DENSITY MATRICES OF SUPERFLUID HELIUM-4. I

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A method proposed earlier is used to calculate the density matrices for the ground state of a system of interacting Bose particles with allowance for many-particle correlations. A general expression from which the calculation of the density matrices in any approximation reduces to simple parametric differentiation is found. A perturbation theory is developed for the logarithm of a density matrix in such a way that each subsequent term of it contains an additional summation with respect to a wave vector compared with the previous term. Corrections whose expressions contain a double summation with respect to the wave vector are calculated explicitly. This corresponds to allowance for the contribution of the three-particle correlations and of those four-particle correlations in the wave function that can be represented by a double Fourier series.

1. Introduction

The phenomenon of Bose-Einstein condensation is one of the examples of the manifestation of the quantum-mechanical principle of the identity of particles on macroscopic scales. Its study in a real Bose fluid, superfluid helium-4, permits verification of the fundamental principles of quantum mechanics and quantum statistics. To establish the connection between the amount of Bose condensate in liquid helium-4 and the spatial structure in the arrangement of the atoms it is necessary to calculate partial density matrices in higher approximations than the ones known in the theory of a weakly nonideal Bose gas [1-3]. In addition, knowledge of the density matrices permits calculation of the equation of state and the thermodynamic functions of the system.

We consider a system of \( N \) \( \text{He}^4 \) atoms in a volume \( V \) at the absolute zero of temperature. By definition [2], the \( s \)-particle density matrix of such a system is

\[
\rho_s(r_1, \ldots, r_s | r'_1, \ldots, r'_s) = V^s \int \cdots \int \psi^*(r'_1, \ldots, r'_s, r_{s+1}, \ldots, r_N) \psi(r_1, \ldots, r_s, r_{s+1}, \ldots, r_N) \, dr_1 \cdots dr_N, \tag{1.1}
\]

where \( \psi(r_1, \ldots, r_N) \) is the ground-state wave function; the vectors \( r_1, \ldots, r_N \) identify the coordinates of the atoms; and \( s = 1, 2, 3, \ldots \), in such a way that in the thermodynamic limit

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The single-particle density matrix determines the momentum distribution of the atoms. The mean number of particles that possess momentum \( \hbar k \) is

\[
N_k = \frac{N}{V} \int e^{-i\hbar k \cdot R} F_1(R) dR, \quad F_1(R) = F_1(r'|r), \quad R = r - r'.
\]  

(1.2)

Hence, the relative number of particles that form the Bose condensate is

\[
\frac{N_0}{N} = \frac{1}{V} \int F_1(R) dR = \lim_{V \to \infty} F_1(R), \quad V \to \infty.
\]  

(1.3)

The mean value of the kinetic energy of the system is

\[
K = \sum_k \frac{\hbar^2 k^2}{2m} N_k = \frac{\hbar^2}{2m} N \lim_{k \to 0} \nabla^2 F_1(R).
\]  

(1.4)

We recall that in the thermodynamic limit the sums over the wave vectors \( k \) are replaced by integrals in accordance with the prescription

\[
\sum_k = V \int \frac{dk}{(2\pi)^3}.
\]

A diagonal element of the two-particle density matrix, the binary distribution function, determines the mean value of the potential energy \( \phi \) of the system with two-body interatomic interaction \( \phi(R) \):

\[
\phi = \frac{1}{2} \rho N \int \Phi(R) F_2(R) dR, \quad F_2(R) = F_2(r_1, r_2| r_1, r_2), \quad R = r_1 - r_2.
\]  

(1.5)

where \( \rho = N/V \) is the density of the atoms. This same expression can be rewritten in terms of the structure factor \( S_k \) of the fluid, which is related to the binary distribution function by a Fourier transformation [4,5]:

\[
S_k = 1 + \rho \int [F_2(R) - 1] e^{-i\hbar k \cdot R} dR.
\]  

(1.6)

Namely, we have

\[
\Phi = \frac{1}{2} \rho N v_0 + \frac{1}{2} \rho \sum_{k \neq 0} v_k (S_k - 1),
\]  

(1.7)

where \( v_k = \int e^{-i\hbar k \cdot R} \Phi(R) dR \) is the Fourier transform of the energy of the interatomic interaction.

The particle momentum distribution and the binary distribution function for a weakly nonideal Bose gas were first found by Bogolyubov in his pioneering studies on the theory of superfluidity [1,2]. In [3], in which the Schrödinger equation was solved by the method of collective variables, the wave functions of a weakly nonideal Bose gas were found, and in [6] they were used to determine the single-particle density matrix in the Bogolyubov approximation in accordance with the definition (1.1). Subsequently, the results of Bogolyubov's theory were reproduced on numerous occasions by various methods, on which we do not need to dwell here. The density matrices calculated in this approximation are not valid for investigation of a strongly nonideal system such as liquid helium-4. The clearest demonstration of this is, for example, the fact that the number of atoms in the Bose condensate is found to be negative. At short distances the binary distribution function is also found to be negative, though, by definition, it is positive.

In [7-9] a method for calculating the density matrices that enables one to avoid these difficulties was developed. It is necessary to develop a perturbation theory for the logarithm of the density matrices, and not for the matrices themselves. In this approach, each successive approximation contains an additional summation with respect to the wave vector \( k \) compared with the previous approximation. This method was used in [7,8] to find the density matrices in the first approximation, the first two terms of the expansions of the matrices in the "coupling constant" giving the results of Bogolyubov's theory. The following approximation was calculated in [9] for the ground state in the case when only