Effective Mass of Atom and Excitation Spectrum in Liquid Helium-4 at \( T = 0 \) K

A. A. Rovenchak

Department for Theoretical Physics, Ivan Franko National University of Lviv
12 Draghomanov St., Lviv, UA-79005, Ukraine
tel: +380 322 979443; e-mail: andrij@krf.franko.lviv.ua

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Abstract

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

**Key words:** liquid helium-4, effective mass, excitation spectrum.

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1 Introduction

The idea of the effective mass of helium atom was suggested by Feynman in 1953 \[1\]. He stated that one should insert the effective mass (being 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 excitation spectrum sound branch 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 receive the value of this quantity basing on the experimental data for the structure factor of liquid helium-4 \[3\], the result of \( 1.70 \) \( m \) was calculated there by Vakarchuk.

In the paper presented we will give the way of the receiving \(^4\)He 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 functions \[5\] are utilized for the calculation of the thermodynamic averages.

The main idea of the paper is 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 efforts. This advantage allows for the development of the further approximations.

In addition, if one accepts the assumption that the phenomena in liquid \(^4\)He are at least partly due to the Bose-condensation being ‘spoiled’ by the interatomic interaction, it turns 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 a very good agreement with the experiment: if the effective mass is about 50% larger than the pure one the Bose-condensation temperature decreases to the value of $\simeq 2$ K.

The Green functions technique provides also a possibility to receive the excitation spectrum of the system. As a result of the mass renormalization, the excitation spectrum is found to be in the better agreement with the experiment in comparison with the Bogoliubov’s or Feynman’s one while the expressions are the same (for the latter two spectra the problem of the so called ‘roton’ minimum overestimation is well-known if one considers the pure mass).

A self-consistent approach was recently applied for the calculation of the $^4$He excitation spectrum by Pashitskii et al [3]. The results of this paper are in an excellent agreement with the experiment. The authors used the ‘semitransparent spheres’ potential for the calculation with some adjusting parameters. In our work, we utilize the potential [6] as an input information for the computations. This potential was received on the basis of the quantum-mechanical equations with the static structure factor as the only experimental data. Since this quantity is quite easily measured directly in the scattering experiments, we consider it as a good approach. Unfortunately, a direct calculation of the potential for the many-body problem cannot be made for the time being.

The paper is organized as follows. The calculating procedure is given in Section 2. The Hamiltonian is written and the equations of motion for the Green functions are solved in random phase approximation (RPA) providing a self-consistent equation for the effective mass extraction.

The numerical results are adduced in Section 3 together with the discussion.

2 Calculation procedure

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

$$
\hat{H} = \sum_{k \neq 0} \left\{ \varepsilon_k \left[ \rho_k \partial_{-k} \rho_{-k} - \partial_k \rho_{-k} \right] + \frac{N}{2V} \nu_k \left[ \rho_k \rho_{-k} - 1 \right] \right\} + \frac{1}{\sqrt{N}} \sum_{k \neq 0} \sum_{q \neq 0} \frac{\hbar^2}{2m} k q \rho_{k+q} \partial_{-k} \partial_{-q},
$$

where the operator $\partial_k = \partial/\partial \rho_{-k}$. Here, $\varepsilon_k$ is the energy spectrum of a free particle, $\varepsilon_k = \hbar^2 k^2 / 2m$, $N$ is the total number of particles in the system, and $V$ is the system volume. In the thermodynamic limit, $N/V = \bar{\nu} = \text{const}$. $\nu_k$ is the Fourier transform of the interatomic potential. 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 $\hat{H}^{(\ast)}$, i. e.,

$$
\hat{H}^{(\ast)} = \sum_{k \neq 0} \left\{ \varepsilon_k^{\ast} \left[ \rho_k \partial_{-k} \rho_{-k} - \partial_k \rho_{-k} \right] + \frac{N}{2V} \nu_k \left[ \rho_k \rho_{-k} - 1 \right] \right\}
$$

where $\varepsilon_k^{\ast} = \hbar^2 k^2 / 2m^{\ast}$ and $m^{\ast}$ is the effective mass of $^4$He atom. It is the only quantity suitable for the ‘effective’ role since we wish to preserve the interatomic potential as the initial information.

One can define $m^{\ast}$ demanding that the effective Hamiltonian [4] leads to the same ground-state energy as the initial Hamiltonian [1], $\langle \hat{H}^{(\ast)} \rangle = \langle \hat{H} \rangle$:

$$
\sum_{k \neq 0} \left\{ \varepsilon_k^{\ast} \left[ \langle \rho_k \partial_{-k} \rangle^{(\ast)} - \langle \partial_k \rho_{-k} \rangle^{(\ast)} \right] + \frac{N}{2V} \nu_k \left[ \langle \rho_k \rho_{-k} \rangle^{(\ast)} - 1 \right] \right\} =
$$

$$
= \sum_{k \neq 0} \left\{ \varepsilon_k \left[ \langle \rho_k \partial_{-k} \rangle - \langle \partial_k \rho_{-k} \rangle \right] + \frac{N}{2V} \nu_k \left[ \langle \rho_k \rho_{-k} \rangle - 1 \right] \right\} + \frac{1}{\sqrt{N}} \sum_{k \neq 0} \sum_{q \neq 0} \frac{\hbar^2}{2m} k q \langle \rho_{k+q} \partial_{-k} \partial_{-q} \rangle,
$$

where $\langle \cdot \rangle$ is the average in the ground state. The Hamiltonian (1) provides the minimum overestimation is well-known if one considers the pure mass).
where the superscript (⋆) near the angle brackets is introduced for the convenience.

One can find the operators product average utilizing two-time temperature Green functions defined as follows [3]:

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

with operators given in the Heisenberg representation, $\theta$ is the Heaviside step function.

$$\langle AB \rangle \equiv \hat{A} G_{BA}(\hbar \omega) = \frac{i}{\hbar} \int_{-\infty}^{+\infty} d\hbar \omega \left. \frac{G_{BA}(\hbar \omega + i\varepsilon) - G_{BA}(\hbar \omega - i\varepsilon)}{e^{\beta \hbar \omega} - 1} \right|_{\varepsilon \to 0}$$

(5)

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

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

$$\begin{align*}
(h\omega + \varepsilon_k)G_{\rho\rho}(k) &= 2\varepsilon_k G_{\rho\vartheta}(k), \\
(h\omega - \varepsilon_k)G_{\rho\vartheta}(k) &= \partial \varepsilon_k G_{\rho\rho}(k) + \frac{1}{2\pi}, \\
(h\omega + \varepsilon_k)G_{\rho\vartheta}(k) &= 2\varepsilon_k G_{\vartheta\vartheta}(k) - \frac{1}{2\pi}, \\
(h\omega - \varepsilon_k)G_{\vartheta\vartheta}(k) &= \partial \varepsilon_k G_{\rho\vartheta}(k).
\end{align*}$$

(6)

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

$$\langle ABC \rangle = \hat{A} G_{C;AB} \equiv \langle C|AB \rangle.$$  

(7)

In other words, we neglect the functions of the type $G_{BC;A} \equiv \langle BC|A \rangle$ 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 the similar procedure with the function $G_{\vartheta \vartheta \vartheta}(k_1, k_2, k_3) \equiv \langle \vartheta_{k_1}|\rho_{k_2}\vartheta_{k_3} \rangle$ we obtain in RPA the following set of equations:

$$\begin{align*}
(h\omega - \varepsilon_{k_2})G_{\vartheta \vartheta \vartheta}(-k_2, k_1 + k_2, -k_1) &= \partial \varepsilon_{k_2} G_{\rho \rho \vartheta}(-k_2, k_1 + k_2, -k_1) - g_{\vartheta \vartheta \vartheta}(\omega) \\
(h\omega + \varepsilon_{k_2})G_{\rho \rho \vartheta}(-k_2, k_1 + k_2, -k_1) &= 2\varepsilon_{k_2} G_{\vartheta \vartheta \vartheta}(-k_2, k_1 + k_2, -k_1) - g_{\rho \rho \vartheta}(\omega),
\end{align*}$$

(8)

where the quadruple Green functions were decoupled in such a way providing for the inhomogeneous set of equations:

$$\langle AB|CD \rangle = \langle BD \rangle \langle A|C \rangle + \langle CA \rangle \langle B|D \rangle + \langle AD \rangle \langle B|C \rangle + \langle CB \rangle \langle A|D \rangle.$$  

(9)

The inhomogeneous terms in Eq. (8) read:

$$\begin{align*}
g_{\rho\rho\vartheta}(\omega) &= \frac{\hbar^2}{2m} \left[ k_1 k_2 2D_{k_1} G_{\rho\rho}(k_1 + k_2) + k_1 k_2 S_{[k_1 + k_2]} G_{\vartheta\vartheta}(k_1) + k_2(k_1 + k_2) D''_{k_1} G_{\vartheta\vartheta}(k_1 + k_2) + k_2(k_1 + k_2) D''_{[k_1 + k_2]} G_{\vartheta\vartheta}(k_1) \right], \\
g_{\vartheta\vartheta\vartheta}(\omega) &= \frac{\hbar^2}{2m} \left[ k_1(k_1 + k_2) D_{k_1} G_{\vartheta\vartheta}(k_1 + k_2) + k_1(k_1 + k_2) D''_{[k_1 + k_2]} G_{\vartheta\vartheta}(k_1) \right] \times 2.
\end{align*}$$  

(10)
The notations for the averages of pair products are listed below:

\[ \langle \rho_{-k}\rho_k \rangle \equiv S_k = \frac{1}{\alpha_k} \coth \left( \frac{\varepsilon_k \alpha_k}{2T} \right), \]

\[ \langle \rho_{-k}\partial_k \rangle \equiv D''_k = \frac{1}{2} \left( \frac{1}{\alpha_k} \coth \left( \frac{\varepsilon_k \alpha_k}{2T} \right) - 1 \right) = \frac{1}{2} (S_k - 1), \]

\[ \langle \partial_{-k}\partial_k \rangle \equiv D_k = \frac{1 - \alpha_k^2}{4\alpha_k} \coth \left( \frac{\varepsilon_k \alpha_k}{2T} \right) = -\frac{\partial \nu}{2\varepsilon_k} S_k. \] (11)

The quantity \( \alpha_k \) is defined as follows:

\[ \alpha_k = (1 + 2\varrho \nu_k/\varepsilon_k)^{1/2}. \] (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 l.h.s. of this equation.

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

\[
-\frac{1}{N} \sum_{k \neq 0} \frac{\varepsilon_k^2}{4} (\alpha_k - 1)^2 = -\frac{1}{N} \sum_{k \neq 0} \frac{\varepsilon_k}{4} (\alpha_k - 1)^2 \\
-\frac{1}{N^2} \sum_{k \neq 0} \sum_{q \neq 0} \left( \frac{\hbar^2}{2m} \right)^2 \frac{kq}{\alpha_k \alpha_q \alpha_p} \left[ \left( \frac{1}{\varepsilon_k \alpha_k + \varepsilon_q \alpha_q} + \frac{1}{\varepsilon_q \alpha_q + \varepsilon_p \alpha_p} \right) \left( \frac{\partial \nu_k \nu_q}{\varepsilon_k \varepsilon_q} + \frac{kp \partial \nu_k}{2\varepsilon_k} + \frac{qq \partial \nu_q}{2\varepsilon_q} \right) \right] \\
+ kp \frac{\partial \nu_k}{2\varepsilon_k} \left( \frac{-\alpha_p}{\varepsilon_k \alpha_k + \varepsilon_q \alpha_q} + \frac{\alpha_q \alpha_p}{\varepsilon_q \alpha_q + \varepsilon_p \alpha_p} \right) - qp \frac{\partial \nu_q}{2\varepsilon_q} \left( \frac{-\alpha_p}{\varepsilon_k \alpha_k + \varepsilon_q \alpha_q} + \frac{\alpha_k}{\varepsilon_k \alpha_k + \varepsilon_q \alpha_q} \right) \right] (13)
\]

where \( p = k + q \). We also consider the specific energy instead of the total one by introducing the factor of \( 1/N \).

### 3 Numerical results and discussion

We use the previously obtained results [8] for the interatomic potential Fourier transform \( \nu_k \). The value of the equilibrium density is \( \varrho = 0.02185 \text{ A}^{-3} \). The mass of helium-4 atom equals \( m = 4.0026 \text{ a.m.u.} \) We transit from the summation over the wave vector to the integration in the usual way: \( \sum_k \rightarrow V \int d\mathbf{k}/(2\pi)^3 \). The value of the upper cut-off for the integration over the wave vector is 16.0 A⁻¹.

The solution of Eq. (13) at the abovelisted conditions is

\[ m^* = 1.58 m. \] (14)

One can also receive the excitations spectrum using Green functions. The solutions of set (3) are proportional to \( 1/((\hbar^2 \omega^2 - \varepsilon_k^2 \alpha_k^2)) \) providing the spectrum \( E_k = \pm \varepsilon_k \alpha_k \) — a very well known result [9]. If one inserts the effective mass into the definitions of \( \varepsilon_k \) and \( \alpha_k \) the obtained curve fits the experimental one quite satisfactory, see Fig. [10].

The phonon branch is reflected quite good providing the sound velocity of approximately 230 m/s vs the experimental 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 the value close to the experimental one.

In addition, the obtained value of the effective mass shifts the temperature of the Bose-condensation from \( T_c = 3.14 \text{ K} \) for the pure mass to \( T_c = 1.99 \text{ K} \) vs the experimental temperature of the lambda transition \( T_\lambda = 2.17 \text{ K} \). We consider the results discussed above as quite good as for such a rough approximation as random phases.
Figure 1: Excitations spectrum of liquid helium-4. Filled circles — experimental data [8]; Solid line — calculated energy.

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