ONE-PARTICLE DENSITY MATRIX OF LIQUID ^{4}He IN THE PAIR CORRELATION APPROXIMATION

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Using the expression for the total density matrix of the system of interacting Bose particles [J. Phys. Stud. **8**, 223 (2004)], the one-particle density matrix for helium-4 in the coordinate representation has been calculated, which reproduces, at low temperatures, the known expression of the Bogolyubov theory and, at high temperatures, the result of the classical liquid theory. The elimination of theoretical infra-red divergences by the renormalization of the one-particle spectrum gives rise to a temperature dependence of the effective atomic mass in the liquid. All final formulas contain the experimentally measurable structural factor of liquid helium-4 extrapolated to the zero temperature rather than the interatomic potential. The temperature $T_c = 2.26$ K of the Bose–Einstein condensation of liquid helium-4 has been calculated. The Bose–Einstein condensate fraction in superfluid ^{4}He has been calculated in a wide temperature range.

1. Introduction

The phenomenon of Bose–Einstein condensation predicted by Einstein for an ideal Bose gas in 1925 attracted a huge, still lasting interest among physicists, both theorists and experimenters, who studied the properties of liquid helium-4 and other quantum liquids. London put forward an idea [1, 2] that superfluidity in liquid helium-4 might be related with the phenomenon of Bose–Einstein condensation in an ideal Bose gas. However, no one has succeeded in establishing this relationship rigorously and unambiguously till now.

Bogolyubov [3] found the dynamic smearing of a Bose-condensate fraction in the framework of a weakly nonideal Bose-gas model. The problem of calculation of the Bose-condensate fraction in liquid helium-4 was considered for the first time by Penrose and Onsager [4]. In that article, the authors, making use of the hard sphere approximation for the wave function of the ground state, obtained a theoretical estimation of about 8% for the Bose-condensate fraction at the zero temperature. Later works gave the values for this quantity that did not differ much [5–10]. The drawback of Bose-condensate fraction calculations for liquid helium-4 is a circumstance that the authors consider various model representations for the ground-state wave function which, however, take only short-range pair interatomic correlations into account. In works [9,11], an attempt was made to calculate the Bose-condensate fraction, taking both short- and long-range correlations into account self-consistently. However, to obtain a specific numerical value, uncontrollable approximations should be made in this case. In a series of works [12–15], the Bose-condensate fraction was calculated from the first principles, making use of the one-particle density matrix concept, and the corresponding value falling within the range from 3.7% to 8.8% at the zero temperature was obtained. Another way to calculate the Bose-condensate fraction involves the Monte-Carlo simulation methods. A number of such researches were carried out in works [16–18]. This approach gives a narrower spread of values concerned: from 7.2% to 9.0%.

Experimental measurements of the Bose-condensate fraction are based on several methods. One of them is based on the analysis of the strongly inelastic scattering of neutrons in liquid helium-4 at a large momentum transfer. This method was applied by a lot of researchers [19–30]. The corresponding values obtained for the Bose-condensate fraction at the temperature $T = 0$ turned out to be from 2.2% to 14.0%. The results obtained from the neutron scattering [31] gave rise to a value of 13.9%. A similar result of 13.3% was obtained somewhat later on with the use of the data concerning the temperature variation of the mean kinetic energy [32]. Recent precise measurements of the dynamic structural factor enabled a value of (7.25 ± 0.75)% to be obtained [33].

In this article, we propose a method for the calculation of s-particle density matrices and a detailed research of the one-particle density matrix of a multiboson system which is obtained from the expression for the total density matrix found in work [34] in a wide temperature range. In Section 2, the basic explicit expressions for the total density matrix of interacting Bose liquids are given, as well as for the s-particle density matrices defined by Bogolyubov. Section 3 contains the calculation of s-particle density matrices.

An expression for the one-particle density matrix of liquid helium-4 in the pair correlation approximation is obtained in Section 4. In the following Section, the method of elimination of divergences that arise in the proposed theory is described, which consists in the renormalization of the free-particle spectrum. The temperature dependence of the effective atomic mass in the liquid is obtained. In Section 6, an expression for the mean kinetic energy of liquid helium-4 is found in the pair correlation approximation. In Section 7, an expression for the Bose-condensate fraction in liquid helium-4 in a wide temperature range is obtained. Last Section 8 contains numerical calculations for the temperature dependence of the Bose-condensate fraction in the pair correlation approximation and for the λ-transition temperature in liquid helium-4.

2. Basic Equations

Consider a system of N spinless interacting Bose particles with mass m each and the coordinates $\mathbf{r}_1, \ldots, \mathbf{r}_N$ which move in volume V. Following Bogolyubov [3, 35], let us introduce s-particle density matrices for this system:

$$F_s(\mathbf{r}_1, \ldots, \mathbf{r}_s|\mathbf{r}'_1, \ldots, \mathbf{r}'_s) = \frac{V^s}{Z_N} \int d\mathbf{r}_{s+1} \ldots \int d\mathbf{r}_N \times$$

$$\times R_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}'_1, \ldots, \mathbf{r}'_s, \mathbf{r}_{s+1}, \ldots, \mathbf{r}_N), \tag{1}$$

$$s = 1, 2 \ldots, N,$$

where $R_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}'_1, \ldots, \mathbf{r}'_N)$ is the total density matrix of the system, and

$$Z_N = \int \ldots \int R_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}_1, \ldots, \mathbf{r}_N) d\mathbf{r}_1 \ldots d\mathbf{r}_N \tag{2}$$

is its partition function with the ratio $s/N \to 0$ in the thermodynamic limit ($N \to \infty$, $V \to \infty$, $N/V = \text{const}$). The diagonal elements of the s-particle density matrices are normalized to unity:

$$\frac{1}{V^s} \int d\mathbf{r}_1 \ldots \int d\mathbf{r}_s F_s(\mathbf{r}_1 \ldots \mathbf{r}_s|\mathbf{r}_1 \ldots \mathbf{r}_s) = 1, \quad V \to \infty.$$

The total density matrix of Bose liquids in the pair correlation approximation was calculated in work [34]:

$$R_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}'_1, \ldots, \mathbf{r}'_N) = R^0_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}'_1, \ldots, \mathbf{r}'_N) \times$$

$$\times P_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}'_1, \ldots, \mathbf{r}'_N), \tag{3}$$

where

$$R^0_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}'_1, \ldots, \mathbf{r}'_N) = \frac{1}{N!} \left(\frac{m^*}{2\pi\beta\hbar^2} \right)^{3/2} \times$$

$$\times \sum_Q \exp \left[-\frac{m^*}{2\beta\hbar^2} \sum_{j=1}^{N} \left(\mathbf{r}_j - \mathbf{r}'_{Qj} \right)^2 \right] \tag{4}$$

is the density matrix of an ideal Bose gas, and the summation over Q means the summation over all $N!$ permutations of indices that enumerate particle coordinates. The factor that takes the particle-to-particle interaction into account is

$$P_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}'_1, \ldots, \mathbf{r}'_N) = e^U, \tag{5}$$

where

$$U = c_0 + \sum_{\mathbf{q} \neq 0} c_1 \rho'_\mathbf{q} \rho_{-\mathbf{q}} - \frac{1}{2} \sum_{\mathbf{q} \neq 0} c_2 \left[\rho_\mathbf{q} \rho_{-\mathbf{q}} + \rho'_\mathbf{q} \rho'_{-\mathbf{q}} \right], \tag{6}$$

$$c_0 = -\beta E_0 + \frac{1}{2} \sum_{\mathbf{q} \neq 0} \ln \left[\frac{\alpha_q \tanh\left(\frac{\beta E_q}{2}\right)}{\tanh\left(\frac{\beta \varepsilon_q}{2}\right)} \right] +$$

$$+ \sum_{\mathbf{q} \neq 0} \ln \left[\frac{1 - \exp\left(-\beta\varepsilon_q\right)}{1 - \exp\left(-\beta E_q\right)} \right],$$

$$c_1 = \frac{1}{2} \left[\frac{\alpha_q}{\sinh(\beta E_q)} - \frac{1}{\sinh(\beta\varepsilon_q)} \right],$$

$$c_2 = \frac{1}{2} [\alpha_q \coth(\beta E_q) - \coth(\beta\varepsilon_q)], \tag{7}$$

$$\lambda_q = 2 \Big[c_2 - c_1 \Big]. \tag{8}$$

In addition, in expressions (4)–(7), the following notations were introduced: $\beta = 1/T$ is the inverse temperature of the Bose gas;

$$\rho_\mathbf{q} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-i\mathbf{q}\mathbf{r}_j}, \qquad \rho'_\mathbf{q} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-i\mathbf{q}\mathbf{r}'_j} \tag{9}$$

are the Fourier coefficients of particle concentration fluctuations; $\varepsilon_q = \hbar^2 q^2/2m^*$ is the energy of a free particle; and m^* is the "bare" effective mass which makes allowance for a contribution made by direct many-particle correlations. The following expression for the effective mass extrapolated to a wide temperature range was proposed by us in work [37]:

$$\frac{m}{m^*} = 1 - \frac{1}{3N}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q^2}{(1+\lambda_q)(2+\lambda_q)}. \tag{10}$$

Here, the quantity λ_q (see Eq. (8)) is taken at $m^* = m$: $\lambda_q = \lambda_q|_{m^*=m}$.

The next quantity,

$$E_q = \alpha_q \frac{\hbar^2 q^2}{2m}, \tag{11}$$

which enters formula (6) is the spectrum of Bogolyubov elementary excitations. Here,

$$\alpha_q = \sqrt{1 + \frac{2N}{V}\nu_q \Big/ \frac{\hbar^2 q^2}{2m}} \tag{12}$$

is the Bogolyubov factor, ν_q is the Fourier transform of the potential energy of the particle-to-particle pair interaction; and

$$E_0 = \frac{N(N-1)}{2V}\nu_0 - \sum_{\mathbf{q}\neq 0}\frac{\hbar^2 q^2}{8m}(\alpha_q - 1)^2 \tag{13}$$

is the ground state energy of a multiboson system in the Bogolyubov approximation [3].

3. Calculations of s-particle density matrices

To carry out the integration in formula (1), let us apply the method that was proposed in work [38]. We separately select $N-s$ coordinates of particles to be integrated over:

$$\rho_{\mathbf{q}} = \xi_{\mathbf{q}} + \sqrt{\frac{N-s}{N}}\rho_{\mathbf{q}}^{(N-s)}, \tag{14}$$

$$\rho'_{\mathbf{q}} = \xi'_{\mathbf{q}} + \sqrt{\frac{N-s}{N}}\rho_{\mathbf{q}}^{(N-s)},$$

and the remaining ones define the s-particle density matrix:

$$\xi_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{j=1}^{s} e^{-i\mathbf{q}\mathbf{r}_j}, \qquad \xi'_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{j=1}^{s} e^{-i\mathbf{q}\mathbf{r}'_j}, \tag{15}$$

$$\rho_{\mathbf{q}}^{(N-s)} = \frac{1}{\sqrt{N-s}}\sum_{j=s+1}^{N} e^{-i\mathbf{q}\mathbf{r}_j}. \tag{16}$$

Note that, for $s=0$, we have $\rho_{\mathbf{q}}^{(N)} = \rho_{\mathbf{q}}$ and $\xi_{\mathbf{q}} = \xi'_{\mathbf{q}} = 0$. Due to the separation of variables, expression (6) can be written in the form

$$U = c_0 + \sum_{\mathbf{q}\neq 0} c_1 \xi'_{\mathbf{q}}\xi_{-\mathbf{q}} - \frac{1}{2}\sum_{\mathbf{q}\neq 0} c_2\left(\xi_{\mathbf{q}}\xi_{-\mathbf{q}} + \xi'_{\mathbf{q}}\xi'_{-\mathbf{q}}\right) -$$

$$-\frac{1}{2}\frac{N-s}{N}\sum_{\mathbf{q}\neq 0}\lambda_q \rho_{\mathbf{q}}^{(N-s)}\rho_{-\mathbf{q}}^{(N-s)} -$$

$$-\frac{1}{2}\sqrt{\frac{N-s}{N}}\sum_{\mathbf{q}\neq 0}\lambda_q \rho_{\mathbf{q}}^{(N-s)}\left(\xi'_{-\mathbf{q}} + \xi_{-\mathbf{q}}\right). \tag{17}$$

Now, taking expressions (14)–(17) into account, the s-particle density matrix for interacting Bose particles can be written as the averaged total density matrix of the ideal Bose gas:

$$F_s(\mathbf{r}_1,\ldots,\mathbf{r}_s|\mathbf{r}'_1,\ldots,\mathbf{r}'_s) = F_s^0(\mathbf{r}_1,\ldots,\mathbf{r}_s|\mathbf{r}'_1,\ldots,\mathbf{r}'_s)\times$$

$$\times\frac{Z_N^0}{Z_N}e^{c_0 + \sum\limits_{\mathbf{q}\neq 0} c_1\xi'_{\mathbf{q}}\xi_{-\mathbf{q}} - \frac{1}{2}\sum\limits_{\mathbf{q}\neq 0} c_2\left(\xi_{\mathbf{q}}\xi_{-\mathbf{q}} + \xi'_{\mathbf{q}}\xi'_{-\mathbf{q}}\right)}\times$$

$$\times\left\langle e^{-\frac{1}{2}\frac{N-s}{N}\sum\limits_{\mathbf{q}\neq 0}\lambda_q\rho_{\mathbf{q}}^{(N-s)}\rho_{-\mathbf{q}}^{(N-s)}} e^{-\frac{1}{2}\sqrt{\frac{N-s}{N}}\sum\limits_{\mathbf{q}\neq 0}\lambda_q\rho_{\mathbf{q}}^{(N-s)}\eta_{\mathbf{q}}}\right\rangle_0. \tag{18}$$

Here, the notation

$$\eta_{\mathbf{q}} = \xi'_{-\mathbf{q}} + \xi_{-\mathbf{q}} \tag{19}$$

is introduced, and the averaging is carried out on the basis of the total density matrix of the ideal Bose gas:

$$\langle\ldots\rangle_0 =$$

$$= \frac{\int d\mathbf{r}_{s+1}\ldots d\mathbf{r}_N R_N^0(\mathbf{r}_1,\ldots,\mathbf{r}_N|\mathbf{r}'_1,\ldots,\mathbf{r}'_s,\mathbf{r}_{s+1},\ldots,\mathbf{r}_N)\{\ldots\}}{\int d\mathbf{r}_{s+1}\ldots d\mathbf{r}_N R_N^0(\mathbf{r}_1,\ldots,\mathbf{r}_N|\mathbf{r}'_1,\ldots,\mathbf{r}'_s,\mathbf{r}_{s+1},\ldots,\mathbf{r}_N)}. \tag{20}$$

Then, the first exponential factor in the angle brackets in formula (18) is expressed in terms of the functional integral,

$$e^{-\frac{1}{2}\frac{N-s}{N}\sum\limits_{\mathbf{q}\neq 0}\lambda_q\rho_{\mathbf{q}}^{(N-s)}\rho_{-\mathbf{q}}^{(N-s)}} =$$

$$= \int(d\varphi)\, e^{-\frac{1}{2}\sum\limits_{\mathbf{q}\neq 0}\varphi_{\mathbf{q}}\varphi_{-\mathbf{q}}+\sum\limits_{\mathbf{q}\neq 0}\sqrt{-\lambda_q\frac{N-s}{N}}\rho_{\mathbf{q}}^{(N-s)}\varphi_{\mathbf{q}}}, \qquad (21)$$

where

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

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

The primed product means that $\varphi_{\mathbf{q}}$ with $\mathbf{q}$-subscripts from any half-space of their possible values are taken into consideration. Then, the substitution of variables $\theta_{\mathbf{q}} = \frac{1}{2}\sqrt{-\lambda_q}\eta_{\mathbf{q}} + \varphi_{\mathbf{q}}$ is made. For such a linear transformation, the Jacobian matrix is equal to unity. Hence, the s-particle density matrix (18) looks now like

$$F_s(\mathbf{r}_1,\dots,\mathbf{r}_s|\mathbf{r}_1',\dots,\mathbf{r}_s') = \frac{Z_N^0}{Z_N}F_s^0(\mathbf{r}_1,\dots,\mathbf{r}_s|\mathbf{r}_1',\dots,\mathbf{r}_s')\times$$

$$\times e^{c_0+\sum\limits_{\mathbf{q}\neq 0}c_1\xi_{\mathbf{q}}'\xi_{-\mathbf{q}}-\frac{1}{2}\sum\limits_{\mathbf{q}\neq 0}c_2\left(\xi_{\mathbf{q}}\xi_{-\mathbf{q}}+\xi_{\mathbf{q}}'\xi_{-\mathbf{q}}'\right)} I^{(N-s)}, \qquad (22)$$

where $I^{(N-s)}$ is the functional integral

$$I^{(N-s)} = \int(d\theta)e^{-\frac{1}{2}\sum\limits_{\mathbf{q}\neq 0}\theta_{\mathbf{q}}\theta_{-\mathbf{q}}}\times$$

$$\times e^{\frac{1}{2}\sum\limits_{\mathbf{q}\neq 0}\sqrt{-\lambda_q}\eta_{\mathbf{q}}\theta_{\mathbf{q}}+\frac{1}{8}\sum\limits_{\mathbf{q}\neq 0}\lambda_q\eta_{\mathbf{q}}\eta_{-\mathbf{q}}}\times$$

$$\times\exp\left\{\sum_{n\geq 1}\frac{1}{n!}\left[\prod_{i=1}^{n}\sum_{\mathbf{q}_i\neq 0}\sqrt{-\lambda_{q_i}\frac{N-s}{N}}\theta_{\mathbf{q}_i}\right]M_n^{(N-s)}\right\}. \qquad (23)$$

The notation $M_n^{(N-s)}$ is used to designate a chain of irreducible averages of the product of $\rho_{\mathbf{q}}^{(N-s)}$ quantities [39, 40]. In particular, two first averages are

$$M_1^{(N-s)} = \langle\rho_{\mathbf{q}}^{(N-s)}\rangle_0,$$

$$M_2^{(N-s)} = \langle\rho_{\mathbf{q}}^{(N-s)}\rho_{-\mathbf{q}}^{(N-s)}\rangle_0 - \langle\rho_{\mathbf{q}}^{(N-s)}\rangle_0\langle\rho_{-\mathbf{q}}^{(N-s)}\rangle_0. \qquad (24)$$

The expression for partition function (2) can be rewritten in terms of the functional integral $I^{(N-s)}$ at $s=0$:

$$Z_N = Z_N^0 e^{c_0} I^{(N)}. \qquad (25)$$

In the approximation where the sum over the wave vector is replaced by its first term, the functional integral $I^{(N-s)}$ (23) is easily calculated:

$$I_0^{(N-s)} = \exp\left[\frac{1}{8}\sum_{\mathbf{q}\neq 0}\lambda_q\eta_{\mathbf{q}}\eta_{-\mathbf{q}}\right]\times$$

$$\times\exp\left[-\frac{1}{2}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q(1-\frac{s}{N})\left[M_1^{(N-s)}\right]^2}{1+\lambda_q(1-\frac{s}{N})M_2^{(N-s)}}\right]\times$$

$$\times\exp\left[-\frac{1}{2}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q\sqrt{1-\frac{s}{N}}M_1^{(N-s)}\eta_{\mathbf{q}}}{1+\lambda_q(1-\frac{s}{N})M_2^{(N-s)}}\right]\times$$

$$\times\exp\left[-\frac{1}{8}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q\eta_{\mathbf{q}}\eta_{-\mathbf{q}}}{1+\lambda_q\left(1-\frac{s}{N}\right)M_2^{(N-s)}}\right]\times$$

$$\times\exp\left[-\frac{1}{2}\sum_{\mathbf{q}\neq 0}\ln\left[1+\lambda_q\left(1-\frac{s}{N}\right)M_2^{(N-s)}\right]\right].$$

Now, the final expression for the s-particle density matrix (22) is

$$F_s(\mathbf{r}_1,\dots,\mathbf{r}_s|\mathbf{r}_1',\dots,\mathbf{r}_s') = F_s^0(\mathbf{r}_1,\dots,\mathbf{r}_s|\mathbf{r}_1',\dots,\mathbf{r}_s')\times$$

$$\times\frac{I_0^{(N-s)}}{I_0^{(N)}}e^{\sum\limits_{\mathbf{q}\neq 0}c_1\xi_{\mathbf{q}}'\xi_{-\mathbf{q}}-\frac{1}{2}\sum\limits_{\mathbf{q}\neq 0}c_2\left(\xi_{\mathbf{q}}\xi_{-\mathbf{q}}+\xi_{\mathbf{q}}'\xi_{-\mathbf{q}}'\right)}. \qquad (26)$$

Therefore, in order to calculate the s-particle density matrix, one has to calculate the corresponding functional integrals (23) and the s-particle density matrix for the ideal Bose gas.

4. One-particle Density Matrix

It is known that the thermodynamics of a system can be constructed with the help of lowest density matrices, in particular, one- and two-particle ones. Our task is to calculate the one-particle density matrix.

Expression (26) at $s=1$ reads

$$F_1(\mathbf{r}_1|\mathbf{r}_1') = F_1^0(\mathbf{r}_1|\mathbf{r}_1')\frac{I_0^{(N-1)}}{I_0^{(N)}}\times$$

$$\times\exp\left[\frac{1}{N}\sum_{\mathbf{q}\neq 0}c_1\left(e^{i\mathbf{q}(\mathbf{r}_1-\mathbf{r}_1')}-1\right)-\frac{1}{2N}\sum_{\mathbf{q}\neq 0}\lambda_q\right], \qquad (27)$$

where

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

$$\times\exp\left[\frac{1}{8}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q^2(1-\frac{1}{N})M_2^{(N-1)}\eta_{\mathbf{q}}\eta_{-\mathbf{q}}}{1+\lambda_q\left(1-\frac{1}{N}\right)M_2^{(N-1)}}\right]\times$$

$$\times\exp\left[-\frac{1}{2}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q\sqrt{1-\frac{1}{N}}M_1^{(N-1)}\eta_{\mathbf{q}}}{1+\lambda_q(1-\frac{1}{N})M_2^{(N-1)}}\right]\times$$

$$\times\exp\left[-\frac{1}{2}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q(1-\frac{1}{N})\left[M_1^{(N-1)}\right]^2}{1+\lambda_q(1-\frac{1}{N})M_2^{(N-1)}}\right]\times$$

$$\times\exp\left[-\frac{1}{2}\sum_{\mathbf{q}\neq 0}\ln\left[1+\lambda_q\left(1-\frac{1}{N}\right)M_2^{(N-1)}\right]\right]. \qquad (28)$$

Here,

$$S_0(q) = \langle\rho_{\mathbf{q}}\rho_{-\mathbf{q}}\rangle_0 \qquad (29)$$

is the N-particle structural factor of the ideal Bose gas. As seen from Eq. (28), in order to calculate the one-particle density matrix (27) in the pair correlation approximation, it is necessary to calculate two first quantities (24).

Carrying out the averaging (20), let us write the expressions for $\langle\rho_{\mathbf{q}}^{(N-1)}\rangle_0$ and $\langle\rho_{\mathbf{q}}^{(N-1)}\rho_{-\mathbf{q}}^{(N-1)}\rangle_0$ as follows:

$$\langle\rho_{\mathbf{q}}^{(N-1)}\rangle_0 = \frac{\sqrt{N-1}}{V}\int d\mathbf{r}_2 e^{-i\mathbf{q}\mathbf{r}_2}\frac{F_2^0(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_1',\mathbf{r}_2)}{F_1^0(\mathbf{r}_1|\mathbf{r}_1')}, \qquad (30)$$

$$\langle\rho_{\mathbf{q}}^{(N-1)}\rho_{-\mathbf{q}}^{(N-1)}\rangle_0 = 1+\frac{N-2}{V^2}\times$$

$$\times\int d\mathbf{r}_2\int d\mathbf{r}_3 e^{-i\mathbf{q}(\mathbf{r}_3-\mathbf{r}_2)}\frac{F_3^0(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3|\mathbf{r}_1',\mathbf{r}_2,\mathbf{r}_3)}{F_1^0(\mathbf{r}_1|\mathbf{r}_1')}. \qquad (31)$$

Here, F_1^0, F_2^0, and F_3^0 are the one-, two-, and three-particle density matrices, respectively, for the ideal Bose gas.

In order to calculate the s-particle density matrix of the ideal Bose gas, we use the known technique of secondary quantization [35, 36, 39]. Since the intermediate expressions are cumbersome, the details of calculations are not presented. The first density matrices look like

$$F_1^0(\mathbf{r}_1|\mathbf{r}_1') = \frac{n_0}{N}+g_{11'}, \qquad (32)$$

$$F_2^0(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_1',\mathbf{r}_2) =$$

$$= \frac{N}{N-1}\left[F_1^0(\mathbf{r}_1|\mathbf{r}_1')+\frac{n_0}{N}\left[g_{12}+g_{21'}\right]+g_{12}g_{21'}\right], \qquad (33)$$

$$F_3^0(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3|\mathbf{r}_1',\mathbf{r}_2',\mathbf{r}_3') = \frac{N^2}{(N-1)(N-2)}\times$$

$$\times\left[\left(\frac{n_0}{N}\right)^3+\left(\frac{n_0}{N}\right)^2(g_{11'}+g_{12'}+g_{13'}+g_{21'}+g_{22'}+\right.$$

$$+g_{23'}+g_{31'}+g_{32'}+g_{33'})+\frac{n_0}{N}\Big(g_{11'}g_{22'}+g_{11'}g_{23'}+$$

$$+g_{11'}g_{32'}+g_{11'}g_{33'}+g_{12'}g_{21'}+g_{12'}g_{23'}+g_{12'}g_{31'}+$$

$$+g_{13'}g_{31'}+g_{13'}g_{21'}+g_{13'}g_{32'}+g_{22'}g_{13'}+g_{22'}g_{31'}+$$

$$+g_{22'}g_{33'}+g_{21'}g_{32'}+g_{23'}g_{32'}+g_{23'}g_{31'}+g_{33'}g_{12'}+$$

$$+g_{33'}g_{21'}\Big)+g_{11'}g_{22'}g_{33'}+g_{11'}g_{23'}g_{32'}+g_{12'}g_{23'}g_{31'}+$$

$$+g_{13'}g_{32'}g_{21'}+g_{12'}g_{21'}g_{33'}+g_{22'}g_{13'}g_{31'}\Big], \tag{34}$$

where

$$g_{ij'}\equiv g(|\mathbf{r}_i-\mathbf{r}'_j|),\quad g(|\mathbf{r}_i-\mathbf{r}'_j|)=\frac{1}{N}\sum_{\mathbf{p}\neq 0} n_p e^{i\mathbf{p}(\mathbf{r}_i-\mathbf{r}'_j)},$$

$$n_p=\frac{1}{z^{-1}e^{\beta\varepsilon_p}-1} \tag{35}$$

is the average number of particles in the ideal Bose gas with the spectrum ε_p, z is its activity, and the parameter n_0/N is the Bose-condensate fraction of free particles with a renormalized spectrum. The activity z is determined from the condition

$$\sum_{\mathbf{p}} n_p=N. \tag{36}$$

Expressions (32)–(34) coincide with their counterparts in work [41].

After simple but rather cumbersome calculations, averages (30) and (31) read

$$\langle\rho_{\mathbf{q}}^{(N-1)}\rangle_0=\frac{\sqrt{N-1}}{N}\frac{1}{F_1^0(\mathbf{r}_1|\mathbf{r}'_1)}\times$$

$$\times\Bigg[n_q\frac{n_0}{N}\left[e^{-i\mathbf{q}\mathbf{r}_1}+e^{-i\mathbf{q}\mathbf{r}'_1}\right]+\frac{1}{2N}\sum_{\substack{\mathbf{p}\neq 0\\ \mathbf{p}+\mathbf{q}\neq 0}} n_p n_{|\mathbf{p}+\mathbf{q}|}\times$$

$$\times\left[e^{i\mathbf{p}(\mathbf{r}_1-\mathbf{r}'_1)}e^{-i\mathbf{q}\mathbf{r}'_1}+e^{-i\mathbf{p}(\mathbf{r}_1-\mathbf{r}'_1)}e^{-i\mathbf{q}\mathbf{r}_1}\right]\Bigg], \tag{37}$$

$$\langle\rho_{\mathbf{q}}^{(N-1)}\rho_{-\mathbf{q}}^{(N-1)}\rangle_0=S_0(q)+\frac{1}{N-1}\left[S_0(q)-1+f_{\mathbf{q}}\right],$$

$$f_{\mathbf{q}}=\frac{1}{F_1^0(\mathbf{r}_1|\mathbf{r}'_1)}\Bigg[n_q^2\frac{n_0}{N}\left[e^{i\mathbf{q}(\mathbf{r}_1-\mathbf{r}'_1)}+e^{-i\mathbf{q}(\mathbf{r}_1-\mathbf{r}'_1)}\right]+$$

$$+\frac{1}{N}\sum_{\substack{\mathbf{p}\neq 0\\ \mathbf{p}+\mathbf{q}\neq 0}} n_p^2 n_{|\mathbf{p}+\mathbf{q}|}\left[e^{i\mathbf{p}(\mathbf{r}_1-\mathbf{r}'_1)}+e^{-i\mathbf{p}(\mathbf{r}_1-\mathbf{r}'_1)}\right]\Bigg], \tag{38}$$

where

$$S_0(q)=1+2\frac{n_0}{N}n_q+\frac{1}{N}\sum_{\substack{\mathbf{p}\neq 0\\ \mathbf{p}+\mathbf{q}\neq 0}} n_p n_{|\mathbf{p}+\mathbf{q}|} \tag{39}$$

is the structural factor of the ideal Bose gas.

Now, let us return to the consideration of the one-particle density matrix (27). Since $\eta_{\mathbf{q}}\sim 1/\sqrt{N}$ (19) and $M_1^{(N-1)}\sim 1/\sqrt{N}$ (37), then the ratio $I_0^{(N-1)}/I_0^{(N)}$ in formula (27) in the thermodynamic limit and in the adopted approximation looks like

$$\frac{I_0^{(N-1)}}{I_0^{(N)}}=\exp\left[\frac{1}{4N}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q^2 S_0(q)}{1+\lambda_q S_0(q)}\left[e^{i\mathbf{q}(\mathbf{r}_1-\mathbf{r}'_1)}-1\right]\right]\times$$

$$\times\exp\left[\frac{1}{2N}\sum_{\mathbf{q}\neq 0}\lambda_q-\frac{1}{2}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q}{1+\lambda_q S_0(q)}\eta_{\mathbf{q}}M_1^{(N-1)}\right]\times$$

$$\times\exp\left[-\frac{1}{2N}\sum_{\mathbf{q}\neq 0}\frac{\lambda_q}{1+\lambda_q S_0(q)}f_{\mathbf{q}}\right]. \tag{40}$$

Ultimately, the expression for the one-particle density matrix (27) can be written as

$$F_1(\mathbf{R})=F_1^0(\mathbf{R})p_1(\mathbf{R})\times$$

$$\times\exp\left[\frac{1}{F_1^0(\mathbf{R})}\left(2\frac{n_0}{N}J_1(\mathbf{R})+J_2(\mathbf{R})\right)\right], \tag{41}$$

where

$$p_1(\mathbf{R})=$$

$$=\exp\left[\frac{1}{4N}\sum_{\mathbf{q}\neq 0}\left(\frac{\lambda_q^2 S_0(q)}{1+\lambda_q S_0(q)}+4c_1\right)\left(e^{i\mathbf{q}\mathbf{R}}-1\right)\right], \tag{42}$$

$$J_1(\mathbf{R})=$$

$$=-\frac{1}{2N}\sum_{\mathbf{q}\neq \mathbf{0}}\frac{\lambda_q}{1+\lambda_q S_0(q)}\left[n_q+n_q(1+n_q)e^{i\mathbf{q}\mathbf{R}}\right], \tag{43}$$

$$J_2(\mathbf{R})=$$

$$=-\frac{1}{N^2}\sum_{\mathbf{q}\neq \mathbf{0}}\frac{\lambda_q}{1+\lambda_q S_0(q)}\sum_{\substack{\mathbf{p}\neq 0\\ \mathbf{p}+\mathbf{q}\neq 0}} n_p n_{|\mathbf{p}+\mathbf{q}|}(1+n_p)e^{i\mathbf{p}\mathbf{R}}, \tag{44}$$

$$\mathbf{R}=\mathbf{r}_1-\mathbf{r}'_1.$$

5. Renormalization of the One-particle Spectrum and Elimination of Infra-red Divergences

Since $n_p \sim 1/p^2$ as $\mathbf{p} \to 0$, the second term J_2 in the exponent in expression (41) diverges as $\mathbf{R} \to 0$:

$$J_2(0) \sim \int_0^\infty dp/p^2 \to \infty. \tag{45}$$

This is the so-called infra-red divergence. The idea of the elimination of such divergences was proposed in work [41] and applied in work [37]. Therefore, we shall not discuss these calculations in detail.

Let us consider expression (41) in the linear approximation for the exponent:

$$F_1(\mathbf{R}) = p_1(\mathbf{R}) \left[F_1^0(\mathbf{R}) + 2\frac{n_0}{N} J_1(\mathbf{R}) + J_2(\mathbf{R}) \right]. \tag{46}$$

Those divergences can be eliminated by renormalizing the free-particle spectrum. We choose it in the form

$$\bar{\varepsilon}_p = \varepsilon_p + \Delta_p - \Delta_0, \tag{47}$$

where Δ_p is a correction to the free-particle spectrum, which is to be determined. Accordingly, the distribution of Bose particles with a new spectrum looks like

$$\bar{n}_p = \frac{1}{\bar{z}^{-1} e^{\bar{\varepsilon}_p} - 1}, \tag{48}$$

where $\bar{z}$ is the renormalized activity.

Consider expression (46). Using the method of elimination of divergences [37, 41], we obtain the following expression for a correction to the free-particle spectrum:

$$\Delta_p = \frac{1}{N\beta} \sum_{\mathbf{q}\neq 0} \frac{\lambda_q}{1 + \lambda_q \bar{S}_0(q)} \bar{n}_{|\mathbf{p}+\mathbf{q}|}. \tag{49}$$

We write the corresponding expression for the one-particle density matrix (46) in the form

$$F_1(\mathbf{R}) = \bar{p}_1(\mathbf{R}) \left[\bar{F}_1^0(\mathbf{R}) + 2\frac{n_0}{N} \bar{J}_1(\mathbf{R}) \right]. \tag{50}$$

Here, the renormalized distribution $\bar{n}_p$ (48) can be substituted everywhere instead of the particle distribution n_p (35), because such an operation does not violate the limits of the adopted approximation. Bars above the quantities mean that they are expressed in terms of the renormalized free-particle distribution (48).

Expression (49) coincides with the corresponding expression in works [37, 41]. We obtained an equation of the integral type to find Δ_p. If the interaction is switched off ($\alpha_q = 1$), the correction to the spectrum $\Delta_p = 0$, $\bar{\varepsilon}_p = \varepsilon_p$, and the activity $\bar{z} = z_0$. Since $\Delta_p = 0$ at $T = 0$, the quantity Δ_p is only a temperature-induced correction to the energy spectrum ε_p, which enables the temperature of the Bose–Einstein condensation of the ideal gas to be shifted.

Expression (47) can be written as

$$\bar{\varepsilon}_p = \frac{\hbar^2 p^2}{2\bar{m}(p)}, \tag{51}$$

where the quantity $\bar{m}(p)$ is interpreted as the total effective mass of a particle which depends on the particle wave vector $\mathbf{p}$. It is clear that we are interested in the behavior of $\bar{m}(p)$ as $\mathbf{p} \to 0$, and we shall understand the quantity $\bar{m} = \bar{m}(0)$ as the total effective mass of the particle. At small $\mathbf{p}$-values, the renormalized spectrum of free particles (47) can be written in the form

$$\bar{\varepsilon}_p = \frac{\hbar^2 p^2}{2\bar{m}}, \tag{52}$$

$$\frac{m}{\bar{m}} = [1 + F(T)] \left[1 - \frac{1}{3N} \sum_{\mathbf{q}\neq 0} \frac{\lambda_q^2}{(1+\lambda_q)(2+\lambda_q)} \right],$$

where

$$F(T) = \frac{1}{2\pi^2 \rho} \int_0^\infty q^2 dq \frac{\lambda_q}{1 + \lambda_q \bar{S}_0(q)} \bar{n}_q (1 + \bar{n}_q) \times$$

$$\times \left[\frac{2}{3} \beta \varepsilon_q (1 + 2\bar{n}_q) - 1 \right]. \tag{53}$$

We recall once more that the details of such calculations are reported in work [37].

Note that the one-particle density matrix (50) has to satisfy the condition

$$F_1(\mathbf{r}_1|\mathbf{r}_1) = 1 \tag{54}$$

which declares that the number of particles in the system is N. Actually, it is a condition for the determination of the renormalized activity $\bar{z}$ rather than z_0, because our expressions include the renormalized spectrum of free particles, but not that of the ideal Bose gas.

6. Mean Kinetic Energy

Using the one-particle density matrix (50), it is possible to calculate the mean kinetic energy of the system, $\langle K\rangle$. By definition,

$$\langle K\rangle = -N\frac{\hbar^2}{2m}\left[\nabla^2 F_1(\mathbf{R})\right]_{\mathbf{R}=0}. \tag{55}$$

In the approximation of one sum over the wave vector, the expression for the mean kinetic energy reads

$$\langle K\rangle = \sum_{\mathbf{q}\neq 0}\frac{\hbar^2 q^2}{2m}\frac{1}{\bar z^{-1}e^{\beta\bar\varepsilon_q}-1}+$$

$$+\sum_{\mathbf{q}\neq 0}\left[\frac{\bar m}{2m}\frac{\lambda_q}{1+\lambda_q\bar S_0(q)}\frac{\partial\bar S_0(q)}{\partial\beta}+\frac{1}{4}\frac{\hbar^2 q^2}{2m}\frac{\lambda_q^2\bar S_0(q)}{1+\lambda_q\bar S_0(q)}\right]+$$

$$+\frac{1}{2}\sum_{\mathbf{q}\neq 0}\frac{\hbar^2 q^2}{2m}\left(\frac{\alpha_q}{\mathrm{sh}(\beta E_q)}-\frac{1}{\mathrm{sh}(\beta\bar\varepsilon_q)}\right). \tag{56}$$

Here, we used expression (39) and the relation

$$\frac{\partial\bar n_p}{\partial\beta} = -\frac{\hbar^2 p^2}{2\bar m}\bar n_p(1+\bar n_p). \tag{57}$$

The activity $\bar z$, the total effective mass $\bar m$, and the Bose-condensate fraction of free particles n_0/N are not differentiated with respect to β.

In work [45], the same expression for the mean kinetic energy, as expression (56) at $\bar m = m$, was obtained, but the former expression contains the β-derivative of the Bose-condensate fraction of free particles. Such a discrepancy results from two distinct approaches: namely, in this work, we find the one-particle density matrix by using the total density matrix and then, with the help of formula (55), calculate the mean kinetic energy. At the same time, in work [45], we find it, by directly averaging the operator of kinetic energy with the use of the total density matrix.

7. Bose Condensate

The limiting value of the one-particle density matrix, as its argument tends to infinity, determines the Bose condensate fraction, i.e. the number of particle, whose momentum equals zero:

$$\frac{N_0(T)}{N} = \lim_{\mathbf{R}\to\infty} F_1(\mathbf{R}). \tag{58}$$

Hence, we obtain the following temperature dependence for the Bose-condensate fraction in the pair correlation approximation:

$$\frac{N_0(T)}{N} = \frac{n_0}{N}\bar p_1(\infty)e^{2\bar J_1(\infty)}. \tag{59}$$

In expressions for $\bar p_1(\mathbf{R})$ (see Eq. (42)) and $\bar J_1(\mathbf{R})$ (see Eq. (43)), the terms with the multiplier $e^{i\mathbf{qR}}$, where $\mathbf{q}\neq 0$, quickly oscillate, if $\mathbf{R}\to\infty$, and give zero contributions. Therefore, in this limit, only terms that do not contain this multiplier survive:

$$\bar p_1(\infty) = \exp\left[-\frac{1}{4N}\sum_{\mathbf{q}\neq 0}\left(\frac{\lambda_q^2\bar S_0(q)}{1+\lambda_q\bar S_0(q)}+4c_1\right)\right], \tag{60}$$

$$\bar J_1(\infty) = -\frac{1}{2N}\sum_{\mathbf{q}\neq \mathbf{0}}\frac{\lambda_q}{1+\lambda_q\bar S_0(q)}\bar n_q. \tag{61}$$

The parameter n_0/N is determined from condition (54) in view of expression (50):

$$\frac{n_0}{N} = \frac{1-\bar g(0)}{1+2\bar J_1(0)}, \tag{62}$$

where

$$\bar J_1(0) = -\frac{1}{2N}\sum_{\mathbf{q}\neq \mathbf{0}}\frac{\lambda_q}{1+\lambda_q\bar S_0(q)}\bar n_q(\bar n_q+2). \tag{63}$$

The quantity $\bar g(0)$ is found from formulas (35) and (36):

$$\bar g(0) = \left(\frac{T}{T_c}\right)^{3/2}, \qquad T_c = \frac{2\pi\hbar^2}{\bar m_c}\left[\frac{N}{V}\Big/\zeta(3/2)\right]^{2/3}. \tag{64}$$

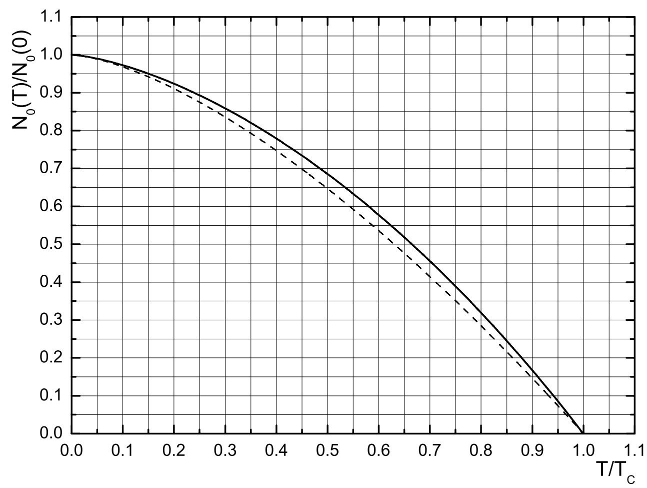
Here, T_c is the Bose–Einstein condensation temperature, $\bar m_c = \bar m(T=T_c)$ is the effective mass of a particle, and $\zeta(3/2)\simeq 2.612$ is the specific value of the Riemann zeta-function.

Ultimately, for the relative amount of the Bose condensate, we obtain

$$N_0(T)\Big/N_0(0) = \frac{\bar p_1(\infty)}{1+2\bar J_1(0)}\left[1-\left(\frac{T}{T_c}\right)^{3/2}\right]\times$$

$$\times\exp\left[\frac{1}{4N}\sum_{\mathbf{q}\neq \mathbf{0}}\frac{(\alpha_q-1)^2}{\alpha_q}+2\bar J_1(\infty)\right], \tag{65}$$

where $N_0(0)$ is the Bose condensate amount in liquid helium-4 at $T=0$. The calculation of $N_0(0)$ is a separate problem which was correctly considered in work [42]: $N_0(0) = 3.7\%$.



Temperature dependences of the Bose-condensate fraction in liquid helium-4 in relative units: ideal Bose gas (dashed curve) and the results of our calculations by formula (65)

8. Numerical Calculations

According to work [37], the quantity α_q can be presented in the main approximation as follows:

$$\alpha_q = \frac{1}{S^{\exp}(q)}. \tag{66}$$

Here, $S^{\exp}(q)$ is the experimental structural factor of liquid helium-4 extrapolated to $T = 0$. Its value can be taken from work [43].

The numerical calculations were carried out for the equilibrium helium density $\rho = 0.02185$ Å^{-3}, the particle mass $m = 4.0026$ amu, the sound velocity $c = 238.2$ m/s (in the limit $T \to 0$ [44]), and the critical temperature of the ideal Bose gas $T_c = 3.138$ K. Since the effective mass is a function of the temperature, expression (64) is, in essence, an equation for the determination of the Bose-condensation temperature T_c. Then, taking advantage of expression (52), we obtain $T_c = 2.26$ K. The calculated value of the Bose-condensation temperature evidently agrees well with the experimental one $T_c^{\exp} = 2.168$ K.

In Fig. 1, the temperature dependence of the Bose-condensate fraction in liquid helium-4 is depicted in relative units. The dependence was calculated by formula (65) with regard for the explicit expressions (60) for $\bar{p}_1(\infty)$, (63) for $\bar{J}_1(0)$, and (61) for $\bar{J}_1(\infty)$.

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ОДНОЧАСТИНКОВА МАТРИЦЯ ГУСТИНИ РІДКОГО ^{4}He В НАБЛИЖЕННІ ПАРНИХ КОРЕЛЯЦІЙ

І.О. Вакарчук, Р.О. Притула

Р е з ю м е

На основі виразу для повної матриці густини системи взаємодіючих бозе-частинок, знайденого в роботі [J. Phys. Stud. **8**, 223 (2004)], розраховано одночастинкову матрицю густини рідкого гелію-4 в координатному зображенні. У границі низьких температур отримано відомий вираз теорії Боголюбова, а при високих температурах наша теорія відтворює результат теорії класичних рідин. Усунувши шляхом перенормування одночастинкового спектра інфрачервоні розбіжності, що виникають у теорії, отримано температурну залежність ефективної маси атома в рідині. Усі кінцеві вирази записано через експериментально вимірюваний структурний фактор рідкого гелію-4, екстрапольований до $T \to 0$, замість потенціалу взаємодії. Розраховано температуру бозе-ейнштейнівської конденсації рідкого гелію-4: $T_c = 2,26$ K. Зроблено чисельний розрахунок температурної залежності бозе-конденсатної фракції в надплинному ^{4}He.