

Effective mass of atom and the excitation spectrum in liquid helium-4 at $T = 0$ K

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A self-consistent approach is applied for calculations within the two-time temperature Green function formalism in the random phase approximation for superfluid ^4He . The effective mass of the ^4He atom is computed as $m^* = 1.58 m$. The excitation spectrum is found to be in a satisfactory agreement with experiment. The sound velocity is calculated as 230 m/s. The Bose-condensation temperature with the effective mass taken into consideration is estimated as 1.99 K.

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1. Introduction

The idea of the effective mass of the helium atom in superfluid phase was suggested by Feynman in 1953 [1]. He stated that one should insert the effective mass (slightly larger than the mass of a «pure» atom m) in the expressions for the density matrix.

Isihara and Samulski [2] used the effective mass $m^* = 1.71 m$ in order to obtain a good agreement of the sound branch of the excitation spectrum with the experimental data on the sound velocity.

While in both these cases the effective mass was introduced phenomenologically, it appeared to be possible to obtain the value of this quantity on the basis of experimental data for the structure factor of liquid helium-4 [3], and a result of $1.70 m$ was calculated there by Vakarchuk.

The main idea of the present paper is to give a way of obtaining the ^4He atom effective mass by means of a self-consistent equation. The expressions are written within the collective variables formalism as described by Bogoliubov and Zubarev [4]. Two-time temperature Green's functions [5] are utilized for the calculation of the thermodynamic averages.

We also intend to show the possibility of an essentially simple approach to the problem of the many-boson system with strong interaction, such as liquid helium-4. The method applied does not require much computational effort. This advantage allows for the development of further approximations.

In addition, if one accepts the assumption that the phenomena in liquid ^4He are at least partly due to the

Bose condensation being «spoiled» by the interatomic interaction, it turns out to be possible to estimate the lambda transition temperature as the critical temperature of the ideal Bose gas. We show that such an approach leads to very good agreement with experiment: if the effective mass is about 50 % larger than the pure one, the Bose condensation temperature decreases to a value of $\simeq 2$ K.

The Green function technique also provides a possibility of obtaining the excitation spectrum of the system. As a result of the mass renormalization, the excitation spectrum is found to be in better agreement with experiment than the Bogoliubov or Feynman spectrum, while the expressions are the same (the latter two spectra suffer from the well-known problem of the so-called «roton» minimum overestimation if one considers the pure mass).

A self-consistent approach was recently applied for the calculation of the ^4He excitation spectrum by Pashitskii et al. [6]. The results of that paper are in excellent agreement with experiment. The authors used the «semitransparent spheres» potential for the calculation, with some adjustable parameters.

A new interpretation of the roton region of the helium excitation spectrum was given by Kruglov and Collett [7]. They considered the so-called roton cluster as a bound state of 13 atoms and solved the nonlinear Schrödinger equation for this system surrounded by the condensate. This approach reflects the experimental data for the roton branch of the excitation curve very well.

In our work, we utilize the potential of Ref. 8 as input information for the computations. This potential was obtained on the basis of the quantum-mechanical equations with the static structure factor as the only experimental datum. Since this quantity is quite easily measured directly in the scattering experiments, we consider this a good approach. Unfortunately, a direct calculation of the potential for the many-body problem cannot be carried out at the present time.

The paper is organized as follows. The calculation procedure is given in Sec. 2. The Hamiltonian is written and the equations of motion for the Green functions are solved in the random phase approximation (RPA), providing a self-consistent equation for the effective mass extraction. The numerical results are adduced and discussed in Sec. 3.

2. Calculation procedure

The Hamiltonian of the Bose system in the collective variables representation reads [4]:

$$\hat{\mathcal{H}} = \sum_{\mathbf{k} \neq 0} \left\{ \varepsilon_{\mathbf{k}} [\rho_{\mathbf{k}} \partial_{-\mathbf{k}} - \partial_{\mathbf{k}} \rho_{-\mathbf{k}}] + \frac{N}{2V} v_{\mathbf{k}} [\rho_{\mathbf{k}} \rho_{-\mathbf{k}} - 1] \right\} + \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \neq 0} \sum_{\substack{\mathbf{q} \neq 0 \\ \mathbf{k} + \mathbf{q} \neq 0}} \frac{\hbar^2}{2m} \mathbf{k} \mathbf{q} \rho_{\mathbf{k} + \mathbf{q}} \partial_{-\mathbf{k}} \partial_{-\mathbf{q}}, \quad (1)$$

where the operator $\partial_{\mathbf{k}} = \partial / \partial \rho_{-\mathbf{k}}$. Here $\varepsilon_{\mathbf{k}}$ is the energy spectrum of a free particle, $\varepsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$, N is the total number of particles in the system, and V is the system volume, and $v_{\mathbf{k}}$ is the Fourier transform of the interatomic potential in the thermodynamic limit, $N/V = \varrho = \text{const}$. The item with one summation over the wave vector \mathbf{k} in Eq. (1) corresponds to the random phase approximation, and the second one is the correction. Let us assume that our system is described by exactly RPA Hamiltonian $\hat{\mathcal{H}}^{(*)}$, i.e.,

$$\hat{\mathcal{H}}^{(*)} = \sum_{\mathbf{k} \neq 0} \left\{ \varepsilon_{\mathbf{k}}^* [\rho_{\mathbf{k}} \partial_{-\mathbf{k}} - \partial_{\mathbf{k}} \rho_{-\mathbf{k}}] + \frac{N}{2V} v_{\mathbf{k}} [\rho_{\mathbf{k}} \rho_{-\mathbf{k}} - 1] \right\}, \quad (2)$$

where $\varepsilon_{\mathbf{k}}^* = \hbar^2 k^2 / 2m^*$ and m^* is the effective mass of the ${}^4\text{He}$ atom. It is the only quantity suitable for the «effective» role, since we wish to preserve the interatomic potential as the initial information.

Such a definition of the effective mass means that we partly transfer the interaction and the higher-order correction onto the kinetic term in the energy. This approach correlates with that of Feynman [1]. As was also shown by Vakarchuk [9], the mass renormalization obtained in a similar fashion leads to the expression obtained for the effective mass of ${}^3\text{He}$ impu-

rity in ${}^4\text{He}$ but with the «pure» mass of the ${}^3\text{He}$ atom replaced by that of ${}^4\text{He}$ atom.

We define m^* by demanding that the effective Hamiltonian (2) leads to the same ground-state energy as the initial Hamiltonian (1), $\langle \hat{\mathcal{H}}^{(*)} \rangle = \langle \hat{\mathcal{H}} \rangle$:

$$\begin{aligned} & \sum_{\mathbf{k} \neq 0} \left\{ \varepsilon_{\mathbf{k}}^* [\langle \rho_{\mathbf{k}} \partial_{-\mathbf{k}} \rangle^{(*)} - \langle \partial_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle^{(*)}] + \right. \\ & \quad \left. + \frac{N}{2V} v_{\mathbf{k}} [\langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle^{(*)} - 1] \right\} = \\ & = \sum_{\mathbf{k} \neq 0} \left\{ \varepsilon_{\mathbf{k}} [\langle \rho_{\mathbf{k}} \partial_{-\mathbf{k}} \rangle - \langle \partial_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle] + \right. \\ & \quad \left. + \frac{N}{2V} v_{\mathbf{k}} [\langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle - 1] \right\} + \\ & + \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \neq 0} \sum_{\substack{\mathbf{q} \neq 0 \\ \mathbf{k} + \mathbf{q} \neq 0}} \frac{\hbar^2}{2m} \mathbf{k} \mathbf{q} \langle \rho_{\mathbf{k} + \mathbf{q}} \partial_{-\mathbf{k}} \partial_{-\mathbf{q}} \rangle, \quad (3) \end{aligned}$$

where the superscript $(*)$ near the angle brackets is introduced for convenience.

One can find the operator product average by utilizing two-time temperature Green functions defined as follows [5]:

$$\langle \langle A(t) | B(t') \rangle \rangle = i\theta(t - t') \langle [A(t), B(t')] \rangle, \quad (4)$$

with the operators given in the Heisenberg representation, θ is the Heaviside step function.

$$\begin{aligned} \langle AB \rangle & \equiv \hat{\mathcal{A}} G_{BA}(\hbar\omega) = \\ & = \frac{i}{\hbar} \int_{-\infty}^{+\infty} d\hbar\omega \frac{G_{BA}(\hbar\omega + i\varepsilon) - G_{BA}(\hbar\omega - i\varepsilon)}{e^{\beta\hbar\omega} - 1} \Big|_{\varepsilon \rightarrow +0}, \quad (5) \end{aligned}$$

where G_{BA} stands for $\langle \langle B | A \rangle \rangle$ and the operator $\hat{\mathcal{A}}$ is introduced for convenience. We set the time arguments in the operators $A(t)$, $B(t')$ to coincide: $t - t' = 0$. This will provide the static properties of the system under consideration. In the above expression, β is the inverse temperature, $\beta = 1/T$.

Now we proceed to the equations of motion for the Green functions $G_{\rho\rho}(\mathbf{k}) \equiv \langle \langle \rho_{\mathbf{k}} | \rho_{-\mathbf{k}} \rangle \rangle$, $G_{\rho\partial}(\mathbf{k}) \equiv \langle \langle \rho_{\mathbf{k}} | \partial_{-\mathbf{k}} \rangle \rangle$, etc. It is easy to obtain the following set of equations in the RPA:

$$\begin{aligned} (\hbar\omega + \varepsilon_{\mathbf{k}}) G_{\rho\rho}(\mathbf{k}) & = 2\varepsilon_{\mathbf{k}} G_{\partial\rho}(\mathbf{k}), \\ (\hbar\omega - \varepsilon_{\mathbf{k}}) G_{\partial\rho}(\mathbf{k}) & = \varrho v_{\mathbf{k}} G_{\rho\rho}(\mathbf{k}) + \frac{1}{2\pi}, \\ (\hbar\omega + \varepsilon_{\mathbf{k}}) G_{\rho\partial}(\mathbf{k}) & = 2\varepsilon_{\mathbf{k}} G_{\partial\partial}(\mathbf{k}) - \frac{1}{2\pi}, \\ (\hbar\omega - \varepsilon_{\mathbf{k}}) G_{\partial\partial}(\mathbf{k}) & = \varrho v_{\mathbf{k}} G_{\rho\partial}(\mathbf{k}). \quad (6) \end{aligned}$$

Here φ is equilibrium density.

Next, let us consider the triple product average $\langle ABC \rangle$. One can obtain it utilizing either the Green function $G_{C,AB} \equiv \langle\langle C|AB \rangle\rangle$ or $G_{BC,A} \equiv \langle\langle BC|A \rangle\rangle$. We suggest the first possibility to fulfill

$$\langle ABC \rangle = \hat{\mathcal{A}} G_{C,AB} \equiv \langle\langle C|AB \rangle\rangle. \quad (7)$$

In other words, we neglect the functions of the type $G_{BC,A} \equiv \langle\langle BC|A \rangle\rangle$ for the sake of simplicity (when applying this to Eq. (6) it means that only the RPA term of the Hamiltonian (1) is taken into consideration when constructing the equations of motion). Having performed a similar procedure with the function $G_{\partial,\rho\partial}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \equiv \langle\langle \partial_{\mathbf{k}_1} | \rho_{\mathbf{k}_2} \partial_{\mathbf{k}_3} \rangle\rangle$, we obtain in the RPA the following set of equations:

$$\begin{aligned} & (\hbar\omega - \varepsilon_{k_2})G_{\partial,\rho\partial}(-\mathbf{k}_2, \mathbf{k}_1 + \mathbf{k}_2, -\mathbf{k}_1) = \\ & = \varphi v_{k_2} G_{\rho,\rho\partial}(-\mathbf{k}_2, \mathbf{k}_1 + \mathbf{k}_2, -\mathbf{k}_1) - g_{\partial\rho\partial}(\omega), \\ & (\hbar\omega + \varepsilon_{k_2})G_{\rho,\rho\partial}(-\mathbf{k}_2, \mathbf{k}_1 + \mathbf{k}_2, -\mathbf{k}_1) = \\ & = 2\varepsilon_{k_2} G_{\partial,\rho\partial}(-\mathbf{k}_2, \mathbf{k}_1 + \mathbf{k}_2, -\mathbf{k}_1) - g_{\rho\rho\partial}(\omega), \end{aligned} \quad (8)$$

where the quadruple Green functions were decoupled in such a way as to provide the inhomogeneous set of equations:

$$\begin{aligned} \langle\langle AB|CD \rangle\rangle &= \langle BD \rangle \langle\langle A|C \rangle\rangle + \langle CA \rangle \langle\langle B|D \rangle\rangle + \\ &+ \langle AD \rangle \langle\langle B|C \rangle\rangle + \langle CB \rangle \langle\langle A|D \rangle\rangle. \end{aligned} \quad (9)$$

The inhomogeneous terms in Eq. (8) read:

$$\begin{aligned} g_{\rho\rho\partial}(\omega) &= \frac{\hbar^2}{2m} [\mathbf{k}_1 \mathbf{k}_2 2D_{k_1} G_{\rho\rho}(\mathbf{k}_1 + \mathbf{k}_2) + \\ &+ \mathbf{k}_1 \mathbf{k}_2 S_{|\mathbf{k}_1 + \mathbf{k}_2|} G_{\partial\partial}(\mathbf{k}_1) + \\ &+ \mathbf{k}_2(\mathbf{k}_1 + \mathbf{k}_2) D_{k_1}'' G_{\partial\rho}(\mathbf{k}_1 + \mathbf{k}_2) + \\ &+ \mathbf{k}_2(\mathbf{k}_1 + \mathbf{k}_2) D_{|\mathbf{k}_1 + \mathbf{k}_2|}'' G_{\rho\partial}(\mathbf{k}_1)], \\ g_{\partial\rho\partial}(\omega) &= \frac{\hbar^2}{m} [\mathbf{k}_1(\mathbf{k}_1 + \mathbf{k}_2) D_{k_1} G_{\partial\rho}(\mathbf{k}_1 + \mathbf{k}_2) + \\ &+ \mathbf{k}_1(\mathbf{k}_1 + \mathbf{k}_2) D_{|\mathbf{k}_1 + \mathbf{k}_2|}'' G_{\partial\partial}(\mathbf{k}_1)]. \end{aligned} \quad (10)$$

The notations for the averages of pair products are listed below:

$$\begin{aligned} \langle \rho_{-\mathbf{k}} \rho_{\mathbf{k}} \rangle &\equiv S_k = \frac{1}{\alpha_k} \coth \frac{\varepsilon_k \alpha_k}{2T}, \\ \langle \rho_{-\mathbf{k}} \partial_{\mathbf{k}} \rangle &\equiv D_k'' = \frac{1}{2} \left(\frac{1}{\alpha_k} \coth \frac{\varepsilon_k \alpha_k}{2T} - 1 \right) = \frac{1}{2} (S_k - 1), \\ \langle \partial_{-\mathbf{k}} \partial_{\mathbf{k}} \rangle &\equiv D_k = \frac{1 - \alpha_k^2}{4\alpha_k} \coth \frac{\varepsilon_k \alpha_k}{2T} = -\frac{\varphi v_k}{2\varepsilon_k} S_k. \end{aligned} \quad (11)$$

The quantity α_k is defined as follows:

$$\alpha_k = \left(1 + 2 \frac{\varphi v_k}{\varepsilon_k} \right)^{1/2}. \quad (12)$$

Now, if we turn back to correlation (3), the meaning of the asterisk as a superscript becomes clear: one should substitute m with m^* in the left hand side of this equation.

In the ground state ($T = 0$ K), hyperbolic cotangents in Eq. (11) equal to unity. Therefore, a self-consistent equation for the extraction of m^* becomes as follows:

$$\begin{aligned} -\frac{1}{N} \sum_{k \neq 0} \frac{\varepsilon_k^*}{4} (\alpha_k^* - 1)^2 &= -\frac{1}{N} \sum_{k \neq 0} \frac{\varepsilon_k}{4} (\alpha_k - 1)^2 - \\ &- \frac{1}{N^2} \sum_{k \neq 0} \sum_{\substack{q \neq 0 \\ \mathbf{k} + \mathbf{q} = 0}} \left(\frac{\hbar^2}{2m} \right)^2 \frac{\mathbf{k}\mathbf{q}}{\alpha_k \alpha_q \alpha_p} \times \\ &\times \left[\mathbf{k}\mathbf{p} \frac{\varphi v_k}{2\varepsilon_k} \left(\frac{-\alpha_p}{\varepsilon_k \alpha_k + \varepsilon_q \alpha_q} + \frac{\alpha_q \alpha_p}{\varepsilon_q \alpha_q + \varepsilon_p \alpha_p} \right) - \right. \\ &- \mathbf{q}\mathbf{p} \frac{\varphi v_q}{2\varepsilon_q} \left(\frac{\alpha_p}{\varepsilon_k \alpha_k + \varepsilon_q \alpha_q} + \frac{\alpha_k}{\varepsilon_q \alpha_q + \varepsilon_p \alpha_p} \right) + \\ &+ \left. \left(\frac{1}{\varepsilon_k \alpha_k + \varepsilon_q \alpha_q} + \frac{1}{\varepsilon_q \alpha_q + \varepsilon_p \alpha_p} \right) \times \right. \\ &\times \left. \left(\mathbf{k}\mathbf{q} \frac{\varphi v_k \varphi v_q}{\varepsilon_k \varepsilon_q} + \mathbf{k}\mathbf{p} \frac{\varphi v_k}{2\varepsilon_k} + \mathbf{q}\mathbf{p} \frac{\varphi v_q}{2\varepsilon_q} \right) \right], \end{aligned} \quad (13)$$

where $\mathbf{p} = \mathbf{k} + \mathbf{q}$. We also consider the specific energy instead of the total one by introducing the factor of $1/N$. One should notice that for the non-interacting system, when $v_k = 0$, the above equation is satisfied trivially ($\alpha_k = \alpha_k^* = 1$ in this case). In particular, the triple product average $\langle \rho_{\mathbf{k} + \mathbf{q}} \partial_{-\mathbf{k}} \partial_{-\mathbf{q}} \rangle$ in (3) equals to zero providing a well-known expression for the ideal Bose-gas (IBG) energy:

$$E_{IBG} = \sum_{k \neq 0} \frac{\varepsilon_k}{2} \left[\coth \frac{\varepsilon_k}{2T} - 1 \right] = \sum_{k \neq 0} \frac{\varepsilon_k}{e^{\varepsilon_k/T} - 1}.$$

3. Numerical results and discussion

We use the previously obtained results [8] for the Fourier transform v_k of the interatomic potential. The value of the equilibrium density is $\varphi = 0.02185 \text{ \AA}^{-3}$. The mass of the helium-4 atom is $m = 4.0026 \text{ a.m.u.}$ We pass from the summation over the wave vector to integration in the usual way: $\sum_{\mathbf{k}} \rightarrow V \int d\mathbf{k} / (2\pi)^3$.

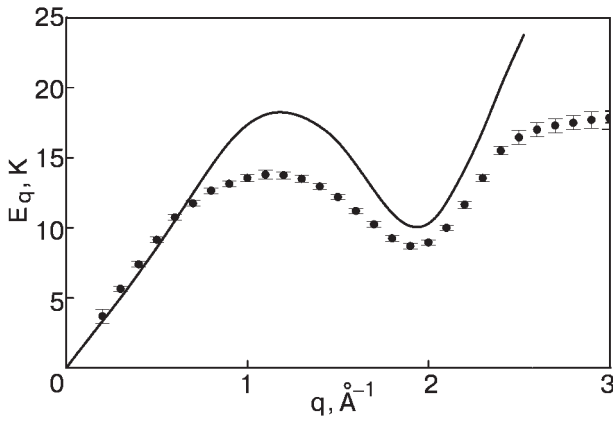


Fig. 1. Excitations spectrum of liquid helium-4. Filled circles — experimental data [10]; Solid line — calculated energy.

The value of the upper cutoff for the integration over the wave vector is 16.0 \AA^{-1} .

The solution of Eq. (13) at the above-listed conditions is

$$m^* = 1.58 m. \quad (14)$$

One can also obtain the excitations spectrum using Green's functions. The solutions of set (6) are proportional to $1/(\hbar^2\omega^2 - \varepsilon_k^2\alpha_k^2)$ providing the spectrum $E_k = \pm \varepsilon_k\alpha_k$, which is a very well known result [4]. If one inserts the effective mass into the definitions of ε_k and α_k , the obtained curve fits the experimental one in a quite satisfactory manner (see Fig. 1).

The phonon branch is reflected quite well, providing a sound velocity of approximately 230 m/s versus the experimental one 238 m/s at $T = 0.8 \text{ K}$ [11] or 240 m/s at $T = 0.1 \text{ K}$ [12]. The so-called «roton» minimum also has a value close to the experimental one.

In addition, the value obtained for the effective mass shifts the temperature of the Bose condensation from $T_c = 3.14 \text{ K}$ for the pure mass to $T_c = 1.99 \text{ K}$,

versus the experimental temperature of the lambda transition $T_\lambda = 2.17 \text{ K}$. We consider the results discussed above to be quite good for such a rough approximation as random phases.

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