

Theory of structure and thermodynamic function of liquid ^4He (Review Article)

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A new method of calculation of the density matrix of a many-boson system is proposed. The calculation of thermodynamic and structure functions at finite temperatures based on density matrix of Bose liquid is made. The structure factor of liquid ^4He at $T = 0$ K is used as an input information for numerical calculation instead of the interatomic potential. We found a good agreement of the calculated quantities with experimental data.

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1. Introduction

Significant step in the microscopic description of interacting Bose systems was made by Bogoliubov in Ref. 1, where for the first time the method of approximate second quantization was used for dilute Bose gas at low temperatures. It was the first correct theoretical description of Bose systems where usual perturbation theory is not applicable.

Perhaps, the first attempts to build the theory of liquid ^4He from the first principles were done by Feynman. In series of papers [2,3] the density matrix of interacting bosons was written in terms of path integrals and the importance of the “trajectories” of the particles that give the main contribution at λ -point and at low temperatures was discussed. It is in this Ref. 2 the effective mass of Bose par-

ticles was introduced for the first time in order to take partially into account the effect of the interatomic interaction. The well-known formula that links excitation spectrum of Bose system with structure factor was written in Ref. 4.

For the first time the collective variables approach was used to build ground-state wave-function of Bose system by Bogoliubov and Zubarev in Ref. 5. The results for the thermodynamic function of the model with condensate had been reproduced at weak-coupling limit. The one-particle density matrix calculated in Ref. 6 for the first time was written in an exponential form. As it turned out later this behavior of the one-particle density matrix is correct not only for three-dimensional systems. In particular, it reproduces correctly the density matrix of the exactly solvable one-dimensional model with δ -repulsion between particles.

Later, the method of collective variables in the theory of Bose systems was developed by Vakarchuk and Yukhnovskii. In Ref. 7 the ground-state properties of the interacting many-boson system were studied. The wavefunction of the first excited state and the equation for the excitation spectrum were built in Ref. 8. It was shown in the first order of perturbation theory that correction to the sound velocity and damping of the spectrum coincide with the results of field-theoretical approach [9]. The method of collective variables combined with field-theoretic approaches was used in Refs. 10–12 to describe the ground-state properties of Bose systems.

Notwithstanding a great number of papers concerned with the microscopic study of Bose system's properties, a good description of the thermodynamic and structure functions of liquid ${}^4\text{He}$ in the whole temperature range has not yet been created. In Ref. 13 the density matrix formalism with the functional optimization of the Jastrow wavefunction parameters was used to describe the properties of liquid helium. The results for internal energy agree well with experimental data for the temperatures below the critical one. It was shown that by taking into account the dynamic two-particle correlations only one can obtain the value of the critical temperature 3.4 K. Thus for a good agreement with experiments one needs to take into account higher-order approximations, which are specifically related to the concept of effective mass of the helium atom in a liquid. In Refs. 14 and 15 the variational calculations were used to obtain the properties of Bose liquid at finite temperatures. The density matrix was written as a product of two multipliers. The first one was chosen in exponential form and described the phonon contribution. The second multiplier was written in the form of a permanent and described the one-particle contribution.

Very interesting and as it seemed simple problem to be solved in the microscopic theory of liquid helium is a problem of the critical temperature calculation. Since London's assumption [16] that the λ -transition in liquid ${}^4\text{He}$ is the Bose condensation deformed by the interatomic interaction theorists did many attempts to calculate the critical temperature of liquid ${}^4\text{He}$ (see Refs. 17–19). In recent years much attention has been paid to the study of the atom's effective mass in liquid helium. Various scholars were mostly concerned with the value of the effective mass at $T \rightarrow 0$. Isihara and Samulski [20] have used the value of $m^*/m = 1.71$ to agree the theoretically calculated sound branch of the excitation spectrum with the corresponding experimental data. In Ref. 21 the effective mass $m^*/m = 1.70$ was obtained on the basis of the liquid ${}^4\text{He}$ structure factor measurements. In Ref. 22 the interatomic potential was preserved as the input information, but in part the contribution of higher correlations was "transferred" to the kinetic energy term. In this way the mass of particles was renormalized that is somehow in correlation with the approach of Ref. 2. As a result of such a renormalization the value of

$m^*/m = 1.58$ was obtained using Green's function method. It was shown in Ref. 23 that the above-mentioned mass renormalization leads to the expressions obtained for the effective mass of the ${}^3\text{He}$ impurity atom in liquid ${}^4\text{He}$ but with the replacement of the "pure" ${}^3\text{He}$ atom mass by the ${}^4\text{He}$ atom mass.

In this article we did not intend to make a full review of works on the theory of liquid ${}^4\text{He}$. We reviewed only a small part related to the present studies. In the present paper we will briefly summarize our results in the theory of liquid helium at finite temperatures. First of all we will discuss the possible way of the density matrix calculation taking into account the two-particle interatomic correlations. The presence of off-diagonal long-range order of the one-particle density matrix, which can be calculated using the density matrix [24] is the indication of the phase transition in this approach. The order parameter of the theory is the value $(N_0/N)^{1/2}$, where N_0/N is the relative number of Bose condensate [25]. Then we will compare calculated thermodynamic and structure functions of liquid ${}^4\text{He}$ with experimental data.

2. Density matrix

Consider the N set of spinless Bose particles with the mass m moving in volume V . The Hamiltonian of the system is

$$\hat{H} = \hat{K} + \hat{\Phi}, \quad (1)$$

where the first term is the operator of the kinetic energy

$$\hat{K} = -\frac{\hbar^2}{2m} \sum_{j=1}^N \nabla_j^2. \quad (2a)$$

The second term presents the potential energy of the two-particle interaction between the particles with the coordinates $x = (\mathbf{r}_1, \dots, \mathbf{r}_N)$

$$\hat{\Phi} = \sum_{1 \leq i < j \leq N} \Phi(|\mathbf{r}_i - \mathbf{r}_j|). \quad (2b)$$

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:

$$e^{-\beta \hat{H}} \psi_n(x) = e^{-\beta E_n} \psi_n(x), \quad (3)$$

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 Eq. (3) by $\varphi(x)$. We will integrate it over all the coordinates x :

$$\int \varphi(x) e^{-\beta \hat{H}} \psi_n(x) dx = e^{-\beta E_n} \int \varphi(x) \psi_n(x) dx, \quad (4)$$

where

$$\int dx = \int d\mathbf{r}_1 \dots \int d\mathbf{r}_N. \quad (5)$$

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

$$\int \varphi(x) \psi_n(x) dx \neq 0. \quad (6)$$

Then making use of the self-conjugation of the operator \hat{H} we shall transfer it in Eq. (4) 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:

$$e^{-\beta \hat{H}} \varphi(x) = \int \varphi(x') R_N(x' | x) dx', \quad (7)$$

where

$$R_N(x' | x) = \sum_n \psi_n^*(x) e^{-\beta E_n} \psi_n(x') \quad (8)$$

is the density matrix in the coordinate representation.

In fact, Eq. (7) 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:

$$\langle x | e^{-\beta \hat{H}} | \varphi \rangle = \int \langle x | e^{-\beta \hat{H}} | x' \rangle \langle x' | \varphi \rangle dx', \quad (9)$$

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

It is clear that formula (7) or (9) 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 (8). Here most significant heuristically is an arbitrary choice of the function $\varphi(x)$ on condition that it is nonorthogonal to the eigenfunctions of the \hat{H} operator and the existence of integral (6).

Should the interparticle interaction be switched off, the density matrix will transfer into that of the ideal Bose system of N particles. That is why we will try to construct the density matrix of the system of N 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:

$$R_N(x' | x) = R_N^0(x' | x) P_N(x' | x), \quad (10)$$

where at temperature $T \neq 0$

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

$$= \frac{1}{N!} \left(\frac{m^*}{2\pi\beta\hbar^2} \right)^{3N/2} \sum_Q \exp \left[-\frac{m^*}{2\beta\hbar^2} \sum_{j=1}^N (\mathbf{r}'_j - \mathbf{r}_{Qj})^2 \right], \quad (11)$$

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 (11) 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.

We would like to base our analysis on the precise Eq. (7) and suggest a consistent method for the calculations 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:

$$\begin{aligned} P_N(x' | x) &= \\ &= \exp \left\{ c_0 + \sum_{\mathbf{q} \neq 0} c_1(q) \rho_{\mathbf{q}}' \rho_{-\mathbf{q}} - \frac{1}{2} \sum_{\mathbf{q} \neq 0} c_2(q) [\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho_{\mathbf{q}}' \rho_{-\mathbf{q}}'] \right\}, \end{aligned} \quad (12)$$

where the Fourier coefficients of the particles density fluctuations

$$\rho_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}_j}, \quad \rho_{\mathbf{q}}' = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{q}\mathbf{r}'_j}, \quad (13)$$

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 Eq. (7).

We have confined ourselves to the consideration of two-particle interparticle correlations in expression (12). 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 (12). 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 Boltzman factor $\exp(-\beta\Phi)$, where Φ is the potential energy of the interparticle interaction thus equaling the second term in Hamiltonian (1).

Finally, we must also choose an appropriate φ function which is contained in Eq. (7) and meets requirement (6). In our case we will adjust it from the class of such functions:

$$\varphi(x) = \exp \left[\sum_{\mathbf{q} \neq 0} \lambda(q) \rho_{\mathbf{q}} \right], \quad (14)$$

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

The detailed calculation of the density matrix of Bose system can be found in Ref. 26. The result is

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

$$\times \exp \left\{ -\frac{1}{4} \sum_{\mathbf{q} \neq 0} \left(\alpha_q \coth[\beta E(q)] - \coth \left[\beta \frac{\hbar^2 q^2}{2m^*} \right] \right) (\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}) + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \left(\frac{\alpha_q}{\sinh[\beta E(q)]} - \frac{1}{\sinh \left[\beta \frac{\hbar^2 q^2}{2m^*} \right]} \right) \rho_{\mathbf{q}} \rho'_{-\mathbf{q}} \right\}, \quad (15)$$

where the ground-state energy in Bogoliubov's approximation [1] is

$$E_0 = \frac{N(N-1)}{2V} v_0 - \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{8m} (\alpha_q - 1)^2, \quad (16)$$

and Bogoliubov's elementary excitation spectrum [1] is

$$E(q) = \alpha_q \frac{\hbar^2 q^2}{2m}, \quad \alpha_q = \sqrt{1 + \frac{2N}{V} v_q \frac{\hbar^2 q^2}{2m}}. \quad (17)$$

Expression (15) for the density matrix 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.

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 $v_q = 0$, i. e., $\alpha_q = 1$ we will obtain from (15) that for any temperature

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

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 [27]. Applying the method of coherent states it was also found in [28]. With the help of wave functions of the many-boson Bogoliubov–Zubarev system [5] it was calculated in [29,30]. Using our notations it looks as follows:

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

$$\left. - \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{\alpha_q}{\sinh[E(q)/T]} \left[(\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}) \cosh \frac{E(q)}{T} - (\rho'_{\mathbf{q}} \rho'_{-\mathbf{q}} + \rho_{\mathbf{q}} \rho_{-\mathbf{q}}) \right] \right\}. \quad (18)$$

This expression holds true only for $T \rightarrow 0$. If $\alpha_q = 1$, then from (18) we obtain an expression for the ideal gas density matrix

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

$$\left. - \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{1}{\sinh(\hbar^2 q^2 / 2mT)} \left[(\rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho'_{-\mathbf{q}}) \cosh \left(\frac{\hbar^2 q^2}{2mT} \right) - (\rho_{\mathbf{q}} \rho'_{-\mathbf{q}} + \rho'_{\mathbf{q}} \rho_{-\mathbf{q}}) \right] \right\}, \quad (19)$$

which does not coincide with the precise expression (11) for $m^* = m$.

It is curious that Eqs. (18) and (19) prompt to us how one can formally obtain our result for the density matrix. Thus we have the equation

$$R_N(x|x') = R_N^0(x|x') \frac{R_N(x|x')(\text{from (18)})}{R_N^0(x|x')(\text{from (19)})}. \quad (20)$$

If we use Eqs. (18) and (19) in the right-hand part of this equation for the density matrices relation, we will immediately arrive at Eq. (15) 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 (18), for instance by solving Bloch's equation directly, as suggested in [30], the result will be the following. Firstly, we will obtain in the (18) 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 (13)). Besides, there also arise corrections $\sim \sum_{\mathbf{q} \neq 0} (...)/N$ to the zeroth ap-

proximation coefficient functions around $\rho_{\mathbf{q}} \rho_{-\mathbf{q}}$ in (18) (again systematized as regards the primed and the non-primed 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 Eq. (20) and by the same reasoning we arrive at (15) with the known value of m^* . Now from Eq. (20) we can also answer the question why Eq. (15) 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 consideration the contribution of the many particle correlations in Eq. (12) 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 Sec. 5.

If we direct the temperature towards zero, i. e., $\beta \rightarrow \infty$ then from (15) 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 (8) 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

$$\psi_0(x) = \frac{1}{\sqrt{V^N}} \left(\prod_{\mathbf{q} \neq 0} \sqrt{\alpha_q} \right) \exp \left[-\frac{1}{4} \sum_{\mathbf{q} \neq 0} (\alpha_q - 1) \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \right] \quad (21)$$

coincides with that discovered for the first time by Bogoliubov and Zubarev [5].

Finally we will consider the classical limit $\hbar \rightarrow 0$ of the density matrix diagonal elements (15) when $\rho'_{\mathbf{q}} = \rho_{\mathbf{q}}$. The energy E_0 from (16) in this limit transforms into

$$E_0 = \frac{N(N-1)}{2V} v_0 - \sum_{\mathbf{q} \neq 0} \frac{N}{2V} v_q. \quad (22)$$

Then, the first logarithm under the sum over \mathbf{q} in the exponent in (15) (together with the factor 1/2) is reduced at $\hbar \rightarrow 0$ to $\ln \alpha_q$ and the second one to $\ln(1/\alpha_q)$; they cancel each other, the factor at $\rho_{\mathbf{q}} \rho_{-\mathbf{q}}$ equaling

$$v_q^* = \alpha_q \tanh \left[\frac{\beta}{2} E(q) \right] - \tanh \left[\beta \frac{\hbar^2 q^2}{4m^*} \right],$$

$$v_q^* = \beta \frac{N}{V} v_q, \quad \hbar \rightarrow 0. \quad (23)$$

We have made use of the fact that at high temperatures $m^* \rightarrow m$. In the $R_N^0(x|x)$ matrix from (11) 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 Φ is given by Eq. (2b).

Thus from Eq. (15) for the density matrix 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 λ -transition point.

3. Structure functions

The density matrix of many-boson system allows to obtain thermodynamic properties and to calculate the structure functions of the system. In particular, the structure factors which are averaged products of Fourier transforms of particle fluctuation contain very important information about the system. Nowadays only pair structure factor is the quantity which may be measured precisely in x-ray, electron or neutron scattering experiments [31,32].

3.1. Partition function and pair structure factor

Let us write down the partition function of the interacting bosons in coordinate representation

$$Z_N = \int d\mathbf{r}_1 \dots \int d\mathbf{r}_N R_N(\mathbf{r}_1, \dots, \mathbf{r}_N | \mathbf{r}_1, \dots, \mathbf{r}_N). \quad (24)$$

Using representation (10) for the density matrix let us rewrite Eq. (24) as an average value over the states of ideal Bose gas

$$Z_N = Z_N^0 e^{c_0} \left\langle \exp \left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \lambda_q \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \right) \right\rangle_0, \quad (25)$$

where

$$Z_N^0 = \prod_{\mathbf{q}} \left(1 - z_0 e^{-\beta \varepsilon_q} \right)^{-1}$$

is partition function, z_0 is fugacity of ideal Bose gas,

$$\lambda_q = \alpha_q \tanh \left(\frac{\beta E_q}{2} \right) - \tanh \left(\frac{\beta \varepsilon_q^*}{2} \right), \quad \varepsilon_q^* = \frac{\hbar^2 q^2}{2m^*}. \quad (26)$$

Let us write down the quantity in the brackets $\langle \dots \rangle_0$ in terms of functional integral

$$\begin{aligned} & \exp \left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \lambda_q \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \right) = \\ & = \int (d\varphi) \exp \left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \varphi_{\mathbf{q}} \varphi_{-\mathbf{q}} + \sum_{\mathbf{q} \neq 0} \sqrt{-\lambda_q} \rho_{\mathbf{q}} \varphi_{\mathbf{q}} \right), \quad (27) \end{aligned}$$

here

$$\int (d\varphi) \equiv \prod'_{\mathbf{q} \neq 0} \int_{-\infty}^{\infty} \frac{d\varphi_{\mathbf{q}}^c}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{d\varphi_{\mathbf{q}}^s}{\sqrt{\pi}},$$

$$\varphi_{\mathbf{q}} = \varphi_{\mathbf{q}}^c + i\varphi_{\mathbf{q}}^s, \quad \varphi_{-\mathbf{q}}^c = \varphi_{\mathbf{q}}^c, \quad \varphi_{-\mathbf{q}}^s = -\varphi_{\mathbf{q}}^s.$$

We have to take into account variables $\varphi_{\mathbf{q}}$ only from half space of possible wave-vector \mathbf{q} values due to symmetry $\varphi_{\mathbf{q}}^* = \varphi_{-\mathbf{q}}$. The prime near product signifies this fact. Now, the partition function takes the form

$$Z_N = Z_N^0 e^{c_0} I, \quad (28)$$

where functional integral I is

$$\begin{aligned} I = & \int (d\varphi) \exp \left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \varphi_{\mathbf{q}} \varphi_{-\mathbf{q}} \right) \times \\ & \times \exp \left\{ \sum_{n \geq 1} \frac{1}{n!} \left[\prod_{i=1}^n \sum_{\mathbf{q}_i \neq 0} \sqrt{-\lambda_{q_i}} \varphi_{\mathbf{q}_i} \right] M_n(\mathbf{q}_1, \dots, \mathbf{q}_n) \right\}, \quad (29) \end{aligned}$$

here $M_n(\mathbf{q}_1, \dots, \mathbf{q}_n)$ are irreducible averages [33] of the products $\rho_{\mathbf{q}_1} \dots \rho_{\mathbf{q}_n}$. The first two are

$$\langle \rho_{\mathbf{q}} \rangle_0 = 0, \quad \langle \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \rangle_0 = S_0(q). \quad (30)$$

The problem of the partition function calculation is reduced to calculation of the functional integral (29).

Let us pass to the calculation of average value of a product $\rho_{\mathbf{q}_1} \dots \rho_{\mathbf{q}_n}$

$$\begin{aligned} \langle \rho_{\mathbf{q}_1} \dots \rho_{\mathbf{q}_n} \rangle & = \frac{1}{Z_N} \int d\mathbf{r}_1 \dots \int d\mathbf{r}_N R_N^0(\mathbf{r}_1, \dots, \mathbf{r}_N | \mathbf{r}_1, \dots, \mathbf{r}_N) \rho_{\mathbf{q}_1} \dots \rho_{\mathbf{q}_n} \exp \left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \lambda_q \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \right) = \\ & = \frac{e^{c_0}}{Z_N} Z_N^0 \left\langle \int (d\varphi) \exp \left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \varphi_{\mathbf{q}} \varphi_{-\mathbf{q}} \right) \left\{ \prod_{i=1}^n \frac{1}{\sqrt{-\lambda_{q_i}}} \frac{\partial}{\partial \varphi_{\mathbf{q}_i}} \right\} \exp \left(\sum_{\mathbf{q} \neq 0} \sqrt{-\lambda_q} \rho_{\mathbf{q}} \varphi_{\mathbf{q}} \right) \right\rangle_0. \quad (31) \end{aligned}$$

Here we formed average over the density matrix of ideal Bose gas and then used the representation (27) for the exponent term. Next, carrying out integration n times by parts over $\varphi_{\mathbf{q}}$ and then "extend" exponential function in the right hand side of the formula through derivatives. Finally taking into account Eq. (29) averages (31) read

$$\langle \rho_{\mathbf{q}_1} \dots \rho_{\mathbf{q}_n} \rangle = \frac{1}{\sqrt{-\lambda_{q_1}} \dots \sqrt{-\lambda_{q_n}}} \overline{\left(-\frac{\partial}{\partial \varphi_{\mathbf{q}_1}} + \varphi_{-\mathbf{q}_1} \right) \dots \left(-\frac{\partial}{\partial \varphi_{\mathbf{q}_n}} + \varphi_{-\mathbf{q}_n} \right)}, \quad (32)$$

where line denotes following averaging

$$\overline{(\dots)} = \frac{\int (d\varphi) \exp \left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \varphi_{\mathbf{q}} \varphi_{-\mathbf{q}} \right) \exp \left\{ \sum_{n \geq 1} \frac{1}{n!} \left[\prod_{i=1}^n \sum_{\mathbf{q}_i \neq 0} \sqrt{-\lambda_{q_i}} \varphi_{\mathbf{q}_i} \right] M_n(\mathbf{q}_1, \dots, \mathbf{q}_n) \right\} (\dots)}{\int (d\varphi) \exp \left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \varphi_{\mathbf{q}} \varphi_{-\mathbf{q}} \right) \exp \left\{ \sum_{n \geq 1} \frac{1}{n!} \left[\prod_{i=1}^n \sum_{\mathbf{q}_i \neq 0} \sqrt{-\lambda_{q_i}} \varphi_{\mathbf{q}_i} \right] M_n(\mathbf{q}_1, \dots, \mathbf{q}_n) \right\}}. \quad (33)$$

Now the problem of calculation of averages $\langle \rho_{\mathbf{q}_1} \dots \rho_{\mathbf{q}_n} \rangle$ is reduced to the calculation of functional integral I .

The partition and structure functions are calculated in detail in Ref. 34.

3.2. Calculation of functional integral I

We restrict our consideration of Eq. (29) to the so-called pair-particle correlation approximation

$$I_0 = \exp\left(-\frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln[1 + \lambda_q S_0(q)]\right),$$

then partition function (28) and two-particle structure factor $S(q)$ (32) of Bose liquid in the pair-particle correlation approximation are

$$Z_N = Z_N^0 \exp\left(c_0 - \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln[1 + \lambda_q S_0(q)]\right),$$

$$S(q) = \frac{S_0(q)}{1 + \lambda_q S_0(q)}. \quad (34)$$

Note that partition function and pair structure factor of Bose liquid in the approximation of pair-particle correlation coincide with the corresponding formulas obtained in Ref. 26.

4. Energy

4.1. Initial equations

The quantum-statistical approach based on the density matrix of Bose liquid will be used in this section for the calculation of the internal energy of the system

$$E = \langle \hat{K} \rangle + \langle \hat{\Phi} \rangle.$$

Using density matrix (10) let us write down the kinetic energy term (2a) in the following way:

$$\langle \hat{K} \rangle = \frac{1}{Z_N} \times$$

$$\times \int d\mathbf{r}_1 \dots \int d\mathbf{r}_N \left[\hat{K} R_N(\mathbf{r}'_1, \dots, \mathbf{r}'_N | \mathbf{r}_1, \dots, \mathbf{r}_N) \right]_{\mathbf{r}'_1 = \mathbf{r}_1, \dots, \mathbf{r}'_N = \mathbf{r}_N}$$

The kinetic energy term in the pair-particle correlation approximation is calculated in details in Ref. 35

$$\langle \hat{K} \rangle = \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \frac{1}{z_0^{-1} e^{\beta \varepsilon_q^*} - 1} + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \frac{\lambda_q}{1 + \lambda_q S_0(q)} \frac{\partial S_0(q)}{\partial \beta} +$$

$$+ \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \lambda_q^2 S(q) + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \left[\frac{\alpha_q}{\sinh[\beta E(q)]} - \frac{1}{\sinh[\beta \varepsilon_q^*]} \right]. \quad (35)$$

The derivative of the fugacity z_0 of the ideal Bose gas with respect to parameter β should be carried out in the formula for $S_0(q)$.

Let us use ρ -representation for the potential energy operator $\hat{\Phi}$ (2b):

$$\hat{\Phi} = \frac{N(N-1)}{2V} v_0 + \frac{N}{2V} \sum_{\mathbf{q} \neq 0} v_q (\rho_{\mathbf{q}} \rho_{-\mathbf{q}} - 1). \quad (36)$$

For the average value of the potential energy we have

$$\langle \hat{\Phi} \rangle = \frac{N(N-1)}{2V} v_0 + \frac{N}{2V} \sum_{\mathbf{q} \neq 0} v_q [S(q) - 1]. \quad (37)$$

Let us write down the quantity v_q using Eq. (17) and experimentally measured structure factor of the system at $T \rightarrow 0$. The quantity v_0 should be eliminated through sound velocity c at zero temperature [35].

Thus, the average value of the potential energy in the pair-particle correlation approximation reads

$$\langle \hat{\Phi} \rangle = N \frac{mc^2}{2} + \frac{1}{16} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \frac{1}{\alpha_q} \left(\alpha_q - \frac{1}{\alpha_q} \right)^2 +$$

$$+ \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} (\alpha_q^2 - 1) [S(q) - 1]. \quad (38)$$

4.2. Internal energy

Taking into account Eqs. (35) and (38) for the internal energy we have

$$E = N \frac{mc^2}{2} + \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \frac{1}{z_0^{-1} e^{\beta \varepsilon_q^*} - 1} + \frac{1}{2} \frac{m^*}{m} \sum_{\mathbf{q} \neq 0} \frac{\lambda_q}{1 + \lambda_q S_0(q)} \frac{\partial S_0(q)}{\partial \beta} + \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} (\lambda_q^2 + \alpha_q^2 - 1) S(q) +$$

$$+ \frac{1}{2} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \left[\frac{\alpha_q}{\sinh[\beta E(q)]} - \frac{1}{\sinh[\beta \varepsilon_q^*]} \right] + \frac{1}{16} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \left(1 - \frac{1}{\alpha_q^2} \right) \left(\alpha_q - \frac{1}{\alpha_q} - 4\alpha_q^2 \right). \quad (39)$$

Obviously, if the interaction between particles is turned off ($\alpha_q = 1$) Eq. (39) reduces to the internal energy of ideal Bose gas. The ground-state energy of many-boson system is

$$E_0 = N \frac{mc^2}{2} - \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \left(1 - \frac{1}{\alpha_q} \right)^3 \left(\alpha_q^2 + \frac{3}{4} \alpha_q + \frac{1}{4} \right), \quad (40)$$

where kinetic and potential energy terms are

$$\langle \hat{K} \rangle |_{T=0} = \frac{1}{4} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} \frac{(\alpha_q - 1)^2}{\alpha_q}, \quad (41a)$$

$$\begin{aligned} \langle \hat{\Phi} \rangle |_{T=0} &= N \frac{mc^2}{2} + \\ &+ \frac{1}{16} \sum_{\mathbf{q} \neq 0} \frac{\hbar^2 q^2}{2m} (\alpha_q - 1)^2 \frac{(\alpha_q + 1)}{\alpha_q} \left(\frac{1}{\alpha_q^2} + \frac{1}{\alpha_q} - 4 \right). \end{aligned} \quad (41b)$$

Kinetic energy term (41a) and potential energy term (41b) of the ground-state energy of many-boson system in the pair-particle correlation approximation coincide with the corresponding expressions found in Ref. 36.

Let us analyze the Eq. (39) for internal energy at the low-temperature limit. In this region the internal energy coincides with the corresponding formula of Ref. 26. At $T \rightarrow 0$ the internal energy is

$$E = E_0 + \sum_{\mathbf{q} \neq 0} \frac{E(q)}{e^{\beta E(q)} - 1}. \quad (42)$$

To carry out integration at the low-temperature limit it is enough to take into account only long-wavelength behavior of the excitation spectrum $E(q) = \hbar c q$. The result is (Stefan–Boltzmann law)

$$E = E_0 + \frac{V}{2\pi^2 (\hbar c)^3} T^4.$$

Thus, the heat capacity has a correct low-temperature behavior $C_V \sim T^3$.

5. Effective mass of the liquid ${}^4\text{He}$

An effective mass of particles is the free parameter present in the theory. Obviously our next task is to propose the scheme of the effective mass calculation. In order to find effective mass of particles we have to determine the one-particle spectrum of the interacting Bose system in normal state. The fact that leading-order term of the quasi-particle dispersion relation is quadratic in the wave vector \mathbf{p} allows us to associate the coefficient of the spectrum near p^2 with the effective mass of particles.

The thermodynamic potential in random phase approximation (RPA) is

$$\Omega = \Omega_0 + \Omega_1, \quad (43)$$

where the ideal gas contribution

$$\Omega_0 = T \sum_{\mathbf{p}} \ln(1 - z e^{-\beta \varepsilon_p}), \quad z = e^{\beta \mu}, \quad \varepsilon_p = \frac{\hbar^2 p^2}{2m} \quad (44)$$

(μ is chemical potential) and well-known RPA-part of the grand canonical potential

$$\Omega_1 = \frac{N^2}{2V} v(0) - \frac{N}{2V} \sum_{\mathbf{k} \neq 0} v(k) + \frac{1}{2\beta} \sum_q \ln |1 + v(k) \Pi(q)|, \quad (45)$$

where $q = (\omega_n, \mathbf{k})$ and $\omega_n = 2\pi n T$ ($n = 0; \pm 1; \pm 2; \dots$) is the Matsubara frequency and

$$\sum_q = \sum_{\omega_n} \sum_{\mathbf{k} \neq 0}.$$

The polarization operator

$$\Pi(q) = \Pi(\omega_n, \mathbf{k}) = \frac{1}{V} \sum_{\mathbf{k}'} \frac{n_{\mathbf{k}'+\mathbf{k}} - n_{\mathbf{k}'}}{i\omega_n - \varepsilon_{\mathbf{k}'+\mathbf{k}} + \varepsilon_{\mathbf{k}'}}. \quad (46)$$

RPA is a very natural starting point in the theory of liquid ${}^4\text{He}$ because it describes correctly both low- and high-temperature behavior of the system.

5.1. Renormalization of the one-particle spectrum

Let us calculate the correction to the one-particle spectrum in the following way $\Delta \varepsilon_p - \Delta \mu = \delta \Omega_1 / \delta n_p$. The result is

$$\Delta \varepsilon_p = \frac{1}{\beta V} \sum_q \frac{v(k)}{1 + v(k) \Pi(q)} \left\{ \frac{1}{\varepsilon_{|\mathbf{k}-\mathbf{p}|} - \varepsilon_p - i\omega_n} - \frac{1}{\varepsilon_{\mathbf{k}} - i\omega_n} \right\}, \quad (47)$$

and the correction to the chemical potential is

$$\Delta \mu = -\frac{N}{V} v(0) + \frac{1}{2V} \sum_{\mathbf{k} \neq 0} v(k) - \frac{1}{\beta V} \sum_q \frac{v(k)}{1 + v(k) \Pi(q)} \frac{\varepsilon_{\mathbf{k}}}{\varepsilon_{\mathbf{k}}^2 + \omega_n^2}. \quad (48)$$

These Eqs. (47), (48) coincide with the result of Ref. 37 where temperature Green's function technique was used.

Finally, the renormalized quasi-particle spectrum of the interacting Bose system is

$$\varepsilon_p^* = \varepsilon_p + \Delta \varepsilon_p, \quad \mu^* = \mu + \Delta \mu. \quad (49)$$

For self-consistency of our calculations, especially near the critical point, the chemical potential μ should be changed by μ^* in the right-hand side of Eqs. (47), (48) (the critical point is determined by the equation $\mu^* = 0$, respectively). Admittedly, the ideal gas dispersion relation should be replaced by the exact one-particle spectrum, but further analysis will not be influenced by this replacement qualitatively.

The long-wavelength asymptote of the spectrum reads

$$\varepsilon_p^* = \Delta \varepsilon_p^u + \frac{\hbar^2 p^2}{2m^*}, \quad (50)$$

where zero frequency contribution of Eq. (47) is

$$\Delta \varepsilon_p^u = \left(\frac{k_0}{\pi} \right)^2 p \int_0^\infty dx \frac{v(2xp)}{1 + \rho v(2xp) \Pi(0, 2xp)} \left[\frac{x}{2} \ln \left| \frac{x+1}{x-1} \right| - 1 \right], \quad (51)$$

and the effective mass may be written in the following way [38]

$$m/m^* = 1 - \Delta(T), \quad (52)$$

where the quantity

$$\Delta(T) = \frac{1}{3N} \sum_{\mathbf{k} \neq 0} \frac{(\alpha_k - 1)^2}{\alpha_k(\alpha_k + 1)} + \frac{2}{3N} \sum_{\mathbf{k} \neq 0} \left\{ \frac{\alpha_k^2 + 3}{\alpha_k^2 - 1} \left[n(\beta \varepsilon_k) - \frac{1}{\beta \varepsilon_k} \right] - \frac{3\alpha_k^2 + 1}{\alpha_k(\alpha_k^2 - 1)} \left[n(\beta \varepsilon_k) - \frac{1}{\beta \varepsilon_k} \right] + 2 \left[\frac{1}{\beta \varepsilon_k} - \beta \varepsilon_k n(\beta \varepsilon_k) [1 + n(\beta \varepsilon_k)] \right] \right\}. \quad (53)$$

It is argued in Ref. 38 that for the realistic potentials of two-particle interaction zero frequency contribution of quasi-particle spectrum (51) is $\Delta \varepsilon_p^u \sim o(p^2)$ for $T > T_c$ and $\Delta \varepsilon_p^u \sim p^2 \ln p$ at $T = T_c$. So we conclude that non-universal physics is not influenced by $\Delta \varepsilon_p^u$.

The effective mass in the low-temperature region is always larger than its “bare” one which means that the renormalized temperature of the Bose condensation of interacting particles is always lower than the critical temperature of the ideal gas. This is the most important result of Eqs. (52) and (53). At high temperatures carefully calculating the limit of $\beta \rightarrow 0$ it is easy to ascertain that the effective mass tends to the mass of particles. It is important that the temperature-independent part of Eq. (53) coincides with the effective mass of impurity atom in liquid ^4He [23].

5.2. Numerical results

In order to provide numerical calculations of the found quantities for liquid ^4He let us use as an output information experimentally measured structure factor $S^{\text{exp}}(q)$ of the system at $T \rightarrow 0$ instead of Fourier transform of two-particle interaction v_q .

The structure factor of ideal Bose gas at the limit $T \rightarrow 0$ tends to unity $S_0(q) \rightarrow 1$. Therefore the quantity $S(q)$ in Eq. (34) should be changed by experimentally measured structure factor $S^{\text{exp}}(q)$ and taking into account Eq. (26) the quantity $\lambda_q \rightarrow \alpha_q - 1$. Then using Eq. (34) at low-temperature limit we get

$$\alpha_q = \frac{1}{S^{\text{exp}}(q)}. \quad (54)$$

This equation determines the unknown quantity α_q . All thermodynamic and structure functions can be rewritten via α_q .

Our numerical calculations are carried out at the equilibrium density of liquid helium $\rho = 0.02185 \text{ \AA}^{-3}$, mass of particles $m = 4.0026 \text{ a.m.u.}$, sound velocity $c = 238.2 \text{ m/s}$ in the limit of $T \rightarrow 0$ [32], and at the critical temperature of the ideal gas $T_c = 3.138 \text{ K}$. The liquid structure factor extrapolated to $T = 0$ was taken from Ref. 39.

In order to study thermodynamic and structure function of liquid ^4He we have to calculate effective mass of particles. In Fig. 1 the dependence of a dimensionless value of the effective mass m^*/m as a function of temperature is

presented. Formally we extrapolated a curve of the effective mass in the condensate region where obviously it becomes a parameter of the theory.

The first three terms of a low-temperature expansion are ($T \ll mc^2$, $T \ll \hbar^2 \rho^{2/3}/m$)

$$\Delta(T \rightarrow 0) = \Delta_0 + \Delta_1 T - \Delta_{3/2} T^{3/2} + O(T^{5/2}), \quad (55)$$

(T in Kelvins)

where Δ -coefficients are

$$\Delta_0 = \frac{1}{3N} \sum_{\mathbf{k} \neq 0} \frac{(\alpha_k - 1)^2}{\alpha_k(\alpha_k + 1)} = 0.41,$$

$$\Delta_1 = \frac{2}{3N} \sum_{\mathbf{k} \neq 0} \frac{\alpha_k^2 - 1}{\alpha_k^2 \varepsilon_k} = 0.31,$$

$$\Delta_{3/2} = \frac{4}{3} \zeta(3/2) \left(\frac{m}{2\pi \hbar^2} \right)^{3/2} / \rho = 0.24.$$

Then the effective mass equals approximately

$$m^* = m / (0.59 - 0.31T + 0.24T^{3/2}). \quad (56)$$

This formula reproduces the curve in Fig. 1 quite well up to the critical temperature.

Now we are in position to calculate the renormalized temperature of the Bose condensation. We can find T_c using condition $\sum_{\mathbf{p}} n_{\mathbf{p}}^* = N$ at the zero value of the renormalized chemical potential μ^* . A simple calculation gives

$T_c = 1.94 \text{ K}$ that agrees quite well with experimental measurements of the temperature of the λ -transition $T_c^{\text{exp}} = 2.17 \text{ K}$ despite the simplicity of the approximations.

The comparison of experimentally measured and calculated (34) structure factors at different temperatures is presented on Fig. 2. The experimental data is taken from Ref. 31. As it is seen from the Fig. 2 the consistence of the curves is good at low temperatures, but with increasing temperature the long-wavelength asymptote of the calcu-

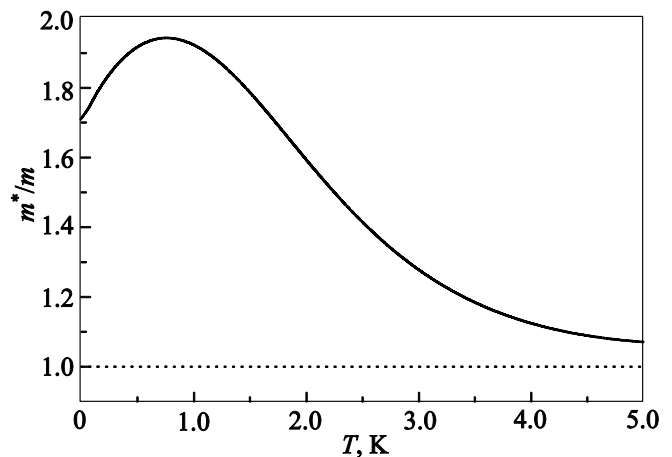


Fig. 1. Temperature dependence of the fraction m^*/m .

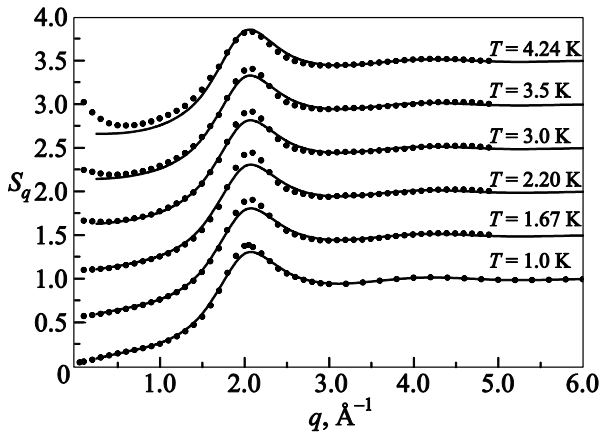


Fig. 2. Structure factor of liquid ^4He at different temperatures. Solid line is calculated pair structure factor, circles is experimental data taken from 31 (for convenience the curves are shifted one from another on 0.5).

lated curve does not coincide with experimental one. The possible reason of this inconsistency is that we do not take into account higher-order approximations.

The results of numerically calculated internal energy (40), kinetic energy (41a) and potential energy (41b) at zero temperature are presented in Table 1. For comparison the experimental data and theoretical predictions of another authors are also brought into the table.

As it is seen from Table 1 the value of the kinetic energy and potential energy obtained in [36] differ from the values obtained in this paper although the formulas coincide. For the numerical calculations provided in Ref. 36 author used experimentally measured structure factor extrapolated to $T = 0$ only for small \mathbf{q} . For other values the structure factor at $T = 0.79$ K [50] was used. In the present numerical calculations we used the experimentally measured structure factor extrapolated to $T = 0$ [39] for all values of \mathbf{q} .

Table 1. Comparison of ground-state energy of liquid ^4He

Reference	E_0/N	K_0/N	Φ_0/N
[40]	-7.1	14.5	-21.6
[41]		14.6	
[42]	-5.56	14.6	-19.82
[43]	-5.73	13.73	-19.46
[44]	-6.02	14.30	-20.32
[45]	-6.85	13.62	-20.47
[46]	-6.10	13.96	-20.06
[47]	-6.97	14.47	-21.44
[48]	-6.96	14.77	-21.73
[49]	-7.13	14.00	-21.14
[36], 1-st order, pair	-6.3	12.1	-18.4
[36], 2-nd order, pair	-9.4	15.2	-24.6
[36]*	-6.4	14.2	-20.6
this paper, 1-st order, pair	-5.2	10.9	-16.1

Notes: [36]* — 2-nd order, pair + three-, four-particle correlations.

The comparison of the theoretically calculated internal energy and experimental measurements for liquid ^4He is presented on Fig. 3.

We calculate heat capacity using the difference method and build the plot of its temperature dependence T/T_c . For capacity we use the Eq. (39) for total energy and expression (56) for effective mass.

A comparison of different heat capacity curves is depicted in Fig. 4. As is seen from the comparison of the calculated curve 1 with the experimental one the agreement is quite good at low temperatures ($0 < T/T_c < 1$). At the temperatures $T/T_c > 1$ the inconsistency occurs: the behavior of the calculated heat capacity is very similar to the behavior of the experimental curve, but shifted upward almost in a parallel way. This inconsistency is related to the fact that three- and four-particle correlations should be taken into account for the quantitative description. The contribution of three- and four-particle correlations, as is shown in Refs. 36, 53, improves significantly the ground-state results and gives a fairly good agreement at $T \rightarrow 0$.

Further, let us calculate the heat capacity of liquid ^4He with taking into account the effective mass of the helium atom in the liquid (curve 2). At low temperatures the heat capacity with taking into account the effective mass of the Bose particles practically coincides with curve 1, which agrees well with experimental data. This shows a weak dependence of the heat capacity on the effective mass below the temperature of phase transition. As is seen from Fig. 4, the calculated curve 2 (unlike curve 1) agrees quite well with the experimental one. It is related to the fact that by using the effective mass we partially take into account a contribution from three- and four-particle correlations. It is not surprising that in close vicinity of the Bose condensation point the theoretically calculated heat capacity deviates most significantly from the experimental curve. It is solely related to the inconsistency of our description near

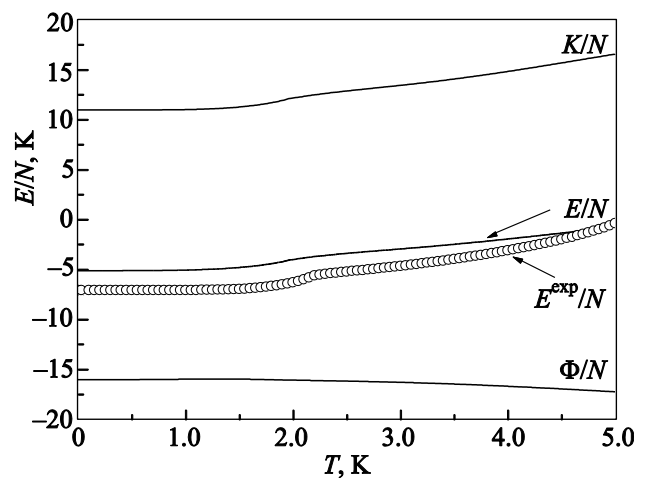


Fig. 3. Internal energy of liquid ^4He : K/N is kinetic energy; Φ/N is potential energy; E/N is internal energy; E^{exp}/N is experimental data taken from Ref. 51.

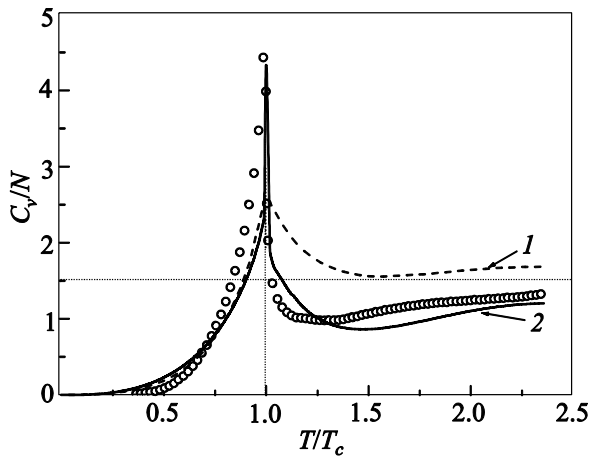


Fig. 4. Heat capacity of liquid ${}^4\text{He}$. Curve 1 is the calculated heat capacity in the pair-correlation approximation (39) [35]; curve 2 is the heat capacity in pair-correlation approximation (39) taking into account the effective mass of the helium atom in liquid (52). The circles show experimental data from Refs. 40, 51, 52.

the critical point because the nonanalytical part (51) of the one-particle spectrum, which makes a significant contribution in the thermodynamic functions at $T \rightarrow T_c$, is disregarded in our approach. One has to use renormalization group methods [54–56] for the correct description of the heat capacity in this temperature region.

6. Conclusions

In this paper we briefly report results on the microscopic theory of liquid ${}^4\text{He}$ at finite temperatures. First of all the method of calculation of the density matrix of interacting Bose system in the pair-particle correlation approximation is discussed. It is shown that obtained density matrix correctly describes low- and high-temperature behavior of the system. In particular, the results obtained coincide with the results of Bogoliubov’s theory at $T \rightarrow 0$. RPA for classical systems is recovered at high-temperature limit. The numerical calculations of the structure functions of liquid ${}^4\text{He}$ provided in the paper demonstrate good agreement with experimental data.

We succeed in deriving quite well an agreement of the internal energy and heat capacity curves of liquid ${}^4\text{He}$ with experimental data practically for all temperatures. The calculation found that for quantitative description of the heat capacity of liquid helium in normal phase one needs to take into account not only collective effects, but deformation of the one-particle spectrum is also needed. It is shown that one-particle spectrum of the interacting Bose system is quadratic in the wave vector, i.e., very similar to the dispersion relation of the ideal gas but with a new mass. This new mass at low temperatures is always greater than the mass of particles, and thus, the presence of the interaction at least in our approximation always lowers the critical temperature. So, an attempt is made to justify microscopi-

cally the idea that the λ -transition in a real quantum liquid is very similar to the Bose–Einstein condensation phenomena of the ideal gas “slightly” deformed by the interaction between the particles.

Hence, the quantum-statistical approach based on the density matrix is suitable for describing thermodynamic properties of such a strongly-interacting Bose liquid as the liquid ${}^4\text{He}$ not only in the limits of low and high temperatures, but for the entire temperature range.

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