Calculation of the He-II quasiparticle spectrum by the method of collective variables

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The method of collective variables (MCV) has been used to calculate the logarithm of the He-II ground-state wave function, ln Ψ₀, to an accuracy of a first correction to the Jastrow function and, in a second approximation, the wave function Ψ₁ of the first excited state and the He-II quasiparticle spectrum. The functions Ψ₀ and Ψ₁ were found as the eigenfunctions of the N-particle Schrödinger equation, and the function Ψ₀ 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 Yukhnovskyi and Vakarchuk.

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I. INTRODUCTION

The structures of the N-particle wave functions of the ground and weakly excited states of helium-II are known in the main 1,2,3,4,5,6,7,8,9,10,11, and the solutions which take into account several first approximations have been obtained. In our opinion, the main unresolved problems concerning the microscopic physics of He-II are the structure of the composed condensate, the nature of the transition, and the 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 1,2,3, an opportunity to determine this spectrum making use of the structure factor has been demonstrated. Feynman intuitively found the structure of the Ψₖ 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,

\[ \Psiₖ(r₁, \ldots, r₉) = ψₖ(r₁, \ldots, r₉)Ψ₀(r₁, \ldots, r₉), \]  \hspace{1cm} (1)

\[ ψₖ = \rho₋ₖ + \sum_{k₁ \neq 0} A₁k₁kₖρ₋ₖ₋ₖ₁, \] \hspace{1cm} (2)

where Ψ₀ is the wave function of the ground state,

\[ ρₖ = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-ikr_j} \] \hspace{1cm} (3)

are collective variables 13, and N is the total number of atoms in helium. However, it has not been shown in Feynman’s works that function (2) is the eigenfunction of the N-particle Schrödinger equation. Feynman’s ideas have been developed in a great number of works (see, e.g., 14,15,16,17,18,19,20). 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 ψₖ and the structure of the function Ψ₀ have been found in works 6,7,8,9,10,11, where Ψ₀ and ψₖ were sought as the eigenfunctions of the Schrödinger equation.

Such an approach has been considered in works 8, where ln Ψ₀ was found in a zeroth-order approximation, while ψₖ and the He-II quasiparticle spectrum in a first one. The obtained spectrum E(k) agreed well with the experiment. In this work, we calculated Ψ₀, ψₖ, and E(k) more accurately. Namely, we found a first correction to ln Ψ₀ and a second ones to ψₖ and E(k). In doing so, we used the equation for Ψ₀, derived in works 8 (below, we coin it as the Vakarchuk equation). Actually, the expansion parameter of the problem was the function 2σ(k)k/k₀ (see Fig. 1), the average value of which within the interval k = 0 ± k₀ was about –1/2; i.e. the parameter was not small. Therefore, the corrections to ln Ψ₀ and E(k), generally speaking, were not small too, and their calculation was of interest.

II. THE GROUND STATE OF HELIUM-II

A more detailed analysis of the equations and the method of determining Ψ₀ were exposed in works 9,10,11. The necessary equations for Ψ₀ and ψₖ were found by Yukhnovskyi and Vakarchuk 5,9,10,24. We shall use differ-
ent notations and different forms of the equations for $\Psi_0$ and $\psi_{k,T}^{11}$ (the latter is partially caused by our desire to reduce the error of numerical solution of the equations11).

The wave function of the ground state of He-II is sought in the form9,11

$$\Psi_0 = e^{S_0},$$  \hspace{1cm} (4)

$$S_0 = \sum_{k \neq 0} \sigma(k) \rho_k \rho_{-k} + \sum_{k_1, k_2 \neq 0} f(k_1, k_2) \rho_{k_1 + k_2} \rho_{-k_1} \rho_{-k_2}.$$  \hspace{1cm} (5)

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

$$f(k_1, k_2) = -\frac{2\sigma(k_1)\sigma(k_2)k_1k_2}{e(k_1 + k_2) + e(k_1) + e(k_2)},$$  \hspace{1cm} (6)

where

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

is valid11. In works24, an equation that connects $\Psi_0$ [Eqs. (11) and (5)] with the He-II structure factor $S(k)$ was derived. We shall write down this equation in approximation9 for $\Psi_0$ and using the notations of work11 as follows:

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

$$\Sigma(q) = \frac{1}{N} \sum_{k \neq 0} \frac{8\sigma(k)\sigma(k + q) + R(k, q)}{|1 - 4\sigma(k)||1 - 4\sigma(k + q)|},$$  \hspace{1cm} (9)

where

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

$$f_s(k, q) = f(k, q) + f(-k - q, k) + f(-k - q, q).$$  \hspace{1cm} (11)

Equations (8) and (9) were derived in work24 from the known equation, which connects $S(k)$ with the pair distribution function $F_2(r)$:

$$S(k) = 1 + n \int (F_2(r) - 1) e^{-ikr} dr,$$  \hspace{1cm} (12)

where $n$ is the concentration of helium atoms.

We note that in Eqs. (8) and (9), the interaction between He$^4$ atoms does not present explicitly, and $\Psi_0$ is connected with the He-II structure factor only, so that such a way of finding $\Psi_0$ allows the problem of descriptions of interaction between He$^4$ atoms at small distances24,11 to be avoided partially: provided strong overlapping of He$^4$ atoms, the description of atomic interaction using the interaction potential becomes inaccurate, because the atomic structure becomes important under such conditions, and it is necessary, generally speaking, to solve a quantum-mechanical problem of interaction of two nuclei and four electrons. The function $\Psi_0$ [Eqs. (11) and (5)], found from Eqs. (11) - (11), takes short-range correlations into account more correctly than that found from the model potential11. For a quite correct account of the atomic structure, one should determine the function $\Psi_0$ for a system of nuclei and electrons rather than $N$ structureless particles. It is a hopeless task. Nevertheless, as one can see below, configurations with atom overlapping are very improbable, so that from the physical point of view, it is quite reasonable to consider atoms as structureless particles.

A single shortcoming made in the course of derivation of $\Psi_0$ from Eqs. (11) - (11) was the break of series (5). But, since the model does not contain fitting parameters, the accuracy of approximation (5) can be estimated by comparing both the theoretical spectrum of He-II quasiparticles and the theoretical potential of interaction 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 work24. We used the smoothed data on $S(k)$, obtained at $T = 1$ K in24, and calculated the dependences $S(k, T = 0)$ by the formula24:

$$S(k, T = 0) = S(k, T) \tanh \frac{E(k)}{2k_BT}.$$  \hspace{1cm} (13)

At $k \leq 0.2$ Å$^{-1}$, we supposed that $S(k, T = 0) \sim k$ (because $S(k = 0, T = 0) = 0^{28}$ and $E(k \rightarrow 0) = ek$ in Eq. (13)). In works24,25, the integral equations (5) and
were not solved and a zeroth-order approximation
\[ 4\sigma(q) = 1 - \frac{1}{S(q)} \]  
was used to determine \( \Psi_0 \).

Below, Eqs. (9)–(11) will be solved numerically, and the solution \( \sigma(k) \), which includes a single correction to the zeroth-order approximation (11), will be obtained; therefore, we shall call this solution a first approximation to \( \sigma(k) \). The solution of the integral equation (9) cannot be found by the iteration method, so that we used the Newton one 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 a zeroth-order approximation and \( -7.16 \text{ K} \) 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 \( \Psi_0 \) is included into the function
\[ S_1(r) = \frac{1}{N} \sum_{k \neq 0} \sigma(k)e^{ikr}, \]
where
\[ \sum_{k \neq 0} \sigma(k)\rho_k\rho_{-k} = \sum_{i,j} S_1(r_i - r_j). \]

The behavior of \( S_1(r) \) at \( r \to 0 \) shows how quickly the function \( \Psi_0 \) decays if the atoms overlap. Fig. 2 represents the function \( S_1(r) \) for a zeroth-order (14) and a first approximation for \( \sigma(k) \), and for \( \sigma(k) \) found in a second approximation, starting from the model potential. One can see that \( S_1(0) \approx -1.7 \) in all these cases. One can separate a two-particle summand of the form \( \sum_{k \neq 0} \sigma(k)\rho_k\rho_{-k} \) from the addend in the r.h.s. of (1), see(10), but a calculation shows that the account of \( \tilde{\sigma}(k) \) renormalizes \( S_1(r) \) very slightly, by a few percent 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. It means that the He\(^4\) atom possesses properties which are intermediate between “soft”- and “hard”-core ones. In case, for example, that 10 pairs of atoms overlap, \( \Psi_0 \) decreases by a factor of \( e^{34} \approx 10^{14} \) as compared to its value for a uniform distribution of atoms without overlapping. Therefore, configurations where many atoms overlap are extremely improbable.

### III. CALCULATION OF THE HE-II QUASIPARTICLE SPECTRUM

Knowing \( \Psi_0 \), one can find the wave function \( \psi_k = \psi_k \Psi_0 \), 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:

\[ \psi_k = \rho_{-k} + \sum_{k_1} \frac{P(k, k_1)}{\sqrt{N}} \rho_{k_1 - k} - \rho_{-k_1} + \sum_{k_1, \neq k_2} \frac{Q(k, k_1, k_2)}{N} \rho_{k_1 + k_2 - k} - \rho_{-k_1} + \cdots \]  

\[ \tilde{E}(k) = E(k) + \int d \mathbf{k}_1 P(k, \mathbf{k}_1)2 \mathbf{k}_1(\mathbf{k} - \mathbf{k}_1)+ \int d \mathbf{k}_1 (-2k_1^2) [Q(k, \mathbf{k}_1, -\mathbf{k}_1) + 2Q(k, \mathbf{k}_1, \mathbf{k}_1)], \]

\[ P(k, \mathbf{k}_1) \left[ e(k_1) + e(\mathbf{k} - \mathbf{k}_1) - \tilde{E}(k) \right] + \int d \mathbf{k}_2 F(k, \mathbf{k}_1, \mathbf{k}_2) = 4\sigma(k_1)M_1 + 2k^2 \sigma(k_1, k - k_1), \]

\[ F(k, \mathbf{k}_1, \mathbf{k}_2) = 4k_2(\mathbf{k} - \mathbf{k}_1 - \mathbf{k}_2)Q(k, \mathbf{k}_1, \mathbf{k}_2) + 2k_2(\mathbf{k}_1 - \mathbf{k}_2)Q(k, \mathbf{k}_1 - \mathbf{k}_2, \mathbf{k}_2), \]

\[ Q(k, \mathbf{k}_1, \mathbf{k}_2) \left[ e(k_1) + e(k_2) + e(\mathbf{k} - \mathbf{k}_1 - \mathbf{k}_2) - \tilde{E}(k) \right] = P_s(k_1, \mathbf{k}_1 + \mathbf{k}_2) * G(k_1, \mathbf{k}_2) + L(k, \mathbf{k}_1, \mathbf{k}_2), \]

\[ P_s(k_1, \mathbf{k}_2) = P(k_1, \mathbf{k}_2) + P(k_1, \mathbf{k}_1 - \mathbf{k}_2), \]

\[ G(k_1, \mathbf{k}_2) = [2\sigma(k_1)k_1 + 2\sigma(k_2)k_2](k_1 + k_2) + 2(k_1 + k_2)^2 \sigma(k_1, k_2), \]
In Eqs. (18)–(24, we converted to the dimensionless variables $\Psi_0$ and $\psi_k$, neglected. In Eqs. (18)–(24, we converted to the dimensionless variables $k' = k/k_0$ and $\tilde{E}(k') = \frac{E(k)2m}{k^2k_0^2}$, where $k_0 = 2\pi/d$ and $d = 3.578$ Å is the average interatomic distance. The primes will be omitted below.

The quasiparticle spectrum, calculated using $\Psi_0$ and $\psi_k$ in a zeroth-order approximation (i.e., $f(k_1, k_2) = 0$, Eq. [14], and $\psi_k = \rho_{-k}$), has the form of Feynman’s known formula[13], which describes the spectrum of a slightly nonideal Bose gas[13]:

$$E(k) = \frac{\hbar^2 k^2}{2mS(k)}.$$  \hspace{1cm} (25)

This spectrum is represented by pluses in Fig. 3.

To find $\psi_k$ in a first approximation, we should assume that $Q(k, k_1, k_2) = 0$. From Eq. [19], we have

$$P(k, k_1) = \frac{4\sigma(k_1)kk_1 + 2k^2f_s(k_1, k - k_1)}{e(k_1) + e(k - k_1) - \tilde{E}(k)}.$$  \hspace{1cm} (26)

The system of equations [18] and [20] was solved by the iteration method. The obtained quasiparticle spectrum, for $\sigma(k)$ in a zeroth-order approximation, is shown in Fig. 3. The spectrum of He-II in the indicated approximations has been found earlier in work[2].

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

In a second approximation, it is necessary to solve the complete system of equations [19]–[21]. Similarly to work[1], 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[13]. In so doing, we used the values of $\sigma(k)$ obtained in a first approximation. The error of the numerical definition of $E(k)$ was about ±10 %; another error of about ±6 % stemmed from measuring $S(k)$ in[25] with an accuracy of ±2 %. The obtained spectrum $E(k)$ is shown in Fig. 3.

Fig. 3: Theoretical He-II quasiparticle spectrum. Pluses correspond to a zeroth-order approximation [23] for $\Psi_0$ and $\psi_k$, triangles to a zeroth-order approximation for $\Psi_0$ and a first one for $\psi_k$, circles to a first approximation for $\Psi_0$ and a second one for $\psi_k$; the solid curve is drawn using the spline method; the dotted curve corresponds to the experimental spectrum[20].

Knowing the structure factor, one can restore the interaction potential between He$^4$ atoms by finding $\sigma(k)$ and $f(k_1, k_2)$ from Eqs. (10)–(11) with known $S(k)$ and substituting the obtained solutions into the following equation for the Fourier-image $\nu(k)$ of the potential: \[ \frac{1}{2} \sigma(k_1)k_1^2 + \frac{n_0(k_1)m}{4k^2} - \sigma^2(k_2)k_2^2 = \frac{1}{N} \sum_{k_2 \neq 0, -k_1} f_s(k_1, k_2)0.5(k_2^2 + k_1k_2). \]  \hspace{1cm} (27)

The potential

$$U(r) = \frac{1}{(2\pi)^3} \int \nu(k)e^{ikr}dk,$$  \hspace{1cm} (28)

where $\nu(k)$ is a solution of Eq. (27), is shown in Fig. 4 for $\sigma(k)$ taken in a zeroth-order and a first approximation. The potential $U(r)$ in a zeroth-order approximation was obtained in work[22] earlier. The potential calculated by us approximately agrees with those obtained in works[11,33,34], but not with Aziz’s potential[35], which possesses a very high barrier of repulsion $U(r = 0) \sim 10^6$ K. This discrepancy might be caused 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 interaction. It is not improbable that some processes (e.g., the scattering of He$^4$ atoms) are better described by Aziz’s potential, while others (in particular, the calculation of $\Psi_0$, $\sigma_k$, and the $E(k)$ spectrum) by 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 “well” with $r_{min} = 2.97$ Å and $U_{min} = -10.8$ K[35].

Fig. 4 also testifies that $U(r)$ for $\sigma(k)$ in a first approximation differs appreciably from that for $\sigma(k)$ in a
zeroth-order one. The potential changes appreciably even if Eqs. (5) and (6) are rewritten in another but equivalent form. The inaccuracy of the $U(r)$ determination stems from the fact that, according to Eqs. (27) and (28), the potential $U(r)$ depends strongly on the $\sigma(k)$ values at $k$’s that are not small, $k = 2k_0 \div 4k_0$, because the summand $\int \sigma(k)k^4dk$ makes a contribution to $U(r)$. The values of $\sigma(k)$ are small at such $k$’s, but the corrections to $\sigma(k)$ turn out to be of about $\sigma(k)$ itself. Therefore, $\sigma(k)$ is not determined exactly at considerable $k$; this circumstance 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 $U(r)$, but 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.

IV. COMPARISON OF DIFFERENT HE-II MODELS

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 are plenty of works dealing with the microscopic description of He-II. Some analysis can be found in reviews. The main approaches are as follows.

(i) Semi-phenomenological methods, where certain equations (like the Gross–Pitayevskii one or that of the model of a “continuous medium”) are postulated and used as a start point to derive the quasiparticle spectrum. Several fitting parameters (FPs) are used at that. The main shortcoming of these methods is 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 $\Psi_0$ and $\psi_k$.

(a) A “straightforward” solution of the $N$-particle Schrödinger equation in the $r$- or the $k$-space (the MCV, see Refs. 37, 38, and this work). Here, both $\Psi_0$ and $\psi_k$ can be determined without introducing FPs.

(b) “Indirect” methods for solving the Schrödinger equation, e.g., the “correlated basis function” and “hypernetted chain” approaches.

(c) Variational methods.

(d) In the “shadow wave function” (SWF) approach, the attempt is made to partially “contract” the whole infinite series of correlational corrections to $\ln \Psi_0$ and $\Psi_k$ into separate simple “shadow” factors. This procedure was argued by a certain reasoning, in particular, by that taking the delocalization of atoms into account means the partial consideration of higher correlations. As was noted in Ref. 17, such a solution is the first iteration of the Schrödinger equation represented in the form of a functional integral. Drawbacks of the models are as follows: the exact solutions for $\ln \Psi_0$ and $\Psi_k$ are infinite series, and it is not clear to a which extent the shadow factors will allow one to evaluate this series; moreover, too much FPs are in use.

FIG. 4: Potential of interaction $U(r)$ between He$^4$ atoms, restored from the structure factor. The solid curve corresponds to a zeroth-order approximation for $\sigma(k)$, and the circles to a first one.

FIG. 5: Fourier image $V(k) = n\nu(k)$ for potentials $U(r)$, shown in Fig. 4, $k_0 = 2\pi/d$. The notations correspond to the same approximations for $\sigma(k)$ as in Fig. 4.
(c) The numerical Monte-Carlo (MC) method,\textsuperscript{12,21-23} which gives the most exact description of the ground state, its energy $E_0$, the structure factor $S(k)$, and the values of all condensates. But the method does not allow one to see the analytic structure of a solution and its details and does not yield the curve $E(k)$.

In approaches c, d, several FPs are used. The main lack of all models a–d from (II) consists in that the exact solutions for $\ln \psi_0$ and $\psi_k$ are infinite correlation series. In practice, one succeeds to consider only 2–3 first terms, whereas the omitted corrections are not small.

(iii) Field-theoretic models.

(a) Studies of the total Hamiltonian $\hat{H}$ in the $k$-space.\textsuperscript{5,13,14,15,14,42,43} 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 $k$-space, in the representation of the operators $\hat{a}_k^+$ and $\hat{a}_k$ for quasiparticles.\textsuperscript{44,45,46} Here, the condensates appear explicitly.

(c) Solution of the equations similar to the Belyaev–Dyson ones.\textsuperscript{33,34}

Models b and c involve FPs.

In our opinion, the most perspective may be the field-theoretic approaches of types (iii,b) and (iii,c), the MC method, or quantum-mechanical methods that have not been discovered yet, which will start from exact microscopic equations, will not use fitting parameters, and where the expansion in a small parameter will be carried out. At the same time, approaches (ii) form a necessary complement to (iii) ones.

V. CONCLUSIONS

To summarize, in this work, using the method of collective variables, the spectrum of He-II quasiparticles has been obtained, and the wave functions of the ground and a first excited state of helium-II have been found approximately, without introducing any fitting parameter into the model. We have solved the equations that had been derived from the exact microscopic equations. A single inaccuracy of the method consisted in breaking the series for $\Psi_0$ and $\psi_k$. The obtained He-II quasiparticle spectrum agrees well with the experimental one. Therefore, we believe that the found solution reflects the microstructure of He-II. This result makes the solution found in works earlier more accurate.

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7

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