ONE-PARTICLE DENSITY MATRIX OF LIQUID $^4$He

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Using the expression for the total density matrix for a system of $N$ interacting Bose particles found in our previous papers, we calculate the one-particle density matrix in the coordinate representation. At low temperatures, the leading approximation of this matrix reproduces the results of the Bogoliubov theory. In the classical limit, the proposed theory reproduces the results of the theory of the classical liquid in the approximation of chaotic phases. From the one-particle density matrix, we find the particle momentum distribution function and the mean kinetic energy of the Bose liquid and investigate the phenomenon of Bose–Einstein condensation.

Keywords: Bose liquid, $\lambda$-transition, Bose condensate

With gratitude and warmth, the author recollects the numerous meetings and conversations with Dmitrii Nikolaevich Zubarev, his advice and constant support, and dedicates this paper to the memory of the scientist who did so much to develop the foundations of statistical mechanics, a person of high culture, fine soul, and exceptional intellectuality.

1. Introduction

This paper continues our studies [1] in which the total density matrix and also the thermodynamic functions of a system of $N$ interacting spinless Bose particles confined in the volume $V$ at the temperature $T$ were calculated in the pair-correlation approximation. Our aim here is to calculate the one-particle matrix, which allows studying the particle momentum distribution and the Bose–Einstein condensation phenomenon and also calculating the mean kinetic energy.

A feature of the results in [1] is that at high temperatures in the semiclassical limit, the diagonal elements of the total density matrix, as they should, transform into the standard Boltzmann factor with the potential energy of the particle system, while at low temperatures ($T \to 0$), we obtain the density matrix with the wave function of the ground state in the Bogoliubov–Zubarev approximation [2]. The thermodynamic functions manifest the same behavior. The expressions obtained in [1] therefore hold in a wide temperature range, and we can expect that they will provide reasonable results for the one-particle density matrix at intermediate temperatures, in particular, in the vicinity of the $\lambda$-transition in liquid $^4$He.

We calculate using a method based on expanding the total density matrix over particle permutations, which was proposed in [3]. Such an approach is natural when studying the $\lambda$-transition related to the Bose–Einstein condensation phenomenon, whose mathematical mechanism is based on taking permutations of larger and larger number of particles into account until permutations of all $N$ particles in the system become equally important at the transition point. Taking into account that the pair-correlation approximation for the ground state and at $T \to 0$, as shown in [4], provides good quantitative results even for such strongly nonideal systems as liquid $^4$He, we can expect from this approach something more than merely qualitative results in the vicinity of the $\lambda$-transition.
The literature on the theory of distribution functions of multibosonic systems is vast; we only note the monographs and the references therein that are well-known to experts, primarily, the fundamental Bogoliubov papers and the pioneering Zubarev paper [5]–[12].

2. The initial equations

We begin with the expression for the total density matrix of a system of \( N \) particles in the volume \( V \) with the Carthesian coordinates \( r_1, \ldots, r_N \) in the \( D \)-dimensional space at the temperature \( T \) [1],

\[
R_N(r_1, \ldots, r_N | r'_1, \ldots, r'_N) = R^0_N(r_1, \ldots, r_N | r'_1, \ldots, r'_N)P_N(r_1, \ldots, r_N | r'_1, \ldots, r'_N),
\]

where the first factor is the density matrix of the ideal Bose gas,

\[
R^0_N(r_1, \ldots, r_N | r'_1, \ldots, r'_N) = \frac{1}{N!} \Delta_N(1, \ldots, N | 1', \ldots, N'),
\]

and the permanent

\[
\Delta_N(1, \ldots, N | 1', \ldots, N') = \begin{vmatrix}
K_{11'} & K_{12'} & K_{13'} & \cdots & K_{1N'} \\
K_{21'} & K_{22'} & K_{23'} & \cdots & K_{2N'} \\
K_{31'} & K_{32'} & K_{33'} & \cdots & K_{3N'} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
K_{N1'} & K_{N2'} & K_{N3'} & \cdots & K_{NN'}
\end{vmatrix}_{+}
\]

is to be expanded as the standard determinant but all its terms must be taken with the plus sign, which is indicated by the subscript + in (2.3). Here and hereafter, to simplify the notation, we also use the notation \((1, \ldots, N) \equiv (r_1, \ldots, r_N)\) and \((1', \ldots, N') \equiv (r'_1, \ldots, r'_N)\) for the particle coordinates. The quantities \( K_{ij'} \) are determined by the expression

\[
K_{ij'} = \frac{1}{V} \sum_{p \neq 0} K_p e^{i\mathbf{p} \cdot (r_i - r'_j)}, \quad K_p = e^{-\beta \hbar^2 p^2 / (2m^*)},
\]

where \( \beta = 1/T \) is the reciprocal temperature. The sum over the wave vector \( \mathbf{p} \) in (2.4) is taken over the integer values of its components that are multiples of \( 2\pi / V^{1/D} \) in the infinite limit, and the sum over \( \mathbf{p} \neq 0 \) becomes the \( D \)-fold integral, \( \sum_{\mathbf{p} \neq 0} \rightarrow V \int d\mathbf{p} / (2\pi)^D \), in passing to the thermodynamic limit \( N \rightarrow \infty \), \( V \rightarrow \infty \), \( N/V = \text{const} \). Obviously \( K_{ij'} = 1/V, T = 0 \), because only the term with \( \mathbf{p} = 0 \) survives in (2.4) at \( T = 0 \), and therefore

\[
K_{ij'} = \left( \frac{m^*}{2\pi\beta\hbar^2} \right)^{D/2} e^{-m^*(r_i - r'_j)^2 / (2\beta m^*)} + \frac{1}{V}. \tag{2.5}
\]

At absolute zero, we therefore have

\[
R^0_N(r_1, \ldots, r_N | r'_1, \ldots, r'_N) = \frac{1}{V^N}, \quad T = 0,
\]

while at high temperatures when the term \( 1/V \) in (2.5) becomes negligible in the thermodynamic limit, we have

\[
R^0_N(r_1, \ldots, r_N | r'_1, \ldots, r'_N) = \frac{1}{N!} \left( \frac{m^*}{2\pi\beta\hbar^2} \right)^{DN/2} \sum_Q \exp \left[ -\frac{m^*}{2\beta m^2} \sum_{j=1}^N (r'_j - r_{Qj})^2 \right], \tag{2.6}
\]