

CALCULATION OF THE He-II QUASIPARTICLE SPECTRUM WITHIN THE METHOD OF COLLECTIVE VARIABLES

M.D. TOMCHENKO

UDC 538.941
© 2005M.M. Bogolyubov Institute for Theoretical Physics, Nat. Acad. Sci. of Ukraine
(14b, Metrolohichna Str., Kyiv 03143, Ukraine; e-mail: mtomchenko@bitp.kiev.ua)

Using the method of collective variables (MCV), we calculate the logarithm of the ground-state wave function of He-II, $\ln \Psi_0$, to an accuracy of the first correction to the Jastrow function, and also we calculate the wave function $\Psi_{\mathbf{k}}$ of the first excited state and the quasiparticle spectrum of He-II, in the second-order approximation. The functions Ψ_0 and $\Psi_{\mathbf{k}}$ were found as the eigenfunctions of the N -particle Schrödinger equation, and the function Ψ_0 was connected to the structure factor of He-II, using the Vakarchuk equation. The model does not contain any fitting parameter or function. The quasiparticle spectrum calculated numerically agrees well with the experiment. Our solution improves the result obtained early by Yukhnovskiy and Vakarchuk.

1. Introduction

The structures of the N -particle wave functions of the ground and weakly excited states of helium-II are known in the main [1–12], and the solutions which take into account several first corrections have been obtained. In our opinion, the main unresolved problems concerning the microscopic physics of He-II are the structure of a composed condensate, nature of the λ -transition, and role of microscopic vortex rings.

The form of the He-II quasiparticle spectrum has been forecasted by Landau for the first time [12]. In Feynman's known works [1–3], an opportunity to determine this spectrum making use of the structure factor has been demonstrated. Feynman intuitively found the structure of the $\Psi_{\mathbf{k}}$ wave function for the state of He-II with a single phonon and approximately deduced the He-II quasiparticle spectrum. According to Feynman and Cohen,

$$\Psi_{\mathbf{k}}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \psi_{\mathbf{k}}(\mathbf{r}_1, \dots, \mathbf{r}_N) \Psi_0(\mathbf{r}_1, \dots, \mathbf{r}_N), \quad (1)$$

$$\psi_{\mathbf{k}} = \rho_{-\mathbf{k}} + \sum_{\mathbf{k}_1}^{\mathbf{k}_1 \neq 0, \mathbf{k}} A \frac{\mathbf{k}_1 \mathbf{k}}{k_1^2} \rho_{\mathbf{k}_1 - \mathbf{k}} \rho_{-\mathbf{k}_1}, \quad (2)$$

where Ψ_0 is the wave function of the ground state,

$$\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{k}\mathbf{r}_j} \quad (\mathbf{k} \neq 0) \quad (3)$$

are collective variables [13], and N is the total number of He atoms. However, it has not been shown in Feynman's works that function (2) is an eigenfunction of the N -particle Schrödinger equation. Feynman's ideas have been developed in a great number of works (see, e.g., [14–20]). The Feynman–Cohen function has been specified in works [5], where the analysis of the total Hamiltonian of the system has been carried out. A more accurate form of the function $\psi_{\mathbf{k}}$ and the structure of the function Ψ_0 have been found in works [6–11], where Ψ_0 and $\psi_{\mathbf{k}}$ were sought as eigenfunctions of the Schrödinger equation.

The idea of the MCV has been proposed in work [13]. This method has been substantiated and developed in works [7–10, 21, 22]. In work [11], taking advantage of the MCV, the Ψ_0 and $\Psi_{\mathbf{k}}$ functions of helium-II have been calculated making use of the model potential of interaction between He⁴ atoms with one fitting parameter. Nevertheless, as was indicated in [9–11], the derivation of the Ψ_0 and $\Psi_{\mathbf{k}}$ wave functions and the He-II quasiparticle spectrum by starting from the He-II structure factor known from the experiment, rather than from a model potential, has significant advantages. In this case, the problem does not contain fitting parameters, and one can avoid the task of the description of atomic interaction at small distances, which arises because of atoms' extension [9–11].

Just this approach has been considered in work [8], where $\ln \Psi_0$ was found in the zero-order approximation, while $\psi_{\mathbf{k}}$ and the He-II quasiparticle spectrum in the first-order one. The obtained spectrum $E(k)$ agreed well with the experiment. In this work, we calculated Ψ_0 , $\psi_{\mathbf{k}}$, and $E(k)$ more accurately. Namely, we found the first correction to $\ln \Psi_0$ and the second ones to $\psi_{\mathbf{k}}$ and $E(k)$. In doing so, we used the equation for Ψ_0 derived in work [22] (below, we name it as the Vakarchuk equation).

Actually, the expansion parameter of the problem was the function $2\sigma(k)k/k_0$ (see Fig. 1), the average value of which within the interval $k = 0 \div k_0$ was about $-1/2$; i.e. the parameter is not small. Therefore, the corrections to $\ln \Psi_0$ and $E(k)$ were not, generally speaking, small, and their calculation was of interest.

2. The Ground State of Helium-II

A more detailed analysis of the equations and the method of determining Ψ_0 were exposed in works [9–11]. The necessary equations for Ψ_0 and $\psi_{\mathbf{k}}$ were found by Yukhnovskiy and Vakarchuk [8–10, 21]. We use different notations and different forms of the equations for Ψ_0 and $\psi_{\mathbf{k}}$ [11] (the latter is partially caused by our desire to reduce the error of the numerical solution of the equations [11]).

The wave function of the ground state of He-II is sought in the form [11, 13]

$$\Psi_0 = e^{S_0}, \quad (4)$$

$$S_0 = \sum_{\mathbf{k} \neq 0} \sigma(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}} + \sum_{\substack{\mathbf{k}_1 + \mathbf{k}_2 \neq 0 \\ \mathbf{k}_1, \mathbf{k}_2 \neq 0}} \frac{f(\mathbf{k}_1, \mathbf{k}_2)}{\sqrt{N}} \rho_{\mathbf{k}_1 + \mathbf{k}_2} \rho_{-\mathbf{k}_1} \rho_{-\mathbf{k}_2}. \quad (5)$$

The corrections of higher orders to S_0 [Eq. (5)] are neglected. In this approximation, the relation

$$f(\mathbf{k}_1, \mathbf{k}_2) = -\frac{2\sigma(k_1)2\sigma(k_2)\mathbf{k}_1\mathbf{k}_2}{e(\mathbf{k}_1 + \mathbf{k}_2) + e(k_1) + e(k_2)}, \quad (6)$$

where

$$e(\mathbf{k}) = k^2(1 - 4\sigma(k)), \quad (7)$$

is valid [11]. In works [21, 22], an equation that connects Ψ_0 [Eqs. (4) and (5)] with the He-II structure factor $S(k)$ was derived. We write down this equation in approximation (5) for Ψ_0 by using the notations of work [11] as follows:

$$4\sigma(q) = 1 - \frac{1}{S(q)} - \Sigma(q), \quad (8)$$

$$\Sigma(q) = \frac{1}{N} \sum_{\mathbf{k} \neq 0} \frac{8\sigma(k)\sigma(\mathbf{k} + \mathbf{q}) + R(\mathbf{k}, \mathbf{q})}{[1 - 4\sigma(k)][1 - 4\sigma(\mathbf{k} + \mathbf{q})]}, \quad (9)$$

where

$$R(\mathbf{k}, \mathbf{q}) = 4f_s(\mathbf{k}, \mathbf{q}) [1 + 2f_s(\mathbf{k}, \mathbf{q})], \quad (10)$$

$$f_s(\mathbf{k}, \mathbf{q}) = f(\mathbf{k}, \mathbf{q}) + f(-\mathbf{k} - \mathbf{q}, \mathbf{q}) + f(-\mathbf{k} - \mathbf{q}, \mathbf{q}). \quad (11)$$

Equations (8) and (9) were derived in work [21] from the known equation which connects $S(k)$ with the binary distribution function $F_2(r)$:

$$S(k) = 1 + n \int (F_2(r) - 1) e^{-i\mathbf{k}\mathbf{r}} d\mathbf{r}, \quad (12)$$

where n is the concentration of helium atoms.

We note that the interaction between He^4 atoms does not present explicitly in Eqs. (8) and (9), and Ψ_0 is connected with the He-II structure factor only. Therefore, such a way of finding Ψ_0 allows one to partially avoid the description of this interaction at small distances [9, 11]: upon a strong overlapping of He^4 atoms, the description of the atomic interaction using a potential becomes inaccurate, because the atomic structure becomes important under such conditions, and it is necessary, generally speaking, to solve the quantum-mechanical problem of the interaction of two nuclei and four electrons. The function Ψ_0 [Eqs. (4) and (5)] found from Eqs. (6)–(11) takes short-range correlations into account more correctly than that found from a model potential [11]. For a quite correct account of the atomic structure, one should determine the function Ψ_0 for a system of nuclei and electrons, rather than for N structureless particles. It is a hopeless task. Nevertheless, as one can see below, configurations with the overlapping of atoms are very improbable. So, from the physical point of view, it is quite reasonable to consider atoms as structureless particles.

A single shortcoming made in the course of the derivation of Ψ_0 from Eqs. (4)–(11) was the truncation of series (5). But, since the model contains no fitting parameters, the accuracy of approximation (5) can be estimated by comparing both the theoretical spectrum of He-II quasiparticles and the theoretical interaction potential between He^4 atoms with experimental ones.

In order to find the wave function of the ground state, one has to know $S(k)$ at the temperature $T = 0$ K. As far as we know, the most exact measurements of $S(k)$ were carried out in work [23]. We used the smoothed data on $S(k)$ obtained at $T = 1$ K in [23] and calculated the dependences $S(k, T = 0)$ by the formula [24]

$$S(k, T = 0) = S(k, T) \tanh \frac{E(k)}{2k_B T}. \quad (13)$$

At $k \leq 0.2 \text{ \AA}^{-1}$, we supposed that $S(k, T = 0) \sim k$ (because $S(k = 0, T = 0) = 0$ [25] and $E(k \rightarrow 0) = ck$ in Eq. (13)). In works [8, 22], the integral equations (8) and (9) were not solved and the zero-order approximation

$$4\sigma(q) = 1 - \frac{1}{S(q)} \quad (14)$$

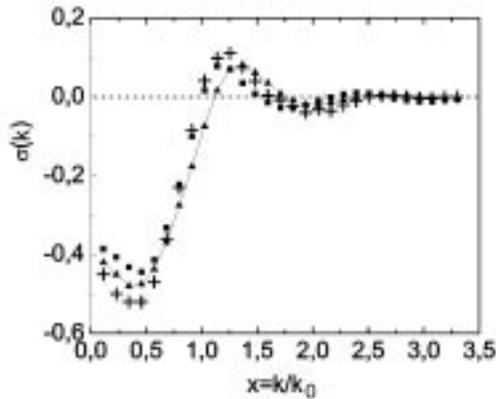


Fig. 1. Dependence of the quantity $\sigma(k)$ on k , k being in units of $k_0 = 2\pi/d = 1.756 \text{ \AA}^{-1}$ and d is the average distance between He-II atoms. Squares mark the zero-order approximation [Eq. (14)] for $\sigma(k)$, pluses the first-order approximation, and triangles the second-order approximation calculated from a model “elliptic” potential with $U(0) = 60 \text{ K}$ [11]

was used to determine Ψ_0 .

Below, Eqs. (6)–(11) will be solved numerically, and the solution $\sigma(k)$, which includes a first correction to the zero-order approximation (14), will be obtained. Therefore, we call this solution as the first approximation to $\sigma(k)$. The solution of the integral equation (8) cannot be found by the iteration method, so that we used the Newton one [26] for this purpose. As a result, two solutions were obtained, one of which, with a smaller energy per atom $E_0 = -1.4 \text{ K}$ ($E_0 = 0.1 \text{ K}$ in the zero-order approximation and -7.16 K in the experiment), being taken as the ground state. This solution for $\sigma(k)$ is shown in Fig. 1.

A significant body of information concerning the properties of Ψ_0 is included into the function

$$S_1(r) = \frac{1}{N} \sum_{\mathbf{k}} \sigma(k) e^{i\mathbf{k}r}, \quad (15)$$

where

$$\sum_{\mathbf{k} \neq 0} \sigma(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}} = \sum_{i,j} S_1(\mathbf{r}_i - \mathbf{r}_j). \quad (16)$$

The behavior of $S_1(r)$ at $r \rightarrow 0$ shows how quickly the function Ψ_0 decays if the atoms overlap. Fig. 2 represents the function $S_1(r)$ for the zero-order (14) and first-order approximations for $\sigma(k)$ and for $\sigma(k)$ found in the second-order approximation starting from a model potential [11]. One can see that $S_1(0) \approx -1.7$ in all those cases. One can separate a two-particle term of the form $\sum_{\mathbf{k} \neq 0} \tilde{\sigma}(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}}$ from the second term on the r.h.s. of (5),

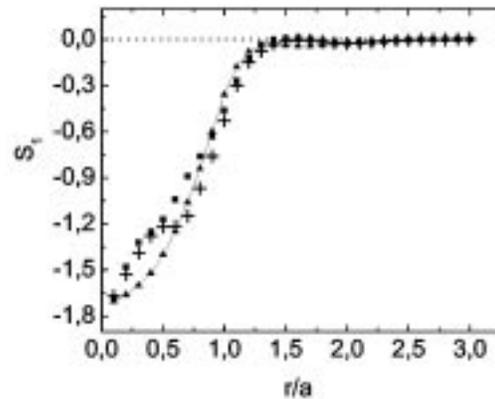


Fig. 2. Function $S_1(r/a)$ [Eq. (15)], where $a = 2.64 \text{ \AA}$ is the “diameter” [32] of a He^4 atom. The notations correspond to the same approximations for $\sigma(k)$ as in Fig. 1

see [11]. But a calculation shows that the account of $\tilde{\sigma}(k)$ renormalizes $S_1(r)$ very slightly, by a few percents only. Thus, provided that two He^4 atoms overlap, the wave function of the ground state diminishes by a factor of $e^{3.4} \approx 30$, so that a sharp reduction does not occur, although the probability density $|\Psi_0|^2$ decreases rather strongly, by a factor of 1000. This means that the He^4 atom possesses properties which are intermediate between “soft”- and “hard”-core ones. In the case, for example, where 10 pairs of atoms overlap, Ψ_0 decreases by a factor of $e^{34} \sim 10^{14}$ as compared to its value for a uniform distribution of atoms without overlapping. Therefore, configurations where many atoms overlap are extremely improbable.

3. Calculation of the He-II Quasiparticle Spectrum

Knowing Ψ_0 , one can find the wave function $\Psi_{\mathbf{k}} = \psi_{\mathbf{k}} \Psi_0$, which describes the state of the system with a single quasiparticle of the phonon type, and the quasiparticle spectrum $E(k)$ from the following equations [11]:

$$\begin{aligned} \psi_{\mathbf{k}} = & \rho_{-\mathbf{k}} + \sum_{\mathbf{k}_1}^{\mathbf{k}_1 \neq 0, \mathbf{k}} \frac{P(\mathbf{k}, \mathbf{k}_1)}{\sqrt{N}} \rho_{\mathbf{k}_1 - \mathbf{k}} \rho_{-\mathbf{k}_1} + \\ & + \sum_{\mathbf{k}_1, \mathbf{k}_2 \neq 0}^{\mathbf{k}_1 + \mathbf{k}_2 \neq \mathbf{k}} \frac{Q(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2)}{N} \rho_{\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}} \rho_{-\mathbf{k}_1} \rho_{-\mathbf{k}_2} + \dots \end{aligned} \quad (17)$$

$$\begin{aligned} \tilde{E}(k) &= e(k) + \int d\mathbf{k}_1 P(\mathbf{k}, \mathbf{k}_1) 2\mathbf{k}_1(\mathbf{k} - \mathbf{k}_1) + \\ &+ \int d\mathbf{k}_1 (-2k_1^2) [Q(\mathbf{k}, \mathbf{k}_1, -\mathbf{k}_1) + 2Q(\mathbf{k}, \mathbf{k}, \mathbf{k}_1)], \end{aligned} \quad (18)$$

$$\begin{aligned} P(\mathbf{k}, \mathbf{k}_1) & \left[e(k_1) + e(\mathbf{k} - \mathbf{k}_1) - \tilde{E}(k) \right] + \\ & + \int d\mathbf{k}_2 F(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2) = 4\sigma(k_1)\mathbf{k}\mathbf{k}_1 + 2k^2 f_s(\mathbf{k}_1, \mathbf{k} - \mathbf{k}_1), \end{aligned} \quad (19)$$

$$\begin{aligned} F(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2) &= 4\mathbf{k}_2(\mathbf{k} - \mathbf{k}_1 - \mathbf{k}_2)Q(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2) + \\ &+ 2\mathbf{k}_2(\mathbf{k}_1 - \mathbf{k}_2)Q(\mathbf{k}, \mathbf{k}_1 - \mathbf{k}_2, \mathbf{k}_2), \end{aligned} \quad (20)$$

$$\begin{aligned} Q(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2) & \left[e(k_1) + e(k_2) + e(\mathbf{k} - \mathbf{k}_1 - \mathbf{k}_2) - \tilde{E}(k) \right] = \\ &= P_s(\mathbf{k}, \mathbf{k}_1 + \mathbf{k}_2) * G(\mathbf{k}_1, \mathbf{k}_2) + L(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2), \end{aligned} \quad (21)$$

$$P_s(\mathbf{k}_1, \mathbf{k}_2) = P(\mathbf{k}_1, \mathbf{k}_2) + P(\mathbf{k}_1, \mathbf{k}_1 - \mathbf{k}_2), \quad (22)$$

$$\begin{aligned} G(\mathbf{k}_1, \mathbf{k}_2) &= [2\sigma(k_1)\mathbf{k}_1 + 2\sigma(k_2)\mathbf{k}_2] (\mathbf{k}_1 + \mathbf{k}_2) + \\ &+ 2(\mathbf{k}_1 + \mathbf{k}_2)^2 f_s(\mathbf{k}_1, \mathbf{k}_2), \end{aligned} \quad (23)$$

$$L(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2) = 2\mathbf{k}(\mathbf{k}_1 + \mathbf{k}_2) f_s(\mathbf{k}_1, \mathbf{k}_2). \quad (24)$$

In (17), the corrections of higher orders to $\psi_{\mathbf{k}}$ are neglected. In Eqs. (18)–(24), we passed to the dimensionless variables $k' = k/k_0$ and $\tilde{E}(k') = \frac{E(k)2m}{\hbar^2 k_0^2}$, where $k_0 = 2\pi/d$ and $d = 3.578 \text{ \AA}$ is the average interatomic distance. The primes will be omitted below.

The quasiparticle spectrum calculated using Ψ_0 and $\psi_{\mathbf{k}}$ in the zero-order approximation (i.e. $f(\mathbf{k}_1, \mathbf{k}_2) = 0$, Eq. (14), and $\psi_{\mathbf{k}} = \rho_{-\mathbf{k}}$) has the form of Feynman's known formula [1] which describes the spectrum of a slightly nonideal Bose gas [13],

$$E(k) = \frac{\hbar^2 k^2}{2mS(k)}. \quad (25)$$

This spectrum is represented by pluses in Fig. 3.

To find $\psi_{\mathbf{k}}$ in the first approximation, we should assume that $Q(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2) = 0$. From Eq. (19), we have

$$P(\mathbf{k}, \mathbf{k}_1) = \frac{4\sigma(k_1)\mathbf{k}\mathbf{k}_1 + 2k^2 f_s(\mathbf{k}_1, \mathbf{k} - \mathbf{k}_1)}{e(k_1) + e(\mathbf{k} - \mathbf{k}_1) - \tilde{E}(k)}. \quad (26)$$

The system of equations (18) and (26) was solved by the iteration method. The obtained quasiparticle spectrum, for $\sigma(k)$ in the zero-order approximation, is shown in Fig. 3. The spectrum of He-II in the indicated approximations has been found earlier in work [8].

We note that the relation $P(\mathbf{k}, \mathbf{k}_1) \sim \frac{\mathbf{k}_1 \mathbf{k}}{k_1^2}$ at $k \rightarrow 0$ and small k_1 is valid for $\psi_{\mathbf{k}}$ in the first approximation, which corresponds to the Feynman-Cohen formula (2).

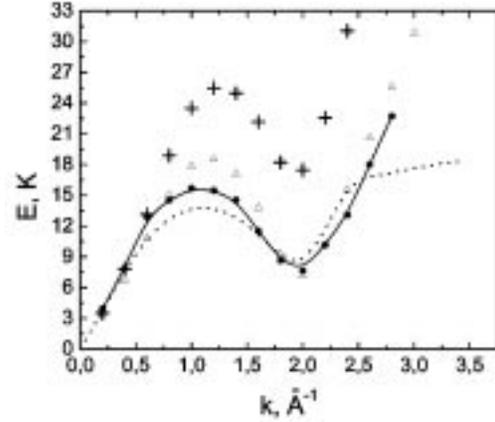


Fig. 3. Theoretical He-II quasiparticle spectrum. Pluses correspond to the zero-order approximation (25) for Ψ_0 and $\psi_{\mathbf{k}}$, triangles to the zero-order approximation for Ψ_0 and the first-order one for $\psi_{\mathbf{k}}$, circles to the first-order approximation for Ψ_0 and the second-order one for $\psi_{\mathbf{k}}$; the solid curve is drawn using the spline method; and the dotted curve corresponds to the experimental spectrum [27]

In the second-order approximation, it is necessary to solve the complete system of equations (18)–(24). Similarly to work [11], we solved these equations numerically. The system of equations (18), (19) as a whole was solved by the iteration method, while Eq. (19) by the method of quadratures [28]. In so doing, we used the values of $\sigma(k)$ obtained in the first-order approximation. The error of the numerical determination of $E(k)$ was about $\pm 10\%$; another error of about $\pm 6\%$ stemmed from measuring $S(k)$ in [23] with an accuracy of $\pm 2\%$. The obtained spectrum $E(k)$ is shown in Fig. 3.

From Fig. 3, one can see that if the number of corrections which are taken into account increases, the agreement between the theoretical and experimental spectra improves. For Ψ_0 and $\psi_{\mathbf{k}}$ determined in the first- and second-order approximations, respectively, we have a good agreement between $E(k)$ and the experiment. The “shoulder” $E(k) \approx 17 \text{ K}$ in the experimental spectrum at $k > 2.5 \text{ \AA}^{-1}$ is connected, in our opinion, with the hybridization of the spectrum that describes a single quasiparticle with a two-roton level [29].

Knowing the structure factor, one can restore the interaction potential between He^4 atoms by finding $\sigma(k)$ and $f(\mathbf{k}_1, \mathbf{k}_2)$ from Eqs. (6)–(11) with known $S(k)$ and substituting the obtained solutions into the following equation for the Fourier transform $\nu(k)$ of the potential [11]:

$$\frac{1}{2}\sigma(k_1)k_1^2 + \frac{n\nu(k_1)m}{4\hbar^2} - \sigma^2(k_1)k_1^2 =$$

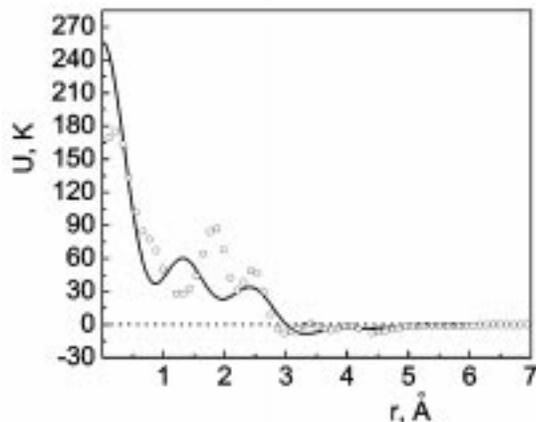


Fig. 4. Interaction potential $U(r)$ between He^4 atoms restored from the structure factor. The solid curve corresponds to the zero-order approximation for $\sigma(k)$, and the circles to the first one

$$= \frac{1}{N} \sum_{\mathbf{k}_2 \neq 0, -\mathbf{k}_1} f_s(\mathbf{k}_1, \mathbf{k}_2) 0.5(k_2^2 + \mathbf{k}_1 \mathbf{k}_2). \quad (27)$$

The potential

$$U(r) = \frac{1}{(2\pi)^3} \int \nu(k) e^{i\mathbf{k}\mathbf{r}} d\mathbf{k}, \quad (28)$$

where $\nu(k)$ (Fig. 5) can be found from (27), is shown in Fig. 4 for $\sigma(k)$ taken in the zero-order and first approximations. The potential $U(r)$ in the zero-order approximation was obtained earlier in [23]. The potential calculated by us agrees approximately with those obtained in works [5, 11, 30, 31], but not with Aziz's potential [33], which possesses a very high barrier of repulsion $U(r=0) \sim 10^6$ K. This discrepancy is probably conditioned by the efficiency of the potential that describes the interaction between He^4 atoms at small distances, as well as by different modeling of such an interaction. It is not improbable that some processes (e.g., the scattering of He^4 atoms) are well described by Aziz's potential. But the certain calculations, e.g. those of Ψ_0 , $\psi_{\mathbf{k}}$, and the $E(k)$ spectrum, are successful with the use of a potential with a much smaller effective barrier $U(0) \sim 100$ K. One can see from Fig. 4 that the found potential has a minimum at $r_{\min} = 3$ Å with the depth $U_{\min} = -7.7$ K, which approximately corresponds to the Lennard-Jones experimental "pit" with $r_{\min} = 2.97$ Å and $U_{\min} = -10.8$ K [33].

Fig. 4 also testifies to that $U(r)$ with $\sigma(k)$ in the first approximation differs appreciably from that with $\sigma(k)$ in the zero-order one. The potential varies appreciably even if Eqs. (8) and (9) are rewritten in another but equivalent form. The inaccuracy of the

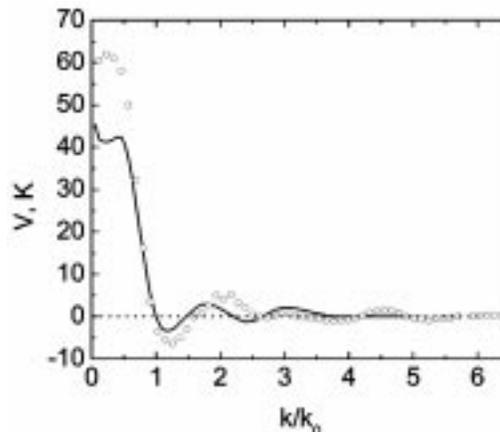


Fig. 5. Fourier image $V(k) = n\nu(k)$ for the potentials $U(r)$ shown in Fig. 4, $k_0 = 2\pi/d$. The curves correspond to the same approximations for $\sigma(k)$ as in Fig. 4

$U(r)$ determination stems from the fact that, according to Eqs. (27) and (28), the potential $U(r)$ depends strongly on the values of $\sigma(k)$ at k which are not small, $k = 2k_0 \div 4k_0$, because the term $\int \sigma(k) k^4 dk$ makes a contribution to $U(r)$. The values of $\sigma(k)$ are small at such k , but the corrections to $\sigma(k)$ turn out to be of about $\sigma(k)$ itself. That is, $\sigma(k)$ is not determined exactly at considerable k , which has almost no influence on the resulting quasiparticle spectrum, but induces a significant error while finding $U(r)$. Thus, we can only estimate the potential $U(r)$. In order to calculate $U(r)$ with a higher accuracy, one must determine the next approximations for $\sigma(k)$ and measure $S(k)$ more precisely.

4. Comparison of Different Models of He-II

Below, we present a short schematic comparison of various methods which are applied in order to explain the microstructure of He-II. In so doing, we do not pretend that our analysis is complete or perfect.

There is a plenty of works dealing with the microscopic description of He-II. Some analysis can be found in reviews [19, 33]. The main approaches are as follows:

- (i) Semiphenomenological methods, where certain equations (like the Gross-Pitaevskii one [34] or that of the model of a "continuous medium" [35]) are postulated and used as a start point to derive the quasiparticle spectrum. In this case, several fitting parameters (FPs) are used. The main shortcoming of these methods is related to that

it is not clear how precisely the initial postulates correspond to the He-II microstructure.

- (ii) Microscopical approaches which are based on the calculation of Ψ_0 and $\psi_{\mathbf{k}}$:
 - a) “Straightforward” solution of the N -particle Schrödinger equation in the \mathbf{r} - [6] or \mathbf{k} -space (the MCV, see [8–11]). Here, both Ψ_0 and $\psi_{\mathbf{k}}$ can be determined without introducing FPs.
 - b) “Indirect” methods for solving the Schrödinger equation, e.g., the “correlated basis function” [16] and “hypernetted chain” [36, 37] approaches.
 - c) Variational methods [1–4, 38].
 - d) A new “shadow wave function” approach [17–20]. At first, the authors hoped that the whole series of correlation corrections to $\ln \Psi_0$ and $\psi_{\mathbf{k}}$ can be convolved into separate simple “shadow” factors. This was explained by the fact that the correlation corrections resulted from the delocalization of atoms (for some reasons, the role of the interaction was not taken into account). However, the further analysis [17, 20] demonstrated that such a simple solution was only the first iteration of a solution of the Schrödinger equation written down in the form of a continual integral, whereas the exact solution is an infinite series for $\ln \Psi_0$ and $\psi_{\mathbf{k}}$ (analogously as it was in cases a – c).

In approaches (ii) b – d , several FPs are used. The main shortcoming of all microscopical methods of type (ii) is that their solutions are given by the series, whose expansion parameters are not small enough.

- (iii) Field-theoretic models.
 - a) Studies of the total Hamiltonian \hat{H} in the \mathbf{k} -space [5, 13–15, 39, 40]. To a certain extent, this case is rather close to item (ii,a). The condensates do not appear explicitly in the equations;
 - b) Studies of the Hamiltonian \hat{H} in the \mathbf{k} -space in the representation of the operators $\hat{a}_{\mathbf{k}}^+$ and $\hat{a}_{\mathbf{k}}$ for quasiparticles [41–43]. In this case, the condensates are explicitly separated;
 - c) Solution of equations similar to the Belyaev–Dyson ones [30, 31].

Models b and c involve FPs.

In our opinion, most perspective may be the field-theoretic approaches. There is a hope that an “ideal” microscopic model of He-II (which will start from exact microscopic equations, will not use fitting parameters, and where the expansions are carried out in small parameters only) can be developed in future just in the field-theoretic approach. At the same time, approach (ii) forms a necessary complement to (iii).

5. Conclusions

To summarize, we have approximately obtained, by using the MCV, the spectrum of He-II quasiparticles and the wave functions of the ground and first excited states of helium-II without introducing any fitting parameter into the model. In this case, we have solved the equations that had been deduced from the exact microscopic equations. A single inaccuracy of the method consists in the truncation of the series for Ψ_0 , $\psi_{\mathbf{k}}$ and $S(k)$. The obtained quasiparticle spectrum of He-II agrees well with the experimental one. Therefore, we believe that the found solution reflects the microstructure of He-II. This result refines the solution found earlier in work [8].

The author is grateful to V.E. Kireev for the discussion of numerical methods and to E.A. Pashytskyi for the discussion of the work and the useful criticism of the previous results.

1. *Feynman R.* // Phys. Rev. — 1954. — **94**. — P. 262–273.
2. *Feynman R.P., Cohen M.* // Phys. Rev. — 1956. — **102**, N 5. — P. 1189–1204.
3. *Feynman R.P.* Statistical Mechanics. A Set of Lectures. — Reading, MA: Addison-Wesley, 1972.
4. *Jastrow R.* // Phys. Rev. — 1955. — **98**, N 5. — P. 1479 — 1484.
5. *Sunakawa S., Yamasaki Sh., Kebukawa T.* // Progr. Theor. Phys. — 1969. — **41**, N 4. — P. 919 — 940; 1970. — **44**, N 3. — P. 565–573.
6. *Feenberg E.* // Ann. Phys. — 1974. — **84**. — P. 128–146.
7. *Vakarchuk I.A., Yukhnovskii I.R.* // Teor. Mat. Fiz. — 1974. — **18**, N 1. — P. 90–107.
8. *Yukhnovskiy I.R., Vakarchuk I.O.* // Visn. AN URSSR. — 1977. — N 9. — P. 32–43.
9. *Vakarchuk I.A., Yukhnovskii I.R.* // Teor. Mat. Fiz. — 1979. — **40**, N 1. — P. 100 — 111.
10. *Vakarchuk I.A., Yukhnovskii I.R.* // Ibid. — 1980. — **42**, N 1. — P. 112–123.
11. *Tomchenko M.D.* // submitted to JETP.
12. *Landau L.* // J. Phys. USSR. — 1947. — **11**. — P. 91–92.
13. *Bogolyubov N.N., Zubarev D.N.* // Zh. Eksp. Teor. Fiz. — 1955. — **28**, N 2. — P. 129 — 139.

14. Bohm D., Salt B. // Rev. Mod. Phys. — 1967. — **39**, N 4. — P. 894–910.
15. Nishiyama T. // Prog. Theor. Phys. — 1971. — **45**, N 3. — P. 730–745.
16. Jackson H. W., Feenberg E. // Rev. Mod. Phys. — 1962. — **34**, N 4. — P. 686 — 693; Lee D. K., Lee F. J. // Phys. Rev. B. — 1975. — **11**, N 11. — P. 4318 — 4330; Chang C.C., Campbell C.E. // Ibid. — 1976. — **13**, N 9. — P. 3779 — 3782; Manousakis E., Pandharipande V. P. // Ibid. — 1984. — **30**, N 9. — P. 5062–5075.
17. Vitiello S. A., Runge K.J., Chester G.V., Kalos M. A. // Phys. Rev. B. — 1990. — **42**, N 1. — P. 228–239.
18. Wu W. S., Vitiello S. A., Reatto L., Kalos M. A. // Phys. Rev. Lett. — 1991. — **67**, N 11. — P. 1446–1449.
19. Reatto L. // J. Low Temp. Phys. — 1992. — **87**, N 3–4. — P. 375–405.
20. Galli D.E., Reatto L., Vitiello S. A. // Ibid. — 1995. — **101**, N 3–4. — P. 755–760.
21. Vakarchuk I.A. // Teor. Mat. Fiz. — 1989. — **80**, N 3. — P. 439 — 451; 1990. — **82**, N 3. — P. 438–449.
22. Vakarchuk I.O., Babin V.V., Rovenchak A.A. // J. Phys. Studies. — 2000. — **4**, N 1. — P. 16 — 22; Vakarchuk I.O., Rovenchak A.A. // Ibid. — 2001. — **5**, N 2. — P. 126–130.
23. Svensson E.C., Sears V.F., Woods A.D.B. et al. // Phys. Rev. B. — 1980. — **21**, N 8. — P. 3638–3651.
24. Feenberg E. // Ann. Phys. — 1972. — **70**. — P. 133–149.
25. Balescu R. Equilibrium and Nonequilibrium Statistical Mechanics. — New York: John Wiley and Sons, 1975.
26. Samarskii A.A., Gulin A.V. Numerical Methods. — Moscow: Nauka, 1989 (in Russian).
27. Donnelly R.J., Donnelly J.A., Hills R.N. // J. Low Temp. Phys. — 1981. — **44**, N 5–6. — P. 471–489.
28. Verlan' A.F., Sizikov V.S. Integral Equations. A Reference Guide. — Kyiv: Naukova Dumka, 1986 (in Russian).
29. Zawadowski A., Ruvalds J., Solana J. // Phys. Rev. A. — 1972. — **5**, N 1. — P. 399–421.
30. Brueckner K.A., Savada K. // Phys. Rev. — 1957. — **106**. — P. 1117 — 1127, 1128 — 1135; Brueckner K.A. Theory of Nuclear Structure. — London: Methuen, 1959.
31. Pashitskii E.A., Mashkevich S.V., Vilchyskyy S.I. // J. Low Temp. Phys. — 2004. — **134**, N 3/4. — P. 851–879.
32. Aziz R.A., Nain V.P.S., Carley J.S. et al. // J. Chem. Phys. — 1979. — **70**, N 9. — P. 4330–4342.
33. Glyde H.R. // J. Low Temp. Phys. — 1995. — **93**, N 5–6. — P. 861–878.
34. Kruglov V.I., Collett M.J. // Phys. Rev. Lett. — 2001. — **87**, N 18. — P. 185302(1–4).
35. Pines D. // Can. J. Phys. — 1987. — **65**. — P. 1357–1367.
36. Campbell C.E. // Phys. Lett. A. — 1973. — **44**, N 7. — P. 471–473.
37. Krotscheck E. // Phys. Rev. B. — 1986. — **33**, N 5. — P. 3158–3167.
38. Jastrow R. // Phys. Rev. — 1955. — **98**. — P. 1479– 1485; McMillan W. L. // Phys. Rev. A. — 1965. — **138**, N 1. — P. 442–452; Schiff D., Verlet L. // Phys. Rev. — 1967. — **160**, N 1. — P. 208–218; Murphy R.D. // Phys. Rev. A. — 1968. — **5**, N 1. — P. 331 — 335; Woo C.-W., Coldwell R.L. // Phys. Rev. Lett. — 1972. — **29**, N 16. — P. 1062–1064; McFarland T., Vitiello S.A., Reatto L. et al. // Phys. Rev. B. — 1994. — **50**. — P. 13577–13587.
39. Rajagopal A.K., Grest G.S. // Phys. Rev. A. — 1974. — **10**. — P. 1395 — 4008, 1837–1851.
40. Rovenchak A.A. // Fiz. Nizk. Temp. — 2003. — **29**, N 2. — P. 145–148.
41. Bogolyubov N.N. // J. Phys. USSR. — 1947. — **11**. — P. 23–33.
42. Evans W.A.B., Imry I. // Nuovo cim. B. — 1969. — **63**, N 1. — P. 155–184.
43. Coniglio A., Mancini F., Maturi M. // Ibid. — P. 227–235.

Received 11.08.04.

Translated from Ukrainian by O.I.Voitenko

ОБЧИСЛЕННЯ СПЕКТРА КВАЗІЧАСТИНОК He-II МЕТОДОМ КОЛЕКТИВНИХ ЗМІННИХ

М.Д. Томченко

Резюме

Методом колективних змінних (МКЗ) обчислено логарифм хвильової функції основного стану He-II, $\ln \Psi_0$, з точністю до першої поправки до функції Джастрова, а також у другому наближенні знайдено хвильову функцію Ψ_k першого збудженого стану He-II і спектр квазічастинок He-II. Ψ_0 та Ψ_k знайдено як власні функції N -частинкового рівняння Шредінгера, крім того, Ψ_0 пов'язується зі структурним фактором He-II за допомогою рівняння Вакарчука. Модель не містить вільних параметрів або функцій. Отриманий чисельно спектр квазічастинок гелію-II добре узгоджується з експериментальним. Знайдений розв'язок уточнює результат, отриманий раніше Юхновським та Вакарчуком.