Calculation of the one-particle and two-particle condensates in He-II at $T = 0$

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We analyze the microstructure of He-II in the framework of the method of collective variables (CV), which was proposed by Bogolyubov and Zubarev and was developed later by Yukhnovskii and Vakarchuk. The logarithm of the ground-state wave function of He-II, $\ln \Psi_0$, is calculated in the approximation of “two sums”, i.e., as a Jastrow function and first (three-particle) correction. In the CV method equations for $\Psi_0$ are deduced from the $N$-particle Schrödinger equation. We also take into account the connection between the structure factor and $\Psi_0$, which allows one to obtain $\Psi_0$ from the structure factor of He-II, not from a model potential of interaction between He-II atoms. It should be emphasized that the model does not have any free parameters or functions. The amount of one-particle ($N_1$) and two-particle ($N_2$) condensates is calculated for the ground state of He-II: we find $N_1 \approx 0.27N$ and $N_2 \approx 0.53N$ in the Jastrow approximation for $\Psi_0$, and, taking into account the three-particle correction to $\ln \Psi_0$, we obtain $N_1 \approx 0.06N$ (which agrees with the experiment) and $N_2 \approx 0.16N$. In the approximation of “two sums”, we also find that the higher $s$-particle condensates ($s \geq 3$) are absent in He-II at $T = 0$.

KEY WORDS: Liquid $^4$He; One-Particle Condensate; Two-Particle Condensate.

1 Introduction

The sum of one-particle condensate (1PC), two-particle condensate (2PC) and higher $s$-particle condensates is usually referred to as the composite condensate. Knowing the structure of the composite condensate in He-II is, without doubt, of great importance [1]–[11]. Except for a purely cognitive interest, it also has a “practical” side, namely, in the field-theoretic approaches to the modelling of He-II microstructure [1] [4] [5] [11], the quasiparticle spectrum of He-II is explicitly expressed through the amount of the 1PC and 2PC, and the dependence on higher condensates is also not excluded. Of interest is the question whether all of He-II atoms belong to the composite condensate at $T = 0$, as was suggested in [7, 8] [11]. The superfluidity of He-II by itself is probably [3] [12] caused by an off-diagonal long-range order (ODLRO).

Our work is devoted to a calculation of the amount of 1PC and 2PC in He-II at $T = 0$. To describe the microstructure of He-II, we use the method of collective variables (CV), which was first proposed by Bogolyubov and Zubarev [13] and was later developed in the works by Yukhnovskii and Vakarchuk [14]–[18]. First, we obtain the ground-state wave function of He-II, $\Psi_0$, and then we calculate the amount of the condensates using the formula of [17, 19] for the $s$-particle density matrices $F_s$. The model does not contain any free parameters or functions: $\Psi_0$ is obtained as an eigenfunction of the $N$-particle Schrödinger equation; we also take into account the connection between $\Psi_0$ and the structure factor $S(k)$ of He-II [17, 19].
As far as we know, the higher \(s\)-particle condensates \((s \geq 3)\) were not calculated previously. The amount of 1PC in He-II at \(T = 0\) was found in many works \([2, 14, 18, 20–24, 11]\) (though only in \([14, 18, 23, 24]\) it was done without free parameters), and the theory agrees with the experiment on the whole. The amount of 2PC in He-II is still unknown. The 1PC was measured in many works, as a number of atoms with momentum equal to zero, but how to measure the 2PC is not yet clear (this issue is beyond of the scope of the article). There are only several theoretical estimates of the 2PC \([6, 8]\), all of which use free parameters. The results of \([6]\) are discussed below in Sec. 4. In \([8]\), a final result was not presented, but some equations were obtained, from which it follows that the proportion between 1PC and 2PC can vary depending on the form of the potential of the interaction between \(\text{He}^4\) atoms. We calculate the amounts of 1PC and 2PC without free parameters, and in more exact approximation as compared with \([14, 18, 6]\).

In \([14]\) and \([18]\), the amount of 1PC was found in the approximation of “one sum” (1S) with the result \(N_1 \approx 0.08N\) and \(N_1 \approx 0.04N\), respectively. Below, we obtain 1PC \((N_1)\) and 2PC \((N_2)\) for He-II at \(T = 0\) in more exact approximation of “two sums” (2S), and we find \(N_1 \approx 0.06N\) and \(N_2 \approx 0.16N\). Our formula for 2PC refines the Ristig’s formula \([6]\) previously obtained by another method in the 1S-approximation for \(\ln \Psi_0\).

In \([19]\) we have found also that (i) in a weakly interacting Bose gas, all atoms belong to 1PC or 2PC at \(T = 0\), and (ii) the higher \(s\)-particle condensates \((s \geq 3)\) are absent in He-II at \(T = 0\) (which was shown in the 2S-approximation).

2 The ground-state wave function of He-II

There exist several methods for calculation of the ground-state wave function of He-II (see also the review \([25]\)): the variational method \([26]\), the “Green’s function Monte Carlo” method \([27]\) and its development, “shadow wave function” (SWF) method \([28]\), the Path Integral Monte Carlo simulations \([22]\), the diffusion Monte Carlo (MC) simulations \([23, 24]\), the “hypernetted chain” (HNC) method \([29, 30]\), (all of these are indirect methods for solving the \(N\)-particle Schrödinger equation), Feenberg’s approach \([31]\) (solving the Schrödinger equation in the \(r\)-space), and the CV-method \([14–19, 32, 33]\) (solving the Schrödinger equation in the \(k\)-space).

The quantum-mechanical models are developed actively and a noticeable progress is already achieved \([19, 32, 24, 25, 28, 30, 34]\). Modern variational methods \([28]\) (SWF), \([29, 30]\) (HNC) reach an accuracy of the order better than 0.1 \(K\), but such models, unfortunately, use several free parameters.

In the CV-method, the equations are deduced from the first principles, namely, from the exact \(N\)-particle Schrödinger equation, and a solution of these equations can be found numerically without using any fitting parameters or functions (which is important) by taking into account the connection between \(\Psi_0\) and \(S(k)\).

All existing models of He-II of which we are aware (except the mentioned CV-approach) use several fitting parameters, at least, in the effective interaction potential (even the MC simulations); in this case, of course, it is not so difficult to obtain two “points”: the ground-state energy and 1PC. In our opinion, the approach without fitting parameters is preferable because, in this case, nothing is introduced in the model “by hand”. In our paper, we use the CV-method since this method does not have any fitting parameters.

According to \([15]\), the ground-state wave function of He-II has the form

\[
\Psi_0 = \frac{e^{S_0}}{\sqrt{Q}}, \quad S_0 = \sum_{j \geq 2} \frac{N^{1-j/2}}{j!} \sum_{\mathbf{k}_1, \ldots, \mathbf{k}_j \neq 0} \delta(\mathbf{k}_1 + \ldots + \mathbf{k}_j) a_j(\mathbf{k}_1, \ldots, \mathbf{k}_j) \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_j},
\]

where \(\delta\) is the Kronecker delta, \(N\) is the total number of atoms in helium, \(Q\) is a normalization
constant, and $\rho_k$ are the collective variables

$$\rho_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-ikr_j}, \quad k \neq 0. \quad (2)$$

The term with $a_n$ in (1) corresponds to $n$-particle correlations in $r$-space. The zero-order approximation for $\Psi_0$, which is also the 1S-approximation, is

$$\ln \Psi_0 = -\frac{1}{2} \ln Q + \sum_{k \neq 0} \frac{a_2(k)}{2} \rho_{k-k}, \quad a_{n \geq 3} = 0. \quad (3)$$

The wave function $\Psi_0$ (3) can be present in the well-known Jastrow form

$$\Psi_0 = \frac{1}{\sqrt{Q}} \prod_{i,j} e^{S_1(r_i-r_j)}, \quad (4)$$

where

$$S_1(r) = \frac{1}{N} \sum_k \frac{a_2(k)}{2} e^{ikr} = \frac{V}{N (2\pi)^3} \int dk \frac{a_2(k)}{2} e^{ikr}, \quad (5)$$

and $V$ is the volume of the system.

The capabilities of computers force us to restrict ourselves to the 2S-approximation for $\Psi_0$; in this case, the sums with $a_2$ and $a_3$ are taken into account in (1), but $a_{n \geq 4} = 0$ (for the “$n$-sum” approximation [17, 18] all sums up to the $n$-th sum over $k$ are included in all expansions). Substitution of $\Psi_0$ (1) into the $N$-particle Schrödinger equation allows one to obtain [15] a chain of equations for $a_n$. In the 2S-approximation, we have

$$a_3(k_1, k_2) = -\frac{2a_2(k_1)a_2(k_2)k_1k_2 + 2a_2(k_1)a_2(k_3)k_1k_3 + 2a_2(k_2)a_2(k_3)k_2k_3}{k_1^2 [1 - 2a_2(k_1)] + k_2^2 [1 - 2a_2(k_2)] + k_3^2 [1 - 2a_2(k_3)]}. \quad (6)$$

Throughout in the paper, we assume $k_3 = -k_1 - k_2 \neq 0$. The $s$-particle density matrices $F_s$ for the ground-state of Bose liquid were found in [17] for the approximation of 1S, and in [17, 19] for the approximation of 2S. Moreover, in [17, 19], an equation connecting $\Psi_0$ with the structure factor $S(k)$ was obtained:

$$2a_2(k) = 1 - \frac{1}{S(k)} - \frac{\Sigma_1(k)}{S(k) [1 - 2a_2(k)]} - \frac{\Sigma_2(k)}{S(k)}, \quad (7)$$

where

$$\Sigma_1(k) = \frac{2}{N} \sum_{q \neq 0} \frac{a_2(q)a_2(k+q) + a_3(k, q) [1 + a_3(k, q)]}{[1 - 2a_2(q)][1 - 2a_2(k+q)]}, \quad (8)$$

$$\Sigma_2(k) = \frac{2}{N} \sum_{q \neq 0} \frac{a_3^2(k, q)}{[1 - 2a_2(q)][1 - 2a_2(k+q)]}, \quad (9)$$

and also the formula for the amount of 1PC ($N_1$) was found:

$$\ln (N_1/N) = I_{1A} + I_{2A} + I_{2B} + I_{2C}, \quad (10)$$

$$I_{1A} = -\frac{1}{N} \sum_{k \neq 0} \frac{a_2^2(k)}{[1 - 2a_2(k)]}; \quad (11)$$

$$I_{2A} = -\frac{1}{8N^2} \sum_{k_1, k_2 \neq 0} \left( \prod_{j=1}^{3} \frac{2a_2(k_j)}{1 - 2a_2(k_j)} \right) \frac{1}{1 - 2a_2(k_1)}, \quad (12)$$
\[ I_{2B} = -\frac{1}{2N^2} \sum_{k_1, k_2 \neq 0} \left( \prod_{j=1}^{3} \frac{1}{1 - 2a_2(k_j)} \right) a_3(k_1, k_2) \ast \left\{ \frac{2a_2(k_1) + a_3(k_1, k_2)}{1 - 2a_2(k_1)} + 2a_2(k_1)[1 - a_2(k_2)] \right\}, \]  
\[ I_{2C} = \frac{1}{2N^2} \sum_{k_1, k_2 \neq 0} a_3^2(k_1, k_2) \prod_{j=1}^{3} \frac{1}{1 - 2a_2(k_j)}. \]  

Note that equations similar to (6), (7) were obtained by other methods by Campbell and Krotschek [29]. Our system of Eqs. (6)–(9) is a little more exact, because in (6) we have \( a_3 \) with \( a_2 \) from (7) (which includes correction \( a_3 \neq 0 \)), but in [29] \( a_3 \) was taken with \( a_2 \) in zeroth approximation (\( a_3 = 0 \) in (7)).

The following asymptotics as \( k \to 0 \) is true [19]:

\[ 2a_2(k \to 0) = -\frac{1 + \Sigma_2(0)}{S(k)}, \]  
\[ E(k \to 0) = ck = \frac{\hbar^2 k^2}{2mS(k)} \left( 1 + \Sigma_2(0) \right), \]  
\[ S(k \to 0) = \frac{\hbar k}{2mc} \left( 1 + \Sigma_2(0) \right), \]

where \( E(k) \) is the quasiparticle spectrum of Bose liquid (see the equations for \( E(k) \) in [16, 35, 33]), and

\[ \Sigma_2(0) = \frac{8}{N} \sum_{q \neq 0} \left( \frac{a_2(q)}{1 - 2a_2(q)} \right)^4 > 0. \]  

In the 1S-approximation [3], for which

\[ 2a_2(k) = 1 - \frac{1}{S(k)}, \quad a_{n \geq 3} = 0, \]

for He-II we obtain \( \Sigma_2(0) = 0.33 \) (from [18, 19]), and, in the 2S-approximation, a numerical solution of (6)–(9) (see Sec. 3) gives \( \Sigma_2(0) = 0.66 \).

### 3 One-particle condensate in He-II at \( T = 0 \)

In the 1S-approximation, the amount of 1PC can be simply found from (10), (11), and (19). For the structure factor \( S(k) \), we use the smoothed experimental data from [36], which is, perhaps, the most exact. We extrapolate this data to \( T = 0 \) according to [37]

\[ S(k, T=0) = S(k, T) \tanh \frac{E(k)}{2k_B T}. \]

At \( T = 0 \), we should have the asymptotic \( S(k=0) = 0 \) [38]; in (20), we take into account that \( E(k \to 0) = ck \). From (10), (11), (19), and (20), we numerically find \( n_1 \equiv \frac{N_1}{N} \cdot 100\% = 27.2\% \).

To calculate \( N_1 \) in the 2S-approximation, we need to know, according to (10)–(14), the functions \( a_2(k) \) and \( a_3(k_1, k_2) \). The function \( a_3 \) is defined in (6), and to obtain \( a_2(k) \) we should solve numerically the integral equation (7) taking into account (6), (8), and (9). We everywhere replace sums by integrals according to the rule [15, 17]

\[ \sum_k \to \frac{V}{(2\pi)^3} \int dk. \]
Equation (7) cannot be solved by iteration; we have succeeded in solving it numerically by the Newton’s method, in which way we found $a_2(k)$. From (6), (10)–(14), and (21), we obtain $n_1 = 6.1\%$, which agrees with the experiment: $n_1^{\text{exp}} \approx 6 – 12\%$ for $T = 0$. We estimate the numerical error for $n_1$ to be $\frac{\delta n_1}{n_1} \approx 0.1$. The properties of $\Psi_0$ and the possibility to obtain the ground-state energy $E_0$ are discussed in more detail in [33].

4 Two-particle condensate

It can be shown in 2S-approximation that the s-particle density matrices $F_s$ of helium-II for $T = 0$ in three dimensions display ODLRO:

$$
\lim_{|r_i - r'_j| \to \infty} F_s(r_1, \ldots, r_s|r'_1, \ldots, r'_s)|_B = F_s(\infty) = [F_s(\infty)]^s = \text{const} > 0,
$$

(22)

where $B$: $|r_i - r_j|$, $|r'_i - r'_j|$ are fixed for any $i, j = 1, \ldots, s$, $i \neq j$.

From the general principles, we write the probability $W_{k_1, k_2}$ of finding the momenta $k_1$ and $k_2$ in two arbitrary atoms, for $T = 0$:

$$
W_{k_1, k_2} = \frac{1}{V^2} \int dr_3 \ldots dr_N \left| \int \Psi_0(r_1, \ldots, r_N)e^{ik_1r_1 + ik_2r_2}dr_1dr_2 \right|^2 =
$$

$$
= \frac{1}{V^4} \int F_2(r_1, r_2|r'_1, r'_2)e^{ik_1(r_1 - r'_1) + ik_2(r_2 - r'_2)}dr_1dr_2dr'_1dr'_2,
$$

(23)

where $F_2$ is the two-particle density matrix.

To obtain the amount of 2PC, we should know $W_{k, -k}$ for $T = 0$. Let us consider first the 1S-approximation for $\Psi_0$ and $F_2$. In this approximation, $\Psi_0$ is defined by (3), and $F_s = F_s^{(1)}$ was found in [17]:

$$
F_s^{(1)}(r_1, \ldots, r_s|r'_1, \ldots, r'_s) = \exp \left\{ \sum_{k \neq 0} \left[ \frac{f_1(k)}{2} (|\xi_k|^2 + |\xi'_k|^2) - \frac{s}{N} \frac{a_2(k)}{1 - 2a_2(k)} \right] + f_2(k)\xi_k\xi'_k \right\},
$$

(24)

where

$$
f_1(k) = a_2(k) + f_2(k), \quad f_2(k) = \frac{a_2^2(k)}{1 - 2a_2(k)},
$$

(25)

$$
\xi_k = \frac{1}{\sqrt{N}} \sum_{j=1}^s e^{-ikr_j}, \quad \xi'_k = \frac{1}{\sqrt{N}} \sum_{j=1}^s e^{-ikr'_j}.
$$

(26)

It is convenient to represent $F_s^{(1)}$ in the form

$$
\ln F_2^{(1)} = \ln F_2(\infty) + \varphi_1(r_1 - r_2) + \varphi_1(r'_1 - r'_2) + \varphi_2(r'_1 - r_1) + \varphi_2(r'_2 - r_2) + \varphi_2(r'_2 - r_1) + \varphi_2(r'_1 - r_2),
$$

(27)

$$
\varphi_i(r) = \frac{1}{N} \sum_{q \neq 0} f_i(q)e^{-iqr}.
$$

(28)

The functions $\varphi_i$ have the property $\varphi_i(r \to \infty) \sim \frac{1}{r} \to 0$. From (23), we obtain

$$
W_{k, -k} = \frac{F_2(\infty)}{V^4} \int dr_1dr_2dr'_1dr'_2 e^{ik(r_1 - r'_1) - ik(r_2 - r'_2)} \exp \left[ \varphi_1(r_1 - r_2) + \varphi_1(r'_1 - r'_2) + \varphi_2(r'_1 - r_1) + \varphi_2(r'_2 - r_2) + \varphi_2(r'_2 - r_1) + \varphi_2(r'_1 - r_2) \right].
$$

(29)
To calculate $W_{k, -k}$ (29), we expand the exponent in (29), with the sum of all $\varphi_i$, in a power series. It can be shown, that only integrals of terms of the form

$$
\varphi_i^l(r_1 - r_2) \varphi_i^2(r'_1 - r'_2) \quad \text{and} \quad \varphi_i^l(r'_1 - r_1) \varphi_i^2(r'_2 - r_2)
$$

(\(l = 1, 2, 3, \ldots\) are all possible natural numbers) are significant for the value of $W_{k, -k}$. The integrals of other sets of $\varphi_i$ are $N$ times smaller or equal to zero. Taking all this into account, we obtain

$$
W_{k, -k} = \frac{F_2(\infty)}{N^2} \left[ \Phi_1^2(k) + \Phi_2^2(k) \right], \quad k \neq 0,
$$

(30)

$$
\Phi_i(k) = \frac{N}{V} \int e^{\varphi_i(r)} e^{ikR} dR, \quad F_2(\infty) = F_1^2(\infty).
$$

(31)

(32)

Following the notation of [6], we rewrite $W_{k, -k}$ (31) in the form

$$
N^2W_{k, -k} = N_k N_{-k} + \chi_k \chi_{-k}, \quad k \neq 0,
$$

(33)

where

$$
N_k = F_1(\infty)\Phi_2(k), \quad \chi_k = F_1(\infty)\Phi_1(k).
$$

(34)

Here, $N_k$ is the amount of atoms with momentum $k$. For $k = 0$, we have $\varphi_2(r) \to 0$ as $r \to \infty$, and $\Phi_2(0) = N$; therefore, $N_{k=0} = NF_1(\infty)$, and we obtain the one-particle condensate $N_1 \equiv N_{k=0}$. In (31) and (34), $F_2(\infty) = F_1^2(\infty)$, and $F_1(\infty)$ correspond to the 1S-approximation: $N_k \equiv F_1(\infty) = e^{F_1}$, see (10), (11).

As it can be seen from (33), $W_{k, -k}$ consists of two terms: the first one, $\frac{N_k^2}{N^2}$, is simply the product of relative numbers of atoms with momenta $k$ and $-k$, this term does not describe correlations. The second term, $\frac{\chi_k^2}{N^2}$, describes correlations in $k$-space in the pairs ($k$, $-k$). It is naturally to relate the two-particle condensate precisely with the correlation term $\frac{\chi_k^2}{N^2}$.

The 2PC was already calculated by Ristig [6] using a different method. In Ristig’s works [6], the 2PC was determined by the quantity

$$
P_2 = \sum_{k \neq 0} \frac{\chi_k^2}{\sum_{k \neq 0} (\chi_k^2 + N_k^2)}.
$$

(35)

The expression $P_2$ can be interpreted as the mean degree of correlation of the pairs of atoms with momenta $k_1 + k_2 = 0$, $k_i \neq 0$. We believe that it is more reasonable to define the number of atoms in 2PC as follows:

$$
N_2 = \sum_{k \neq 0} N_k c_k,
$$

(36)

where $c_k$ is the “correlation factor”,

$$
c_k = \begin{cases}
\frac{|\chi_k|}{N_k} & \text{for } |\chi_k| < N_k, \\
1 & \text{for } |\chi_k| \geq N_k.
\end{cases}
$$

(37)

Using $a_2(k)$ in (19), from (25)–(34) we obtain the functions $\chi_k$ and $N_k$ (see Fig. 1); then from (35)–(37) we find $N_2 \approx 0.53N$ and $P_2 \approx 0.31$. In [6], using the Jastrow approximation [11] for $\Psi_0$ [as in our work [3]], it was found $P_2 \approx 0.09$, but, for $S_1(r)$ in [11]. Ristig applied [6] the popular McMillan’s form

$$
S_1(r) = -\frac{r_0^5}{4r^5}, \quad r_0 = 2.963 \, \text{Å}.
$$

(38)

This form is simple and is convenient for calculation but, at the same time, it is a very crude variational
approximation. Using the CV-method, we find $S(k)$ without any free parameters. Equation (7) was deduced \cite{18, 19} from the equation

\begin{equation}
S(k) = 1 + \frac{N}{V} \int d\mathbf{r} (g(r) - 1)e^{-ikr},
\end{equation}

connecting $S(k)$ with the pair distribution function $g(r)$. Equation (7) was derived in the approximation neglecting $a_{n \geq 4}$ in (1) and neglecting multiple scattering in (39) \cite{43}. As shown in Fig. 2, our result $S_1(r)$ differs greatly from (38); therefore, our result for $P_2$ differs from that obtained in \cite{6} although the formulas for $\chi_k$ \cite[see (45)]{50} and $P_2$ are the same in our work and in \cite{6}. Note that $S_1(r \to \infty) \sim \frac{1}{r^2}$ since $a_2(k \to 0) \sim \frac{1}{k^2}$, see (7).

It should also be noted that we found the function $S_1(r)$ not quite precisely at $r \lesssim d_c \approx 2 \AA$ (at such $r$, two atoms penetrate each other). This is evident from the fact that the function $g(r)$ recovered from Eq. (39) oscillates irregularly at $r \lesssim 1.7 \AA$ (see Fig. 3) and is different from that expected from physical considerations: $g(r) \to 0$ at $r \lesssim d_c$, and $g(r) > 0$. Inaccuracy of the determination of $g(r)$ and $S_1(r)$ at $r \lesssim d_c$ is caused by large relative error of measurement of the value $S(k) - 1$ at $k \approx 2\pi/d_c \approx 3 \AA^{-1}$, probably by neglecting multiple scattering in (39) \cite{43}, and by truncation of expansion (11) [for $S_1(r)$].

Oscillations of $g(r)$ at small $r$ arise mainly \cite{36} from the inaccuracy of measurement of $S(k)$ at large $k$, $k \gtrsim 2\pi/d_c$. Although the values of $S(k)$ are very close to unity at such $k$, $S(k) \approx 1$, the values of $g(r)$ are sensitive to the small oscillations of $S(k)$ in the neighborhood of the unity. At the same time, such a small indefiniteness of $S(k)$ at large $k$ influences insignificantly the amounts of the condensates and quasiparticle spectrum \cite{32}. According to our numerical analysis, the amount of the condensates are sensitive, first of all, to the value of $S(k)$ at the small and middle $k$, $k \lesssim 2\pi/d \approx 1.7 \AA^{-1}$ (where $d = 3.58\AA$ is the mean distance between helium atoms), which corresponds to $r \gtrsim d$ ($g(r)$ is well defined at such $r$). In fact, the condensates are “spread out” in the whole system, so the values of $g(r)$ at large $r$, $r \gtrsim d$, are important for the estimates of the amount of condensates. Moreover, the oscillations of $g(r)$ at small $r$ may be related to the problem of realistic description of the structure of

Fig. 1. The functions $N_k$ and $\chi_k$, where $k$ is in the units of $k_d = 2\pi/d = 1.756\AA^{-1}$. Open circles mark $N_k$ in the 1S-approximation; triangles mark $N_k$ in the 2S-approximation; crosses mark $\chi_k$ in the 1S-approximation; squares mark $\chi_k$ in the 2S-approximation.

Fig. 2. The function $S_1(r/a)$ \cite{50}, where $a = 2.64\AA$ is the diameter \cite{12} of a He$^3$ atom. Open circles correspond to the 1S-approximation for $a_2(k)$; crosses to the 2S-approximation for $a_2(k)$; triangles to the “three sums” approximation for $a_2(k)$ in the approach of \cite{35} with a model elliptical potential with $U(r = 0) = 60 K$; continuous line shows the McMillan’s form \cite{45}.
helium atoms.

Correlations in the pairs \((0, 0)\) are absent [19]; therefore, only atoms with \(k > 0\) belong to the two-particle condensate \((k, -k)\).

In the more exact 2S-approximation, the two-particle condensate is calculated similarly (see [19] for more details). The function \(W_{k,-k}\) is again defined by (31)–(34) with \(\varphi_i\) given by (28), where \(F_i(\infty)\) now correspond to the 2S-approximation [see (10)–(14) for \(\frac{N}{N_1} \equiv F_1(\infty)\)], and we derive more exact formulas for \(f_1(k)\) and \(f_2(k)\):

\[
f_1(k) = a_2(k) + f_2(k) + \delta_1(k),
\]

\[
\delta_1(k) = \frac{1}{N} \sum_{q \neq 0} \frac{a_3(k, q)}{1 - 2a_2(k + q)},
\]

\[
f_2(k) = \frac{a_2^2(k)}{1 - 2a_2(k)} + \delta_2(k) + \delta_3(k),
\]

\[
\delta_2(k_1) = \frac{1}{N} \frac{1}{1 - 2a_2(k_1)} \sum_{k_2 \neq 0} \prod_{j=1}^{3} \frac{a_2(k_j)}{1 - 2a_2(k_j)},
\]

\[
\delta_3(k_1) = \frac{1}{N} \sum_{k_2 \neq 0} \left( \prod_{j=1}^{3} \frac{1}{1 - 2a_2(k_j)} \right) a_3(k_1, k_2)
\]

\[
\times \left[ a_2(k_1) + a_3(k_1, k_2) \left( 1 - a_2(k_2) \right) \right] + a_2(k_1) \left( 1 - 2a_2(k_2) \right) + a_2(k_2) a_2(k_1 + k_2)
\].

The function \(\chi_k\) in the 2S-approximation can be presented in the form

\[
\chi_k = \frac{N}{V} \int dr e^{2S_1(r) + S_2^*(r)} F_1(r) e^{ikr}, \quad k \neq 0,
\]

where \(F_1(r) = \frac{N}{N_1} e^{\varphi_2(r)}\) (this is the one-particle density matrix in the 2S-approximation, see Fig. 4), \(S_1(r)\) is defined according to (5), and

\[
S_2^*(r) = \frac{1}{N} \sum_{k \neq 0} \delta_1(k) e^{ikr},
\]
For the 1S-approximation, we have \( \delta_1(k) \equiv 0, S_2^*(r) = 0 \), and \( F_1(r) = F_1^{(1)}(r) \), so that (45) coincides with the Ristig’s formula for \( \chi_k \) derived earlier [6] (to an accuracy of the factor \( N/V \) appearing as a result of different normalization of \( F_1 \); we also choose the opposite sign for \( \chi_k \)). Formula (45) was not obtained previously.

Using \( a_0(k_1, k_2) \) given by (6), and \( a_2(k) \) as a solution of (7), we find the two-particle condensate according to (44)–(45), (40)–(45): \( N_2 \approx 0.16N, P_2 \approx 0.025 \). The obtained functions \( \chi_k \) and \( N_k \) are shown in Fig. 1.

Note that, in the 2S-approximation, we have, taking into account (13), \( N_{k-0} = \frac{N}{N} \frac{a_2(k)}{2} = \frac{N}{N} \frac{mc}{2 \hbar k} (1 + \Sigma_1(0)) \), \( \chi_{k-0} = -N_{k-0} \). Such an asymptotics for \( N_k \) refines the one found earlier in [44, 45], \( N_{k-0} = \frac{N}{N} \frac{mc}{2 \hbar k} \).

In Fig. 5, we show the function

\[
\chi(r) = \frac{1}{2(2\pi)^3} \int d\mathbf{k} e^{-i\mathbf{k}\mathbf{r}} \chi_k = \frac{N}{V} e^{2S_1(r) + S_2(r)} F_1(r) = \frac{N}{V} e^{\varphi_1(r)}. \tag{47}
\]

The function \( g(r) \) describes the dependence of the correlations in the pairs of two atoms with arbitrary momenta, \( (k_1, k_2) \), on the size of the pair \( r \); and \( \chi(r) \) describes the same for a narrower class of pairs \( (k, -k) \). For infinite separation between the atoms in the pair, correlations disappear; therefore, \( g(\infty) \) and \( \chi(\infty) \) take the values of \( g \) and \( \chi \) for uncorrelated pairs [for a totally chaotic distribution of atoms in the \( \mathbf{r} \)-space, we would have \( g(r) \equiv g(\infty) \) for all \( r \), and similarly for \( \chi(r) \)].

Comparing the functions \( g(r) \) (Fig. 3) and \( \chi(r) \) (Fig. 5), we can see that these functions have similar form, as it could be expected. Atoms interact strongly at a small distance, so the correlations in the pairs are significant at \( r \lesssim 2d \), where the values of \( g(r) \) and \( \chi(r) \) are substantially different from those at infinity.

The authors of [21, 10] believe to warrant the investigations of the possible pairing of He-II atoms in the \( \mathbf{r} \)-space. However, in our opinion, the properties of \( \chi(r) \) and the results of [21] do not
give grounds to talk about the bound states in the \( r \)-space; these properties are indicative only of correlations in pairs. The pairing energy \( E_p \approx -0.05 \) K was found in [21], but this energy is too small for the appearance of real bound pairs because \( E_p \) is two orders of magnitude smaller than the ground-state energy \( E_0 \).

At present, we are not aware of any reliable evidence of the existence of bound pairs of atoms in \( \text{He-II} \). An interesting arguments in favour of the possibility of pairing were presented in [10]. Our analysis cannot exclude the possibility of existence of narrow bound pairs, of atomic size. Electrons should be collectivized in narrow pairs; therefore, such pairs have to be considered as a new kind of “atoms”; in this case, we need to know \( \Psi_0 \) for a mixture of two Bose liquids. However, the closeness of the experimental value of circulation [40] to the value of one quantum, \( \kappa = \hbar/m \), indicates that the number of bound pairs in He-II is very small or equal to zero.

5 The higher condensates

We also investigated correlations (in the \( k \)-space) in groups of \( s \) atoms (\( s \geq 3 \)) under the condition \( k_1 + \ldots + k_s = 0 \) for momenta \( k_i \) of atoms. We were interested in the “nontrivial” part of the \( s \)-particle condensate, which cannot be reduced to the “lower” condensates; so we put \( k_1 + \ldots + k_l \neq 0 \) for all \( l = 1, \ldots, s - 1 \). There is a wide-spread, but not proved, opinion according to which the higher condensates should be present in He-II. We considered the problem in the 2S-approximation, for which the three-particle term with \( a_3 \) is taken into account in ln \( \Psi_0 \), and we expected that at least three-particle condensate would turn out to be nonzero. However, we found [19] that all higher \( s \)-particle condensates (\( s \geq 3 \)) are absent from He-II at \( T = 0 \). An analysis is cumbersome and similar to that for 2PC, see [19] for more detail.

Our results, which consist in the absence of all higher \( s \)-particle condensates (\( s \geq 3 \)) and in the small value of two-particle condensate, should be important for the field-theoretic model of He-II: they can significantly simplify such model and, perhaps, open a possibility of constructing an “ideal” micro-model of He-II.

6 Conclusions

The main results of our paper were already outlined in the introduction. Summarizing, we notice that the CV-method allows one to calculate the quasiparticle spectrum of He-II [11, 32, 33] and also, with lower accuracy, condensates (this work), without any fitting parameters or functions. The equations of the model are deduced from the exact microscopic equations, and the results approximately agree with the experiment. Thus, the model under consideration, undoubtedly, gives an approximate description of the microstructure of He-II.

- However, the calculated amount of one- and two-particle condensates appreciably depends on the number of the corrections \( a_n \) taken into account in ln \( \Psi_0 \). The reason is that the quantity ln \( \Psi_0 \) and the condensates \( N_i \) are expanded in series in a parameter which is not very small (this is the function \( q(k) = a_2(k)k/k_d, k_d = 2\pi/d \), where \( d \) is the mean distance between atoms; the mean value of \( q(k) \) at \( k < k_d \) is not very small, being around \(-1/2\), see Fig. 1 in [19]) and, for condensates, the series stand in the exponent. These difficulties arise in all approaches where condensates are calculated from \( \Psi_0 \), unless the free parameters are chosen so that the corrections “turn out” to be small.

- If, in some quantum mechanical approach, the amount of the condensate changes insignificantly by taking into account the next corrections to ln \( \Psi_0 \) and the condensates, this is, probably, mainly a result of a good choose of fitting parameters. Really, in our model we find a solution from the exact (but truncated) microscopic equations, without free parameters whatsoever, and we clearly see that the corrections to ln \( \Psi_0 \) and especially to the values of the condensates are not small enough, unfortunately. Nevertheless, our results give the approximate estimates of the fraction of the condensates (the amount
of 1PC agrees with the experiment) and, at the same time, the significant value of the corrections show that quantum-mechanical approaches (except, perhaps, the MC methods) do not offer methods for sufficiently precise calculation of the amount of the condensates.

The Monte Carlo method \[23, 24\] is one of the perspective approaches for the calculation of the 1PC and 2PC but, unfortunately, we do not know the error of the numerical definition of 1PC and 2PC for the MC simulations.

The absence of small parameter is a general problem of virtually all (except the MC simulations) known approaches to the description of the microstructure of He-II. Perhaps, in some approaches, in the future, one will succeed in calculating the 1PC, 2PC and higher condensates more exactly, using expansions in small parameters only and without fitting parameters and unjustified postulates. Unfortunately, by now, such an “ideal” micromodel of He-II is not constructed. And it is not clear even, whether it is possible.

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