbf{k}}} - \frac{\partial^2 U}{\partial\rho_{\mathbf{k}}\partial\rho_{-\mathbf{k}}} - \frac{\partial U}{\partial\rho_{\mathbf{k}}}\frac{\partial U}{\partial\rho_{-\mathbf{k}}}\right) \\ &+ \frac{1}{\sqrt{N}}\sum_{\substack{\mathbf{k}\neq 0 \ \mathbf{k}'\neq 0 \\ \mathbf{k}+\mathbf{k}'\neq 0}}\frac{\hbar^2(\mathbf{k}\mathbf{k}')}{2m}\rho_{\mathbf{k}+\mathbf{k}'}\left(\frac{\partial^2 U}{\partial\rho_{\mathbf{k}}\partial\rho_{\mathbf{k}'}} + \frac{\partial U}{\partial\rho_{\mathbf{k}}}\frac{\partial U}{\partial\rho_{\mathbf{k}'}}\right) \\ &+ \frac{N(N-1)}{2V}\nu_0 + \sum_{\mathbf{k}\neq 0}\frac{N}{2V}\nu_k(\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - 1). \end{aligned} \quad (2.7)$$

We substitute in this equation expression (2.4) for the  $U$  function and from the equivalence condition of the coefficient functions at the equal degrees of  $\rho_{\mathbf{k}}$  in the left- and right-hand sides of this equation and again taking into account just the two-particle correlation we find a system of three equations for the unknown quantities  $a_0$ ,  $a_1(q)$  and  $a_2(q)$

$$\begin{aligned} -\frac{da_0}{d\beta} &= -\sum_{\mathbf{q}\neq 0}\frac{\hbar^2 q^2}{2m}[a_2(q) + a_1^2(q)] \\ &+ \frac{N(N-1)}{2V}\nu_0 - \sum_{\mathbf{q}\neq 0}\frac{N}{2V}\nu_q, \end{aligned} \quad (2.8)$$

$$-\frac{da_1(q)}{d\beta} = \frac{\hbar^2 q^2}{2m}a_1(q)[1 - 2a_2(q)], \quad (2.9)$$

$$-\frac{da_2(q)}{d\beta} = \frac{\hbar^2 q^2}{m}[a_2(q) - a_2^2(q)] + \frac{N}{V}\nu_q. \quad (2.10)$$

We begin to solve the system of these equations from equation (2.10) for  $a_2(q)$ . Notwithstanding the fact that this equation is nonlinear its solution can be found analytically which was suggested for the first time in [21] in the framework of the so-called shifts and collective variables method:

$$a_2(q) = -\frac{\alpha_q - 1}{2}\frac{1 - e^{-2\beta E(q)}}{1 + \frac{\alpha_q - 1}{\alpha_q + 1}e^{-2\beta E(q)}}, \quad (2.11)$$

$$\alpha_q = \sqrt{1 + \frac{2N}{V}\nu_q\left/\frac{\hbar^2 q^2}{2m}\right.}, \quad (2.12)$$

where

$$E(q) = \alpha_q\frac{\hbar^2 q^2}{2m} \quad (2.13)$$

is Bogoliubov's elementary excitation spectrum [16].

After this we solve in turn equations (2.9) and (2.8). Fairly simple even though cumbersome transformations taking into account the "initial" condition (2.3) lead to the following result

$$a_1(q) = \lambda(q) \frac{\frac{2\alpha_q}{\alpha_q+1} e^{-\beta E(q)}}{1 + \frac{\alpha_q-1}{\alpha_q+1} e^{-2\beta E(q)}}, \quad (2.14)$$

$$a_0 = -\beta E_0 - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left[ \frac{1 + \frac{\alpha_q-1}{\alpha_q+1} e^{-2\beta E(q)}}{1 + \frac{\alpha_q-1}{\alpha_q+1}} \right] + \sum_{\mathbf{q} \neq 0} \lambda^2(q) \frac{1 - e^{-2\beta E(q)}}{(\alpha_q + 1) \left[ 1 + \frac{\alpha_q-1}{\alpha_q+1} e^{-2\beta E(q)} \right]}, \quad (2.15)$$

where

$$E_0 = \frac{N(N-1)}{2V} \nu_0 - \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{8m} (\alpha_q - 1)^2 \quad (2.16)$$

is the energy of the ground state of the many-boson system in Bogoliubov's approximation [16].

Thus in the approximation of pair correlation we have found explicitly the result of the action of statistical operators on the  $\varphi$  function, i. e., the left-hand side of our main equation (1.5) which taking into account (2.1) looks as follows:

$$e^U = \int \varphi(x') R(x'|x) dx'. \quad (2.17)$$

To go further we must calculate the integral over  $x'$  in the right-hand side of this equation.

### III. THE RIGHT-HAND SIDE OF EQUATION (1.5)

Let us now proceed to the finding of the explicit form of the right-hand side of our main equation (2.17) making use of the postulated form of the (1.8)–(1.10) statistical operator. We have

$$\int \varphi(x') R(x'|x) dx' = \int \dots \int R_N^0(x'|x) \exp \left\{ \sum_{\mathbf{q} \neq 0} \lambda(q) \rho'_{\mathbf{q}} + c_0 + \sum_{\mathbf{q} \neq 0} c_1(q) \rho'_{\mathbf{q}} \rho_{-\mathbf{q}} - \frac{1}{2} \sum_{\mathbf{q} \neq 0} c_2(q) [\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}] \right\} d\mathbf{r}'_1 \dots d\mathbf{r}'_N. \quad (3.1)$$

Let us pass over in this expression from the integration of particles  $\mathbf{r}'_1, \dots, \mathbf{r}'_N$  by the individual coordinates to the integration over the  $\rho'_{\mathbf{q}}$  variables which are determined by formula (1.12). Such a transition is performed by means of Zubarev's [22] transition function which is a product of the Dirac  $\delta$ -function and equation (3.1) and looks as follows:

$$\int \varphi(x') R(x'|x) dx' = \int \dots \int \exp \left\{ \sum_{\mathbf{q} \neq 0} \lambda(q) \rho'_{\mathbf{q}} + c_0 + \sum_{\mathbf{q} \neq 0} c_1(q) \rho'_{\mathbf{q}} \rho_{-\mathbf{q}} - \frac{1}{2} \sum_{\mathbf{q} \neq 0} c_2(q) [\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}] \right\} J_0(\rho') (d\rho'), \quad (3.2)$$

where the weight function

$$J_0(\rho') = \int \dots \int R_N^0(x'|x) \prod'_{\mathbf{q} \neq 0} \delta \left( \rho'_{\mathbf{q}} - \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}'_j} \right) d\mathbf{r}'_1 \dots d\mathbf{r}'_N. \quad (3.3)$$

An element of the  $\rho'_{\mathbf{q}}$  space volume

$$(d\rho') = \prod'_{\mathbf{q} \neq 0} d\rho_{\mathbf{q}}^c d\rho_{\mathbf{q}}^s, \quad (3.4)$$

where  $\rho_{\mathbf{q}}^c, \rho_{\mathbf{q}}^s$  are a real and respectively an imaginary part of the variable  $\rho'_{\mathbf{q}} = \rho_{\mathbf{q}}^c - i\rho_{\mathbf{q}}^s$ . The integration by  $\rho_{\mathbf{q}}^c, \rho_{\mathbf{q}}^s$  takes place in the infinite volume. The prime (') at the product sign in (3.3) and (3.4) means that the values of the wave vector  $\mathbf{q}$  are considered only from the half-space of all of its possible values because there exists the dependence  $\rho_{\mathbf{q}}^{s*} = \rho_{-\mathbf{q}}^s$  or  $\rho_{\mathbf{q}}^{c*} = \rho_{-\mathbf{q}}^c, \rho_{\mathbf{q}}^{s*} = -\rho_{-\mathbf{q}}^s$ .

We will use the integral representation for the  $\delta$ -function and write the transition function (3.3) as

$$\begin{aligned}
 J_0(\rho') &= \int \dots \int R_N^0(x'|x) \int (d\omega) \exp \left[ \pi i \sum_{\mathbf{q} \neq 0} \omega_{\mathbf{q}} \left( \rho'_{\mathbf{q}} - \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}'_j} \right) \right] d\mathbf{r}'_1 \dots d\mathbf{r}'_N \\
 &= \int (d\omega) \exp \left[ \pi i \sum_{\mathbf{q} \neq 0} \omega_{\mathbf{q}} \rho'_{\mathbf{q}} \right] \left\langle \exp \left[ -\pi i \sum_{\mathbf{q} \neq 0} \frac{1}{\sqrt{N}} \omega_{\mathbf{q}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}'_j} \right] \right\rangle,
 \end{aligned} \tag{3.5}$$

here the element of the  $\omega$  space

$$(d\omega) = \prod'_{\mathbf{q} \neq 0} d\omega_{\mathbf{q}}^c d\omega_{\mathbf{q}}^s,$$

where  $\omega_{\mathbf{q}}^c, \omega_{\mathbf{q}}^s$  are a real and respectively an imaginary part of the  $\omega_{\mathbf{q}}$  complex variable linked to  $\rho_{\mathbf{q}}$ , the angle brackets denoting the integration over the individual primed coordinates with the weight equaling the density matrix of the ideal gas:

$$\langle \dots \rangle = \int \dots \int (\dots) R_N^0(x'|x) d\mathbf{r}'_1 \dots d\mathbf{r}'_N. \tag{3.6}$$

The integral from the  $R_N^0(x'|x)$  density matrix itself by  $x'$  equals unity. Indeed,

$$\begin{aligned}
 \int \dots \int R_N^0(x'|x) d\mathbf{r}'_1 \dots d\mathbf{r}'_N &= \frac{1}{N!} \left( \frac{m^*}{2\pi\beta\hbar^2} \right)^{3N/2} \sum_Q \int \dots \int e^{-\frac{m^*}{2\beta\hbar^2} \sum_{j=1}^N (\mathbf{r}'_j - \mathbf{r}_{Qj})^2} d\mathbf{r}'_1 \dots d\mathbf{r}'_N \\
 &= \frac{1}{N!} \left( \frac{m^*}{2\pi\beta\hbar^2} \right)^{3N/2} \sum_Q \int \dots \int e^{-\frac{m^*}{2\beta\hbar^2} \sum_{j=1}^N \mathbf{R}_j^2} d\mathbf{R}_1 \dots d\mathbf{R}_N = 1,
 \end{aligned} \tag{3.7}$$

where we have passed to the new variables of integration

$$\mathbf{R}_j = \mathbf{r}'_j - \mathbf{r}_{Qj},$$

and at the same time we assume that the size of the box where the system of particles is located is already infinite,  $V \rightarrow \infty$ . We will refer to operation (3.6) as to averaging.

Let us now pass over to the calculation of the weight function (3.5). We will reflect the average from the exponent in (3.5) in the form of the exponent from the non-reducible averages limiting ourselves to two-particle correlations again:

$$\begin{aligned}
 J_0(\rho') &= \int (d\omega_{\mathbf{q}}) e^{\pi i \sum_{\mathbf{q} \neq 0} \omega_{\mathbf{q}} \rho'_{\mathbf{q}}} \exp \left\{ -\pi i \sum_{\mathbf{q} \neq 0} \frac{\omega_{\mathbf{q}}}{\sqrt{N}} \left\langle \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}'_j} \right\rangle + \frac{1}{2} \sum_{\mathbf{q}_1 \neq 0} \sum_{\mathbf{q}_2 \neq 0} \frac{(\pi i \omega_{\mathbf{q}_1})(\pi i \omega_{\mathbf{q}_2})}{N} \right. \\
 &\quad \left. \times \left[ \left\langle \sum_{j_1=1}^N e^{-i\mathbf{q}_1 \mathbf{r}'_{j_1}} \sum_{j_2=1}^N e^{-i\mathbf{q}_2 \mathbf{r}'_{j_2}} \right\rangle - \left\langle \sum_{j_1=1}^N e^{-i\mathbf{q}_1 \mathbf{r}'_{j_1}} \right\rangle \left\langle \sum_{j_2=1}^N e^{-i\mathbf{q}_2 \mathbf{r}'_{j_2}} \right\rangle \right] + \dots \right\}.
 \end{aligned} \tag{3.8}$$

Let us calculate the average quantities necessary for us. Thus similarly to (3.7) we have

$$\begin{aligned}
 \left\langle \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}'_j} \right\rangle &= \frac{1}{N!} \left( \frac{m^*}{2\pi\beta\hbar^2} \right)^{3N/2} \sum_Q \sum_{l=1}^N \int \dots \int d\mathbf{r}'_1 \dots d\mathbf{r}'_N e^{-i\mathbf{q}\mathbf{r}'_l} e^{-\frac{m^*}{2\beta\hbar^2} \sum_{j=1}^N (\mathbf{r}'_j - \mathbf{r}_{Qj})^2} \\
 &= \frac{1}{N!} \left( \frac{m^*}{2\pi\beta\hbar^2} \right)^{3N/2} \sum_Q \sum_{l=1}^N \int \dots \int d\mathbf{R}_1 \dots d\mathbf{R}_N e^{-i\mathbf{q}\mathbf{R}_l} e^{-\frac{m^*}{2\beta\hbar^2} \sum_{j=1}^N \mathbf{R}_j^2}
 \end{aligned} \tag{3.9}$$

$$= \frac{1}{N!} \left( \frac{m^*}{2\pi\beta\hbar^2} \right)^{3N/2} \sum_Q \sum_{l=1}^N \left( \frac{2\pi\beta\hbar^2}{m^*} \right)^{3(N-1)/2} e^{-i\mathbf{q}\mathbf{r}_{Ql}} \left( \frac{2\pi\beta\hbar^2}{m^*} \right)^{3/2} e^{-\beta\hbar^2 q^2/2m^*} = \sqrt{N} \rho_{\mathbf{q}} e^{-\beta\hbar^2 q^2/2m^*}.$$

Incidentally, it is not difficult to show that the mean for the many-fermion system equals zero. This is connected with the fact that the  $R_N^0(x'|x)$  density matrix for the fermions is antisymmetric as regards the permutation of the primed  $(\mathbf{r}'_1, \dots, \mathbf{r}'_N)$  coordinates, the value of (1.12) being symmetrical. Otherwise said, for Fermi statistics the  $\varphi$  function from (1.13) does not meet condition (1.4). Thus, it is necessary to find another function which would be non-orthogonal to the wave functions of the many-fermion system. The results of the calculation of the thermodynamic and structure functions for the Fermi particles on the basis of the suggested approach will be published separately.

Our further steps are analogous to those in the case of (3.9):

$$\begin{aligned} \left\langle \sum_{j_1=1}^N e^{-i\mathbf{q}_1 \mathbf{r}'_{j_1}} \sum_{j_2=1}^N e^{-i\mathbf{q}_2 \mathbf{r}'_{j_2}} \right\rangle &= \left\langle \sum_{j_1=1}^N e^{-i(\mathbf{q}_1 + \mathbf{q}_2) \mathbf{r}'_{j_1}} \right\rangle + \sum_{j_1=1}^N \sum_{\substack{j_2=1 \\ (j_1 \neq j_2)}}^N \left\langle e^{-i\mathbf{q}_1 \mathbf{r}'_{j_1} - i\mathbf{q}_2 \mathbf{r}'_{j_2}} \right\rangle \\ &= e^{-\beta \frac{\hbar^2 (\mathbf{q}_1 + \mathbf{q}_2)^2}{2m^*}} \sum_{j_1=1}^N e^{-i(\mathbf{q}_1 + \mathbf{q}_2) \mathbf{r}_{j_1}} + \sum_{j_1=1}^N e^{-i\mathbf{q}_1 \mathbf{r}_{j_1}} \sum_{j_2=1}^N e^{-i\mathbf{q}_2 \mathbf{r}_{j_2}} e^{-\beta \left( \frac{\hbar^2 q_1^2}{2m^*} + \frac{\hbar^2 q_2^2}{2m^*} \right)} - e^{-\beta \frac{\hbar^2}{2m^*} (q_1^2 + q_2^2)} \sum_{j_1=1}^N e^{-i(\mathbf{q}_1 + \mathbf{q}_2) \mathbf{r}_{j_1}}. \end{aligned} \quad (3.10)$$

Now, taking into account (3.9) and (3.10) we will find that

$$\begin{aligned} \left\langle \sum_{j_1=1}^N e^{-i\mathbf{q}_1 \mathbf{r}'_{j_1}} \sum_{j_2=1}^N e^{-i\mathbf{q}_2 \mathbf{r}'_{j_2}} \right\rangle - \left\langle \sum_{j_1=1}^N e^{-i\mathbf{q}_1 \mathbf{r}'_{j_1}} \right\rangle \left\langle \sum_{j_2=1}^N e^{-i\mathbf{q}_2 \mathbf{r}'_{j_2}} \right\rangle &= \left( 1 - e^{-2\beta \frac{\hbar^2 q_1^2}{2m^*}} \right) N \delta(\mathbf{q}_1 + \mathbf{q}_2) \\ &+ \left[ e^{-\beta \frac{\hbar^2}{2m^*} (\mathbf{q}_1 + \mathbf{q}_2)^2} - e^{-\beta \frac{\hbar^2}{2m^*} (q_1^2 + q_2^2)} \right] \sqrt{N} \rho_{\mathbf{q}_1 + \mathbf{q}_2}. \end{aligned} \quad (3.11)$$

Here, the second term will be omitted in the accepted approximation of two-particle correlations when substituting (3.11) in (3.8). Expressions (3.9), (3.11) give correct asymptotics at absolute zero temperature,  $\beta \rightarrow \infty$ , as well.

Further, the weight function in (3.8) can be calculated easily as the integrals by  $\omega_{\mathbf{k}}^c$  and  $\omega_{\mathbf{k}}^s$  are reducible to the Poisson integrals:

$$\begin{aligned} J_0(\rho') &= \int (d\omega) \exp \left[ -\frac{1}{2} \sum_{\mathbf{q} \neq 0} |\pi\omega_{\mathbf{q}}|^2 (1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}) + \pi i \sum_{\mathbf{q} \neq 0} \omega_{\mathbf{q}} \left( \rho'_{\mathbf{q}} - \rho_{\mathbf{q}} e^{-\beta \frac{\hbar^2 q^2}{2m^*}} \right) \right] \\ &= \exp \left\{ -\frac{1}{2} \sum_{\mathbf{q} \neq 0} \frac{|\rho'_{\mathbf{q}} - \rho_{\mathbf{q}} e^{-\beta \frac{\hbar^2 q^2}{2m^*}}|^2}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right\} \prod'_{\mathbf{q} \neq 0} \frac{1}{\pi \left( 1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}} \right)}. \end{aligned} \quad (3.12)$$

Now, just as in (3.12) we can carry out integration in (3.2):

$$\begin{aligned} \int \varphi(x') R(x'|x) dx' &= \exp \left\{ c_0 + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \frac{\lambda^2(q)}{\left[ c_2(q) + \frac{1}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right]} \right\} \\ &\times \exp \left\{ \sum_{\mathbf{q} \neq 0} \lambda(q) \rho_{\mathbf{q}} \left[ c_1(q) + \frac{e^{-\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right] \right\} \left/ \left[ c_2(q) + \frac{1}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right] \right\} \\ &\times \exp \left\{ \frac{1}{2} \sum_{\mathbf{q} \neq 0} \frac{\left[ c_1(q) + \frac{e^{-\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right]^2}{\left[ c_2(q) + \frac{1}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right]} \right\} \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \end{aligned}$$

$$-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \left[ c_2(q) + \frac{e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right] \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \left\} \prod'_{\mathbf{q} \neq 0} \frac{1}{1 + (1 - e^{-2\beta \hbar^2 q^2 / 2m^*}) c_2(q)}. \quad (3.13)$$

Thus, we have also found the right-hand side of the main equation (1.15). Now we can proceed to determining the unknown coefficient functions  $c_0$ ,  $c_1(q)$  and  $c_2(q)$ .

#### IV. EQUATIONS FOR THE $c_n(q)$ COEFFICIENT FUNCTIONS

To satisfy condition (2.17) the exponent factor in (3.3) should equal the  $U$  function from (2.4) for any values of the  $\rho_{\mathbf{q}}$  variable and the arbitrary function  $\lambda(q)$ . From this condition we find the equation for the unknown functions  $c_0$ ,  $c_1(q)$ ,  $c_2(q)$ . Thus, we will equate the coefficients at the identical degrees of  $\rho_{\mathbf{q}}$  in (2.4) as well as in the exponent of the right-hand side part of equation (3.13):

$$a_0 = c_0 + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \lambda^2(q) \left/ \left[ c_2(q) + \frac{1}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right] - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left[ 1 + \left( 1 - e^{-2\beta \hbar^2 q^2 / 2m^*} \right) c_2(q) \right], \quad (4.1)$$

$$a_1(q) = \lambda(q) \left[ c_1(q) + \frac{e^{-\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right] \left/ \left[ c_2(q) + \frac{1}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right], \quad (4.2)$$

$$a_2(q) = \left[ c_1(q) + \frac{e^{-\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right]^2 \left/ \left[ c_2(q) + \frac{1}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right] - \left[ c_2(q) + \frac{e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}} \right]. \quad (4.3)$$

Let us address equation (4.1) taking into account expression (2.5) for  $a_0$  as a result of the arbitrariness of the function  $\lambda(q)$ . We will obtain one more additional equation equaling the multipliers near  $\lambda^2(q)$  on either side in equation (4.1). In equation (4.2) the value of  $\lambda(q)$  falls out as can be seen from (2.4). Thus, we now have three equations for two coefficients  $c_1(q)$  and  $c_2(q)$ . If our theory is consistent, one of the equations from system (4.1)–(4.3) will be satisfied identically:

$$\frac{\frac{2\alpha_q}{\alpha_q+1} e^{-\beta E(q)}}{1 + \frac{\alpha_q-1}{\alpha_q+1} e^{-2\beta E(q)}} = \frac{\bar{c}_1(q)}{\bar{c}_2(q)},$$

$$a_2(q) = \frac{\bar{c}_1^2(q)}{\bar{c}_2(q)} - \bar{c}_2(q) + 1, \quad (4.4)$$

$$\frac{1}{\alpha_q + 1} \frac{1 - e^{-2\beta E(q)}}{1 + \frac{\alpha_q-1}{\alpha_q+1} e^{-2\beta E(q)}} = \frac{1}{2\bar{c}_2(q)},$$

here we have introduced abbreviated notations

$$\bar{c}_1(q) = c_1(q) + \frac{e^{-\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}}, \quad (4.5)$$

$$\bar{c}_2(q) = c_2(q) + \frac{1}{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}}. \quad (4.6)$$

From the third equation of system (4.4) we have

$$\begin{aligned} \bar{c}_2(q) &= \frac{\alpha_q + 1}{2} \frac{1 + \frac{\alpha_q-1}{\alpha_q+1} e^{-2\beta E(q)}}{1 - e^{-2\beta E(q)}} \\ &= \frac{1 + \alpha_q \coth[\beta E(q)]}{2}, \end{aligned}$$

and from (4.6)

$$c_2(q) = \frac{1}{2} \left\{ \alpha_q \coth[\beta E(q)] - \coth \left[ \beta \frac{\hbar^2 q^2}{2m^*} \right] \right\}. \quad (4.7)$$

Now, from the first equation (4.4) we find

$$\bar{c}_1(q) = \frac{\alpha_q}{2 \sinh[\beta E(q)]},$$

and from (4.5) we have

$$c_1(q) = \frac{1}{2} \left\{ \frac{\alpha_q}{\sinh[\beta E(q)]} - \frac{1}{\sinh \left[ \beta \frac{\hbar^2 q^2}{2m^*} \right]} \right\}. \quad (4.8)$$

We can easily check now that the second equation from system (4.4) is indeed met identically as expected.

Finally, from (4.1) we also find the coefficient

$$c_0 = -\beta E_0 + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left( \frac{1 - e^{-2\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-2\beta E(q)}} \right) + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \alpha_q. \quad (4.9)$$

## V. DENSITY MATRIX AND THE PARTITION FUNCTION

With the help of expressions (4.7)–(4.9) taking into account (1.8)–(1.10) we find the explicit expression for the  $N$ -particle density matrix:

$$R_N(x'|x) = R_N^0(x'|x) \exp \left\{ -\beta E_0 + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left( \frac{\alpha_q \tanh \left[ \frac{\beta}{2} E(q) \right]}{\tanh \left[ \beta \frac{\hbar^2 q^2}{4m^*} \right]} \right) + \sum_{\mathbf{q} \neq 0} \ln \left( \frac{1 - e^{-\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-\beta E(q)}} \right) \right\} \\ \times \exp \left\{ -\frac{1}{4} \sum_{\mathbf{q} \neq 0} \left( \alpha_q \coth [\beta E(q)] - \coth \left[ \beta \frac{\hbar^2 q^2}{2m^*} \right] \right) (\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}) \right. \\ \left. + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \left( \frac{\alpha_q}{\sinh [\beta E(q)]} - \frac{1}{\sinh \left[ \beta \frac{\hbar^2 q^2}{2m^*} \right]} \right) \rho_{\mathbf{q}} \rho'_{-\mathbf{q}} \right\}. \quad (5.1)$$

By integrating the density matrix diagonal elements in compliance with (1.6) we obtain the partition function

$$Z_N = \int R_N(x|x) dx, \quad (5.2)$$

from which we will find free energy  $F = -T \ln Z_N$ , and from the latter other thermodynamic functions.

In (5.2) let us pass over from the integration over the individual coordinates  $(\mathbf{r}_1, \dots, \mathbf{r}_N)$  to the integration over the collective variables (1.11) similarly to what was done in (3.1):

$$Z_N = Z_N^0 \exp \left\{ -\beta E_0 + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left( \frac{\alpha_q \tanh \left[ \frac{\beta}{2} E(q) \right]}{\tanh \left[ \beta \frac{\hbar^2 q^2}{4m^*} \right]} \right) + \sum_{\mathbf{q} \neq 0} \ln \left( \frac{1 - e^{-\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-\beta E(q)}} \right) \right\} \int (d\rho) J(\rho) \\ \times \exp \left\{ -\frac{1}{2} \sum_{\mathbf{q} \neq 0} \left( \alpha_q \tanh \left[ \frac{\beta}{2} E(q) \right] - \tanh \left[ \beta \frac{\hbar^2 q^2}{4m^*} \right] \right) \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \right\}, \quad (5.3)$$

where the weight function

$$J(\rho) = \left\langle \prod'_{\mathbf{q} \neq 0} \delta \left( \rho_{\mathbf{q}} - \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}_j} \right) \right\rangle^0, \quad (5.4)$$

here the angular brackets marked with “0” denote the following averaging:

$$\langle \dots \rangle^0 = \frac{1}{Z_N^0} \int (\dots) R_N^0(x|x) dx, \quad (5.5)$$

and the partition function of the ideal gas

$$Z_N^0 = \int R_N^0(x|x) dx. \quad (5.6)$$

We calculate the  $J(\rho)$  weight function from (5.4) in the same way as the  $J_0(\rho')$  function from (3.3), clearly just with a different averaging operation (5.5) instead of (3.6). Thus, by the respective reassignment for  $J(\rho)$  we have expressions (3.5) and (3.8). The necessary average values contained in (3.8) can now be calculated easily as well

$$\left\langle \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}_j} \right\rangle^0 = \sqrt{N} \delta_{\mathbf{q},0},$$

and

$$\left\langle \left( \frac{1}{\sqrt{N}} \sum_{j_1=1}^N e^{-i\mathbf{q}_1 \mathbf{r}_{j_1}} \right) \left( \frac{1}{\sqrt{N}} \sum_{j_2=1}^N e^{-i\mathbf{q}_2 \mathbf{r}_{j_2}} \right) \right\rangle^0$$

$$= S_0(q_1)\delta(\mathbf{q}_1 + \mathbf{q}_2), \quad \mathbf{q}_1 \neq 0, \quad \mathbf{q}_2 \neq 0, \quad (5.7)$$

where  $S_0(q)$  by definition is a pair structure factor of the ideal Bose-gas. The expression for it is well-known

$$S_0(q) = 1 + \frac{1}{N} \sum_{\mathbf{p}} n_p n_{|\mathbf{p}+\mathbf{q}|}, \quad (5.8)$$

where

$$n_p = \frac{1}{z_0^{-1} e^{\beta \frac{\hbar^2 p^2}{2m^*}} - 1} \quad (5.9)$$

is an average number of particles whose momentum equals  $\hbar\mathbf{p}$ , the activity of the ideal gas  $z_0$  being excluded from the condition

$$\sum_{\mathbf{p}} n_p = N. \quad (5.10)$$

Let us also remember the expression for the partition function of the ideal Bose-gas (5.6) the particles of which have the mass  $m^*$

$$Z_N^0 = \exp \left[ - \sum_{\mathbf{q}} \ln \left( 1 - z_0 e^{-\beta \hbar^2 q^2 / 2m^*} \right) \right]. \quad (5.11)$$

The necessary integral over  $\omega_{\mathbf{k}}$  in (3.8) taking into account pair correlations can be easily taken. We will find the weight function (5.4):

$$J(\rho) = \left( \prod'_{\mathbf{q} \neq 0} \frac{1}{\pi S_0(q)} \right) \exp \left[ - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \frac{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}{S_0(q)} \right]. \quad (5.12)$$

Now, taking into account (5.12) the integration over the variables  $\rho_{\mathbf{q}}$  in (5.3) is reduced to the calculation of the Poisson integral:

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$$Z_N = Z_N^0 \exp \left\{ -\beta E_0 + \sum_{\mathbf{q} \neq 0} \ln \left( \frac{1 - e^{-\beta \frac{\hbar^2 q^2}{2m^*}}}{1 - e^{-\beta E(q)}} \right) + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left( \frac{\alpha_q \tanh \left[ \frac{\beta}{2} E(q) \right]}{\tanh \left[ \beta \frac{\hbar^2 q^2}{4m^*} \right]} \right) \right. \\ \left. - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left[ 1 + S_0(q) \left( \alpha_q \tanh \left[ \frac{\beta}{2} E(q) \right] - \tanh \left[ \beta \frac{\hbar^2 q^2}{4m^*} \right] \right) \right] \right\}. \quad (5.13)$$

Expressions (5.1) and (5.13) for the density matrix and for the statistical operator are the starting formulae for the calculation of the thermodynamic and structure functions of the Bose-liquid. Before we pass over to the calculation of these values we will make some preliminary studies.

First of all we will say that we have not obtained the equation for the effective mass  $m^*$ . It is not surprising at all as we were working in the approximation of one sum over the wave vector  $\mathbf{q}$  and the difference between the effective mass  $m^*$  and the initial particle mass  $m$  is proportional to the sum over  $\mathbf{q}$ .

Let us pass to the discussion of the obtained expressions for the partition function and the density matrix. It is apparent that when we switch off the interparticle interaction with  $\nu_q = 0$ , i. e.,  $\alpha_q = 1$  we will obtain from

(5.1) that for any temperature

$$R_N(x|x') = R_N^0(x|x'),$$

and

$$Z_N = Z_N^0.$$

Notwithstanding the naturalness of this condition it will not be met, for instance, by the well-known Penrose formula for the  $N$ -particles density matrix. This formula was also obtained by Feenberg [23]. Applying the method of coherent states it was also found in [24]. With the help of wave functions of the many-boson Bogoliubov–Zubarev system [26] it was calculated in [27, 28]. Using our notations it looks as follows:

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$$R_N(x|x') = \left\{ \prod'_{\mathbf{q} \neq 0} \alpha_q \tanh \frac{E(q)}{2T} \right\} \exp \left\{ - \frac{E_0}{T} - \sum_{\mathbf{q} \neq 0} \ln \left( 1 - e^{-E(q)/T} \right) + \frac{1}{4} \sum_{\mathbf{q} \neq 0} (\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}) \right\}$$

$$- \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{\alpha_q}{\sinh[E(q)/T]} \left[ (\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}) \cosh \frac{E(q)}{T} - (\rho_{\mathbf{q}} \rho'_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho_{-\mathbf{q}}) \right] \Bigg\}. \quad (5.14)$$

This expression holds true only for  $T \rightarrow 0$ . If  $\alpha_q = 1$ , then from (5.14) we obtain an expression for the ideal gas density matrix

$$R_N^0(x|x') = \left\{ \prod'_{\mathbf{q} \neq 0} \tanh \left[ \frac{\hbar^2 q^2}{4mT} \right] \right\} \exp \left\{ - \sum_{\mathbf{q} \neq 0} \ln \left( 1 - e^{-\hbar^2 q^2 / 2mT} \right) + \frac{1}{4} \sum_{\mathbf{q} \neq 0} (\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}) \right. \\ \left. - \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{1}{\sinh(\hbar^2 q^2 / 2mT)} \left[ (\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}) \cosh \left[ \frac{\hbar^2 q^2}{2mT} \right] - (\rho_{\mathbf{q}} \rho'_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho_{-\mathbf{q}}) \right] \right\}, \quad (5.15)$$

which does not coincide with the precise expression (1.9) for  $m^* = m$ . It is not surprising at all as in the  $\rho_{\mathbf{q}}$  representation the kinetic energy operator is not diagonal (which can be shown at least from equation (2.7)). It is just on its off-diagonal part that we are building the perturbation theory in which each subsequent member of the series has in comparison with the previous member an additional summation over the wave vector  $\mathbf{q}$ .

It is curious that formulae (5.14) and (5.15) prompt to us how one can formally obtain our result for the density matrix. Thus we have the equation

$$R_N(x|x') = R_N^0(x|x') \frac{R_N(x|x') \text{(from formula (5.14))}}{R_N^0(x|x') \text{(from formula (5.15))}}. \quad (5.16)$$

If we use expressions (5.14) and (5.15) in the right-hand part of this equation for the density matrices relation, we will immediately arrive at formula (5.1) with  $m^* = m$ . This trick also hints at a possibility of calculating the effective mass  $m^*$ . Thus, should we find the following approximation for the density matrix (5.14), for instance by solving Bloch's equation directly, as suggested in [28], the result will be the following. Firstly, we will obtain in the (5.14) exponent the  $\sim \rho_{\mathbf{q}_1} \rho_{\mathbf{q}_2} \rho_{\mathbf{q}_3}$  members from  $\mathbf{q}_3 = -\mathbf{q}_1 - \mathbf{q}_2$ , viz., a contribution from the three-particle correlations and also a share of the contribution from the four-particle correlations  $\sim \rho_{\mathbf{q}_1} \rho_{-\mathbf{q}_1} \rho_{\mathbf{q}_2} \rho_{-\mathbf{q}_2}$  (appropriately systematized as regards the primed and the nonprimed variables (1.11) and (1.12)). Besides, there also arise corrections  $\sim \sum_{\mathbf{q} \neq 0} (\dots) / N$  to the zeroth approximation coefficient functions around  $\rho_{\mathbf{q}} \rho_{-\mathbf{q}}$  in (5.14) (again systematized as regards the primed and the nonprimed variables). A part of these corrections can be "hidden" quite naturally by renormalizing the particle mass  $m$ . After this fixing of the renormalized mass  $m^*$  we suggest that  $\alpha_q \rightarrow 1$  and find the ideal gas density matrix  $R_N^0(x|x')$  in which instead of  $m$  we will have  $m^*$ . Then we will address formula (5.16) and by the same reasoning we arrive at (5.1) with the known value of  $m^*$ . Now from formula (5.16) we can also answer the question why formula (5.1) holds true for any mass  $m^*$ . The matter is that we multiply and divide by the same value  $R_N^0(x|x')$  "finding" the denominator for all the orders of the perturbation theory by the number of summations over the wave vector.

In the approach suggested here the effective mass also arises in the natural fashion if we take into considera-

tion the contribution of the many particle correlations in expressions (1.10) and (2.4) and if we renormalize the mass by the contributions to be factorized (possibly with the dependence upon the wave vector  $\mathbf{q}$ ). We will not discuss here higher approximations and the discussion of the issue of  $m^*$  will be returned to in Section VIII.

If we direct the temperature towards zero, i. e.,  $\beta \rightarrow \infty$  then from (5.1) with the consideration of the fact that the density matrix of the ideal Bose-gas, which in this case is fully degenerate, equals  $1/V^N$ , we will obtain in compliance with designation (1.6) the following expression

$$R_N(x|x') = e^{-\beta E_0} \psi_0(x') \psi_0(x),$$

where the normalized wave function of the ground state of the interacting Bose-particles system

$$\psi_0(x) = \frac{1}{\sqrt{V^N}} \left( \prod_{\mathbf{q} \neq 0} \sqrt{\alpha_q} \right) \\ \times \exp \left[ - \frac{1}{4} \sum_{\mathbf{q} \neq 0} (\alpha_q - 1) \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \right]$$

coincides with that discovered for the first time by Bogoliubov and Zubarev [26].

Finally we will consider the classical limit  $\hbar \rightarrow 0$  of the density matrix diagonal elements (5.1) when  $\rho'_{\mathbf{q}} = \rho_{\mathbf{q}}$ .

The energy  $E_0$  from (2.16) in this limit transforms into

$$E_0 = \frac{N(N-1)}{2V} \nu_0 - \sum_{\mathbf{q} \neq 0} \frac{N}{2V} \nu_{\mathbf{q}}. \quad (5.17)$$

Then, the first logarithm under the sum over  $\mathbf{q}$  in the exponent in (5.1) (together with the factor  $1/2$ ) is reduced at  $\hbar \rightarrow 0$  to  $\ln \alpha_{\mathbf{q}}$  and the second one to  $\ln(1/\alpha_{\mathbf{q}})$ ; they cancel each other, the factor at  $\rho_{\mathbf{q}} \rho_{-\mathbf{q}}$  equaling

$$\begin{aligned} \nu_{\mathbf{q}}^* &= \alpha_{\mathbf{q}} \tanh \left[ \frac{\beta}{2} E(\mathbf{q}) \right] - \tanh \left[ \beta \frac{\hbar^2 q^2}{4m^*} \right], \\ \nu_{\mathbf{q}}^* &= \beta \frac{N}{V} \nu_{\mathbf{q}}, \quad \hbar \rightarrow 0. \end{aligned} \quad (5.18)$$

We have made use of the fact that at high temperatures  $m^* \rightarrow m$ . In the  $R_N^0(x|x)$  matrix from (1.9) at  $\hbar \rightarrow 0$  only an identical permutation survives

$$R_N^0(x|x) = \frac{1}{N!} \left( \frac{m}{2\pi\beta\hbar^2} \right)^{3N/2}.$$

Consequently, bringing everything together we have the exact classical solution for the density matrix

$$R_N(x|x) = \frac{1}{N!} \left( \frac{m}{2\pi\beta\hbar^2} \right)^{3N/2} e^{-\beta\Phi},$$

where the potential energy  $\Phi$  is given by equation (2.5).

For the partition function (5.13) taking into account the fact that in the classical limit  $\hbar \rightarrow 0$  the struc-

tural factor of the ideal gas (5.8)  $S_0(q) = 1$  we find a well-known expression in the random phase approximation [3, 25]:

$$\begin{aligned} Z_N &= Z_N^0 \exp \left\{ -\beta \frac{N(N-1)}{2V} \nu_0 \right. \\ &\quad \left. - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \left[ \ln \left( 1 + \beta \frac{N}{V} \nu_{\mathbf{q}} \right) - \beta \frac{N}{V} \nu_{\mathbf{q}} \right] \right\}, \end{aligned} \quad (5.19)$$

$$Z_N^0 = \frac{V^N}{N!} \left( \frac{m}{2\pi\beta\hbar^2} \right)^{3N/2}.$$

Thus from expressions (5.1), (5.13) for the density matrix and the partition function we have received all the known limiting cases both in the essentially quantum and classical regions. For that matter we can expect these expressions to give good results also in the intermediate temperature region, in particular in the vicinity of the  $\lambda$ -transition point.

## VI. ENERGY

From expression (5.13) for the partition function we find the energy by the well-known thermodynamic equation:

$$E = \frac{\partial}{\partial \beta} (\beta F) = -\frac{\partial}{\partial \beta} \ln Z_N.$$

Simple calculations give

$$\begin{aligned} E &= E_0 + \sum_{\mathbf{q} \neq 0} \frac{E(\mathbf{q})}{e^{\beta E(\mathbf{q})} - 1} + \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m^{**}} \left[ \frac{1}{z_0^{-1} e^{\frac{\beta \hbar^2 q^2}{2m^{**}}} - 1} - \frac{1}{e^{\beta \frac{\hbar^2 q^2}{2m^{**}}} - 1} \right] \\ &\quad - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \left( \frac{E(\mathbf{q})}{\sinh[\beta E(\mathbf{q})]} - \frac{\hbar^2 q^2 / 2m^{**}}{\sinh[\beta \hbar^2 q^2 / 2m^{**}]} \right) + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \frac{1}{1 + S_0(q) (\alpha_{\mathbf{q}} \tanh[\beta E(\mathbf{q})/2] - \tanh[\beta \hbar^2 q^2 / 4m^{**}])} \\ &\quad \times \left\{ \frac{S_0(q)}{2} \left[ \frac{\alpha_{\mathbf{q}} E(\mathbf{q})}{\cosh^2[\beta E(\mathbf{q})/2]} - \frac{\hbar^2 q^2 / 2m^{**}}{\cosh^2[\beta \hbar^2 q^2 / 4m^{**}]} \right] + \frac{\partial S_0(q)}{\partial \beta} \left( \alpha_{\mathbf{q}} \tanh \left[ \frac{\beta}{2} E(\mathbf{q}) \right] - \tanh \left[ \beta \frac{\hbar^2 q^2}{4m^{**}} \right] \right) \right\}, \end{aligned} \quad (6.1)$$

where the value

$$m^{**} = m^* \left/ \left[ 1 + \beta m^* \frac{\partial}{\partial \beta} \left( \frac{1}{m^*} \right) \right] \right. \quad (6.2)$$

For the actual calculus of the temperature dependence of the energy  $E$  we will write in more detail the ideal

Bose-gas structural factor (5.8) and its derivative with respect to the inverse temperature

$$\frac{\partial S_0(q)}{\partial \beta} = \frac{2}{N} \sum_{\mathbf{p}} \frac{\partial n_{\mathbf{p}}}{\partial \beta} n_{|\mathbf{p}+\mathbf{q}|}, \quad (6.3)$$

which enter (6.1) with the consideration of the Bose-

Einstein condensation phenomenon.

Bose-condensation arises on condition that  $z_0 = 1$  and the critical temperature  $T_c$  is determined from equation (5.10) [1, 4, 6]

$$T_c = \frac{2\pi\hbar^2}{m^*} \left[ \frac{N}{V} / \zeta(3/2) \right]^{2/3}, \quad (6.4)$$

where Riemann  $\zeta$ -function  $\zeta(3/2) = 2.612375\dots$ . As the effective mass also happens to be a function of temperature, expression (6.4) as a matter of fact is the equation for determining the temperature of the Bose-condensation  $T_c$ .

In (5.4) we will single out the terms with the average number of particles  $n_0$  whose momenta equal zero:

$$T \leq T_c, \quad z_0 = 1, \quad (6.5)$$

$$S_0(q) = 1 + 2\frac{n_0}{N}n_q + \frac{1}{N} \sum_{\substack{\mathbf{p} \neq 0 \\ \mathbf{p}+\mathbf{q} \neq 0}} n_p n_{|\mathbf{p}+\mathbf{q}|}.$$

Now, taking into account the temperature dependence of the Bose-condensate fraction for an ideal gas [1, 4]

$$\frac{n_0}{N} = 1 - \left( \frac{T}{T_c} \right)^{3/2},$$

which is also determined from condition (5.10) for the temperatures  $T \leq T_c$ . We find from (6.5) that

$$S_0(q) = \coth \left( \beta \frac{\hbar^2 q^2}{4m^*} \right) - 2 \left( \frac{T}{T_c} \right)^{3/2} n_q$$

$$+ \frac{1}{N} \sum_{\substack{\mathbf{p} \neq 0 \\ \mathbf{p}+\mathbf{q} \neq 0}} n_p n_{|\mathbf{p}+\mathbf{q}|}.$$

In this expression we will pass from the summation over the wave vector  $\mathbf{p}$  to the integration considering the thermodynamic limit  $N \rightarrow \infty$ ,  $V \rightarrow \infty$ ,  $N/V = \rho = \text{const}$  and ultimately we find after integration over angles

$$S_0(q) = \coth \left( \beta \frac{\hbar^2 q^2}{4m^*} \right) - \frac{2(T/T_c)^{3/2}}{e^{\beta \frac{\hbar^2 q^2}{2m^*}} - 1} + \frac{m^*}{4\pi^2 \rho q \hbar^2 \beta} \times \int_0^\infty \frac{p}{e^{\beta \hbar^2 p^2 / 2m^*} - 1} \ln \left| \frac{1 - e^{-\beta \frac{\hbar^2 (p+q)^2}{2m^*}}}{1 - e^{-\beta \frac{\hbar^2 (p-q)^2}{2m^*}}} \right| dp, \quad (6.6)$$

$$T \leq T_c.$$

For the temperatures which are above the critical temperature the Bose-condensate is absent ( $n_0 = 0$ ), that is why from (5.8)

$$S_0(q) = 1 + \frac{m^*}{4\pi^2 \rho q \hbar^2 \beta} \int_0^\infty \frac{p}{z_0^{-1} e^{\beta \hbar^2 p^2 / 2m^*} - 1} \times \ln \left| \frac{1 - z_0 e^{-\beta \frac{\hbar^2 (p+q)^2}{2m^*}}}{1 - z_0 e^{-\beta \frac{\hbar^2 (p-q)^2}{2m^*}}} \right| dp, \quad (6.7)$$

$$T \geq T_c.$$

We carry out analogous calculations also for the structure factor derivative (6.3):

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$$\frac{\partial S_0(q)}{\partial \beta} = 3T \left( \frac{T}{T_c} \right)^{3/2} \frac{m^*/m^{**}}{e^{\beta \frac{\hbar^2 q^2}{2m^*}} - 1} - \frac{\hbar^2 q^2 / 4m^{**}}{\sinh^2 \left( \beta \frac{\hbar^2 q^2}{4m^*} \right)} \left[ 1 - \left( \frac{T}{T_c} \right)^{3/2} \right] - \frac{m^*}{16\pi^2 \rho q \beta m^{**}} \int_0^\infty dp \frac{p^3}{\sinh^2 \left( \beta \frac{\hbar^2 p^2}{4m^*} \right)} \ln \left| \frac{1 - e^{-\beta \frac{\hbar^2 (p+q)^2}{2m^*}}}{1 - e^{-\beta \frac{\hbar^2 (p-q)^2}{2m^*}}} \right|, \quad (6.8)$$

$$T \leq T_c$$

and

$$\frac{\partial S_0(q)}{\partial \beta} = -\frac{m^*}{16\pi^2 \rho q \beta m^{**}} \int_0^\infty dp \frac{p^3}{\sinh^2 \left[ \beta \frac{\hbar^2 p^2}{4m^*} - \frac{\ln z_0}{2} \right]} \left( 1 - \frac{\partial \ln z_0}{\partial \beta} / \frac{\hbar^2 p^2}{2m^{**}} \right) \ln \left| \frac{1 - z_0 e^{-\beta \frac{\hbar^2 (p+q)^2}{2m^*}}}{1 - z_0 e^{-\beta \frac{\hbar^2 (p-q)^2}{2m^*}}} \right|, \quad (6.9)$$

$$T \geq T_c.$$

Let us now analyze the expression for the energy  $E$  from (6.1) in the low-temperature region. If  $T < T_c$  then  $z_0 = 1$  and the contribution of the third term in (6.1) equals zero and the last two terms cancel each other, and this can be seen from (6.6) and (6.8) at  $\beta \rightarrow \infty$ ,  $S_0(q) \rightarrow \coth(\beta\hbar^2 q^2/4m^*)$  and also  $\partial S_0(q)/\partial\beta \rightarrow -\hbar^2 q^2/[4m^{**} \sinh^2(\beta\hbar^2 q^2/4m^*)]$ . Consequently, we obtain Bogoliubov's formula for the energy as a mean value of the energy of the non-interacting elementary excitations:

$$E = E_0 + \sum_{\mathbf{q} \neq 0} \frac{E(q)}{e^{\beta E(q)} - 1}, \quad T \rightarrow 0.$$

In the quasi-classical limit  $\hbar \rightarrow 0$  from (6.1) we can easily find:

$$E = \frac{3}{2}NT + \frac{N(N-1)}{2V}\nu_0 - \frac{T}{2} \sum_{\mathbf{q} \neq 0} \frac{(\beta \frac{N}{V} \nu_q)^2}{1 + \beta \frac{N}{V} \nu_q}. \quad (6.10)$$

This expression corresponds to the random phases approximation also for the partition function (5.19). When arriving at it we took into account that at  $\hbar \rightarrow 0$  the value of  $E_0$  in (6.1) gets canceled together with the second member in the square brackets of the third term since at high temperatures the high values of  $q$  prove to be important when  $\alpha_q \rightarrow 1$ . The fourth term in expression (6.1) at  $\hbar \rightarrow 0$  also tends to zero and from the last fifth term we

find a contribution taking into account that  $S_0(q) \rightarrow 1$  and  $\partial S_0(q)/\partial\beta = 0$  as can be seen from (6.7) and (6.9). Finally, the first term in the square brackets of the second term of the energy  $E$  is the energy of the ideal gas (with the temperature dependence of the effective mass  $m^*$  being taken into account) and in the classical limit it equals  $3NT/2$ .

Hence, both at high and low temperatures our theory yields correct limiting cases. That is why we can expect good results also in the intermediate temperature domain.

## VII. STRUCTURE FACTOR AND THE POTENTIAL ENERGY

By definition the structure factor is the mean quadratic fluctuation of particles density:

$$S(q) = \frac{\int |\rho_{\mathbf{q}}|^2 R_N(x|x) dx}{\int R_N(x|x) dx}. \quad (7.1)$$

For calculating this expression we will use the designation of the partition function (3.2) with integration over variables  $\rho_{\mathbf{q}}$  (5.3) and we will write (7.1) as a functional derivative:

$$S(q) = -2 \frac{\delta \ln Z_N}{\delta \nu_q^*}, \quad (7.2)$$

where the quantity  $\nu_q^*$  is defined by formula (5.18). By means of expression (5.13) we will find from (7.2) that

$$S(q) = \frac{S_0(q)}{1 + S_0(q) (\alpha_q \tanh[\beta E(q)/2] - \tanh[\beta\hbar^2 q^2/4m^*])}. \quad (7.3)$$

At the temperature of absolute zero ( $T = 0$  K) when  $\nu_q^* = (\alpha_q - 1)$ , we have the expression which is yielded by Bogoliubov's theory [16, 26]:

$$S(q) = \frac{1}{\alpha_q}. \quad (7.4)$$

The classical limit  $\hbar \rightarrow 0$  in (7.3) also yields a well-known result for the structure factor in the random phase approximation:

$$S(q) = \frac{1}{1 + \beta \frac{N}{V} \nu_q}. \quad (7.5)$$

We have one more illustration of the consistency of our theory.

Using formula (7.3) we find the mean value of the potential energy (2.5) calculated with the full Hamiltonian (1.1):

$$\langle \Phi \rangle_H = \frac{\int R(x|x) \Phi dx}{\int R(x|x) dx}.$$

Thus,

$$\langle \Phi \rangle_H = \frac{N(N-1)}{2V} \nu_0 + \frac{N}{2V} \sum_{\mathbf{q} \neq 0} \nu_q \left[ \frac{S_0(q)}{1 + S_0(q) (\alpha_q \tanh [\beta E(q)/2] - \tanh [\beta \hbar^2 q^2 / 4m^*])} - 1 \right]. \quad (7.6)$$

In its turn, this expression makes it possible to calculate the mean kinetic energy  $K$  as a difference of the full energy (6.1) and (7.6):

$$K = E - \langle \Phi \rangle_H. \quad (7.7)$$

### VIII. EFFECTIVE MASS

As we have already mentioned in [19] a different method was used to obtain a formula for the density matrix  $R_N(x'|x)$  as a product of the density matrix of the interacting particles with the effective mass  $m^*$  multiplied by the factor  $P_N(x'|x)$  which takes into account the interparticle correlations. Moreover, both for  $P_N(x'|x)$  and for  $m^*$  an expression was found only in the limit  $T = 0$  K. The effective mass is determined by the following equation [19]:

$$\frac{m}{m^*} = 1 - \frac{1}{3N} \sum_{\mathbf{q} \neq 0} \frac{(\alpha_q - 1)^2}{\alpha_q (\alpha_q + 1)}. \quad (8.1)$$

It is curious that this result coincides with the expression for the effective mass  $M^*$  of the impurity atom moving in the liquid  ${}^4\text{He}$  which we obtained in [29] using a completely different method

$$\begin{aligned} \frac{M}{M^*} &= 1 - \frac{1}{3N} \sum_{\mathbf{q} \neq 0} \frac{(\alpha_q - 1)^2}{\alpha_q (1 + \alpha_q \frac{M}{m})} \\ &\times \left[ 1 - \frac{(1 - \frac{M}{m})}{1 + \alpha_q \frac{M}{m}} \right]^2, \end{aligned} \quad (8.2)$$

should the atom of the impurity be taken as equal to the mass  $m$ , i. e., to the mass of the  ${}^4\text{He}$  atom. Expression (8.1) with the square bracket replaced by one was obtained independently in several studies [30–33].

The fact that the “analytical extension” of formula (8.2) in the case when the impurity mass equals that of the liquid atom takes us to expression (8.1) testifies to a certain self-consistency of the theory [19]. The same coincidence of effective masses as shown in [19] cannot be expected at the temperatures not equaling zero. A dependence between the effective mass of the impurity  $M^*$  on the temperature was studied in [34].

It is obvious that for high temperatures the role of interatomic interaction decreases and  $m^* \rightarrow m$  when  $\beta \rightarrow 0$ . Let us consider this question in more detail. Let the impurity atom of the mass  $M$  and the coordinate  $\mathbf{R}$  move in the liquid. The complete Hamiltonian of the system “an atom plus liquid” consists of the sum of the Hamiltonians of the liquid (1.1) plus the Hamiltonian of the impurity

$$H_i = \frac{M\mathbf{v}^2}{2} + \frac{N}{V} \bar{\nu}_0 + \frac{\sqrt{N}}{V} \sum_{\mathbf{q} \neq 0} \bar{\nu}_q e^{i\mathbf{q}\mathbf{R}} \rho_{\mathbf{q}}. \quad (8.3)$$

Here the first term is the kinetic energy of the impurity atom whose velocity equals  $\mathbf{v}$ , the two other terms being its potential energy of the pair interaction with the liquid atoms with the Fourier  $\bar{\nu}_q$  coefficient. As we consider a classical system its partition factor  $Z$  and additional energy  $\Delta E$  to the full energy of the liquid (6.10) can be easily found in the random phase approximation (see (5.19))

$$Z = Z_N Z_i, \quad (8.4)$$

where

$$\begin{aligned} Z_i &= V \left( \frac{M}{2\pi\beta\hbar^2} \right)^{3/2} \exp \left\{ -\beta \frac{N}{V} \bar{\nu}_0 \right. \\ &\left. + \frac{1}{2N} \sum_{\mathbf{q} \neq 0} \frac{(\beta \frac{N}{V} \bar{\nu}_q)^2}{1 + \beta \frac{N}{V} \nu_q} \right\}, \end{aligned} \quad (8.5)$$

and  $Z_N$  can be found from formula (5.19);

$$\begin{aligned} \Delta E &= \frac{3}{2} T + \frac{N}{V} \bar{\nu}_0 - \frac{T}{2N} \sum_{\mathbf{q} \neq 0} \frac{(\beta \frac{N}{V} \bar{\nu}_q)^2}{1 + \beta \frac{N}{V} \nu_q} \\ &- \frac{T}{2N} \sum_{\mathbf{q} \neq 0} \left( \frac{\beta \frac{N}{V} \bar{\nu}_q}{1 + \beta \frac{N}{V} \nu_q} \right)^2. \end{aligned} \quad (8.6)$$

Let us now introduce some effective Hamiltonian of the system “an atom plus liquid” in which the mass of the impurity atom is substituted by the effective mass  $M^*$ , the interaction between the liquid particles  $\nu_q$  is substituted by  $\bar{\nu}_q$  at  $\mathbf{q} \neq 0$  and the interaction between the impurity atom and the liquid is absent. Constants  $\nu_0$  and  $\bar{\nu}_0$  remain invariable at  $\mathbf{q} = 0$  as we are interested

by the renormalization via fluctuation mechanism, when  $\mathbf{q} \neq 0$ . We will introduce the quantities  $M^*$ ,  $\tilde{\nu}_q$  in the way so that the thermodynamic function of the initial system “an atom plus field” and the approximating mod-

el with the effective Hamiltonian should coincide in the respective approximations. For the suggested model with the effective Hamiltonian the partition function can be found easily

$$Z = Z_N^0 V \left( \frac{M^*}{2\pi\beta\hbar^2} \right)^{3/2} \exp \left[ -\beta \frac{N(N-1)}{2V} \nu_0 - \beta \frac{N}{V} \bar{\nu}_0 + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \beta \frac{N}{V} \tilde{\nu}_q - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left( 1 + \beta \frac{N}{V} \tilde{\nu}_q \right) \right]. \quad (8.7)$$

Let us now compare expressions for the partition function of the initial system (8.4) and (8.5) and the model system (8.7):

$$\begin{aligned} & -\frac{3}{2} \ln \frac{M}{M^*} - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \left[ \ln \left( 1 + \beta \frac{N}{V} \tilde{\nu}_q \right) - \beta \frac{N}{V} \tilde{\nu}_q \right] \\ & = \frac{1}{2N} \sum_{\mathbf{q} \neq 0} \frac{(\beta \frac{N}{V} \tilde{\nu}_q)^2}{1 + \beta \frac{N}{V} \tilde{\nu}_q} - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \left[ \ln \left( 1 + \beta \frac{N}{V} \nu_q \right) - \beta \frac{N}{V} \nu_q \right]. \end{aligned} \quad (8.8)$$

Taking into account some arbitrariness in the designation of  $M^*$  and  $\tilde{\nu}_q$  we will equate in (8.8) logarithmic terms. As a result of this we will find the effective potential

$$\tilde{\nu}_q = \nu_q + \frac{\beta \bar{\nu}_q^2}{V (1 + \beta \frac{N}{V} \nu_q)}$$

and in the linear approximation the effective mass:

$$\frac{M}{M^*} = 1 - \frac{1}{3N} \sum_{\mathbf{q} \neq 0} \left( \frac{\beta \frac{N}{V} \bar{\nu}_q}{1 + \beta \frac{N}{V} \nu_q} \right)^2. \quad (8.9)$$

Let us now put in (8.9) that  $M = m$ ,  $\bar{\nu}_q = \nu_q$  and find an expression for the effective mass  $m^*$  in the classical limit  $\hbar \rightarrow 0$ :

$$\frac{m}{m^*} = 1 - \frac{1}{3N} \sum_{\mathbf{q} \neq 0} \left( \frac{\beta \frac{N}{V} \nu_q}{1 + \beta \frac{N}{V} \nu_q} \right)^2. \quad (8.10)$$

Thus, formulae (8.1) and (8.10) determine the effective mass in the limiting cases  $T = 0$  and  $\hbar \rightarrow 0$ . One can rewrite these two formulae using the liquid structure factor  $S(q)$ . At the absolute zero temperature from (8.1)

and (7.4) one can find

$$\frac{m}{m^*} = 1 - \frac{1}{3N} \sum_{\mathbf{q} \neq 0} \frac{[S(q) - 1]^2}{S(q) + 1}, \quad T = 0, \quad (8.11)$$

and from (8.10), (7.5) the high-temperature limit is obtained:

$$\frac{m}{m^*} = 1 - \frac{1}{3N} \sum_{\mathbf{q} \neq 0} [S(q) - 1]^2, \quad T \rightarrow \infty. \quad (8.12)$$

The above expressions might be “sewed together” numerically and the temperature dependence of the effective mass can be obtained. However, both of them are from the source other than the presented paper. Although, this is necessary at  $T = 0$  as the mass  $m^*$  at this condition just drops out from all the expressions, as seen from (5.1).

To reach full self-consistency of our theory at  $T \neq 0$  we need to find the expression for  $m^*$  within the considered approach. One can demand, e. g., by means of special selection of  $m^*$ , the expressions for the kinetic energy (7.7) and that from  $\langle K \rangle = -m dF/dm$  (following from the know theorem about the derivation of the free energy  $F$  by some parameter) or  $\langle K \rangle$  calculated from the density matrix  $R(x'|x)$  from (5.1) to equal. It is clear that

in the exact theory all these expressions coincide, but as a consequence of the pair correlations approximation we use here they differ. To reach the self-consistency of the theory one can utilize the arbitrariness of the parameter  $m^*$  and choose it every time to obtain these formulae to be equal for the kinetic energy at different temperatures.

Let us indicate one more way to determine  $m^*$  via the condition that the pair distribution function of  ${}^4\text{He}$  at zero interatomic distance should equal to zero due to hard core in the interaction potential. Only the numerical calculation can show how all the described approaches to the determination of  $m^*$  concord.

Therefore, if the liquid structure factor measured experimentally [35–38] is used as a source information, the theory of liquid  ${}^4\text{He}$  proposed in this paper gives the connection between the observable quantities in the whole temperature interval, including the vicinity of  $\lambda$ -transition. Such an approach was utilized by the author in [39, 42] for the calculation of different physical properties of  ${}^4\text{He}$  near the absolute zero,  $T \rightarrow 0$  K.

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**САМОУЗГОДЖЕНА ТЕОРІЯ РІДКОГО  $^4\text{He}$**

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Запропоновано новий метод розрахунку повної матриці густини та термодинамічних функцій багато-бозонної системи і знайдено їхні явні вирази в наближенні парних кореляцій для довільних температур. Теорія є самоузгодженою в тому сенсі, що обчислені фізичні величини при низьких температурах збігаються з відповідними виразами теорії Боголюбова, а при високих температурах приводять до результатів теорії класичного неідеального газу в наближенні хаотичних фаз і виявляють фазовий перехід як наслідок бозе-айнштайнівської конденсації, що zdeформована міжчастинковою взаємодією. Усі остаточні формули записані лише через рідинний структурний фактор, який береться як вихідна інформація замість потенціалу взаємодії, і отже зв'язують між собою лише спостережувані величини, що дає також змогу досліджувати таку сильнеідеальну систему, як рідкий  $^4\text{He}$ .