Impurity effective mass in superfluid $^4$He

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Abstract

The system of bose liquid + impurity is considered. The energy spectrum as well as effective mass of impurity is calculated. For the case of the $^3$He atom in superfluid $^4$He numerical calculations are performed.

keywords superfluid helium, impurity, effective mass.

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1 Introduction

A couple of the most interesting questions is to be mentioned within the problem of determining the impurity energy spectrum in superfluid $^4$He, namely the calculation of the impurity effective mass $M^*$ and revealing the spectrum character in the region of wave vectors corresponding to the reverse interatom distance. Within the frames of the thermodynamic approach the effective mass of $^3$He was originally determined on the basis of experimental data for the heat capacity and the spin diffusion coefficient by Bardeen J., Baym G., Pines D. They found the value $M^*/M = 2.34$ for the impurity effective mass and the isolated atom $M$ mass ratio in the case of liquid $^4$He equilibrium density. A microscopic theory of the energy spectrum for the $^3$He impurities in superfluid $^4$He was independently developed in Ref. [1]. They determined the energy of replacement, the effective mass and relative

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change of liquid bulk caused by the replacement of $^4$He with $^3$He. In order to obtain the numerical value of $M^*$, the liquid $^4$He structure factor calculated theoretically by different authors was used. For example, using the data of [7], the value $M^*/M = 1.81$ is obtained. The same problems were considered by Slyusarev and Strzhemechny [4]; they used trial variation function of impure atom and the Brillouin-Wigner perturbation theory with the long wave estimate for the matrix elements of "impurity" and "impurity-phonon". An explicit expression for the impurity effective mass via the $^4$He structure factor as well as the numerical value $M^*/M = 2.4$ on the basis of experimentally measured structure factor were given in this work too. The authors noted the essential non-square behaviour of the spectrum in the wave vector region near $3\,\text{Å}^{-1}$. A similar expression for $M^*$ was obtained by Woo Tan and Massey [5], however, by using the theoretical structure factor they obtained $M^*/M = 1.85$ to be closer to the value found in [3]. The same authors in [6] have improved this result in $M^*/M = 2.37$ by an evaluation of higher corrections to the effective mass of the interaction "impurity-phonon". In [8] variational wave function suitable only for the calculation of the effective mass is chosen. With the help of this function which takes into account the backflow arising from driving the $^3$He atom in the form proposed by Feynman and Cohen for pure $^4$He [9] the value $M^*/M = 1.7$ is obtained. We would like to mention work [10] as well, in which the spectrum of the impurity and its dampings were investigated by means of the dynamic structure factor for small values of the wave vector $M^*/M = 2.35$, as well as in the region of roton minimum $^4$He. "One-parameter" trial wave function without an application of the perturbations theory of Brillouin-Wigner is used in [11] for the calculation of the impurity branch of spectrum. For the effective mass two first corrections are explicitly calculated, each of which contains one sum over a wave vector more than the previous one. Using experimental data for the structure factor, in the case of the $^3$He atom the value $M^*/M = 1.73$ is obtained.

In the present work the calculation of the impurity spectrum will be carried out on the basis of the polaron-type Hamiltonian where liquid helium + impurity system is simulated in the approximation of one sum over a wave vector. We propose to pass in the Hamiltonian to other variables so that impurity coordinates should be dropped out, and further to develop the perturbation theory not for the interaction "liquid-impurity", but for an additional "anharmonic" term, which results from such a transformation of
independent variables. In a zero approximation of the approach the result for the spectrum of an impurity of the second order of the perturbation theory for a potential of the interaction "liquid - impurity" is reconstituted, but without the assumption of the smallness of the "liquid - impurity" interaction. Numerical estimates of an effective mass of the $^3\text{He}$ atom in superfluid $^4\text{He}$ on the basis of experimental values of the structural factor for liquid $^4\text{He}$ are also carried out.

2 Notations

The object of our study is a model of the system "superfluid $^4\text{He}$ + impurity", based on the following Hamiltonian:

$$H = \frac{P^2}{2M} + H_{He^4} + H_{int}$$  \hspace{1cm} (1)

The first term in (1) represents a kinetic energy of the impurity atom (practically, it is the $^3\text{He}$ atom), the mass of which we have denoted as $M$. We take the Hamiltonian of superfluid helium in an approximation of noninteracting elementary perturbations

$$H_{He^4} = E_0 + \sum_{q \neq 0} E_q b_q^\dagger b_q$$

with the Bogoliubov spectrum $E_q$ and energy of a ground state $E_0$ [12] :

$$E_0 = \frac{N(N-1)}{2V} \nu_0 - \frac{1}{4} \sum_{q \neq 0} \frac{\hbar^2 q^2}{2m} (\alpha_q - 1)^2$$

$$E_q = \frac{\hbar^2 q^2}{2m} \alpha_q, \quad \alpha_q = \sqrt{1 + \frac{2N}{V} \nu_q / \frac{\hbar^2 q^2}{2m}}$$

where the letters $N$ and $V$ denote the number of particles of a liquid and the volume of the system respectively, $m$ is the mass of atom $^4\text{He}$ and $\nu_q$ is Fourie-image of a pair potential of interparticle interaction in superfluid $^4\text{He}$. The operators of creation-anihilation of the elementary perturbations $b_q^\dagger, b_q$ satisfy the commutative relations of Bose

$$[b_q, b_k^\dagger] = \delta (q - k).$$
The part of Hamiltonian (1) which corresponds to the interaction between a liquid and impurity, is expressed in the following form

\[
H_{\text{int}} = \frac{N}{V} w_0 + \sqrt{\frac{N}{V}} \sum_{q \neq 0} \frac{w_q}{\sqrt{\alpha_q}} e^{iqR} \left( b_q^\dagger + b_q \right).
\]

Here \( R \) is a coordinate of an impurity, \( w_q \) is Fourier-image of a potential of interaction between the \(^4\text{He} \) atom and the impurity atom.

3 Calculation of the impurity spectrum

In order to treat the problem it is convenient to pass from (1) to a unitary equivalent Hamiltonian

\[
H_* = U H U^\dagger
\]

with the help of the transformation

\[
U = \exp \left( i \sum_{q \neq 0} (qR) b_q^\dagger b_q \right), \quad U^\dagger = U^{-1}.
\]

Transformation (3) enables us to lose impurity coordinates, but, instead of that, results in the emergence of anharmonic terms.

The operator of impulse \( P \) of an impurity now can be considered as a \( c \)-number and one can identify a spectrum of impurity by the energy of a ground state which corresponds to \( H_* \).

The Hamiltonian \( H_* \), as well as input \( H \), cannot be diagonalized exactly, therefore for further calculations we use the theory of perturbations. It is
natural in the next step to divide $H_*$ into a problem that we supposes an exact solution,

$$H_0^* = \frac{N}{V} w_0 + E_0 + \frac{P^2}{2M} +$$

$$+ \sum_{q \neq 0} \left\{ \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} qP \right) b_q^\dagger b_q + \frac{\sqrt{N}}{V} w_q \frac{\alpha_q}{\sqrt{\alpha_q}} \left( b_q^\dagger + b_q \right) \right\}$$

and into perturbation

$$H_{int}^* = \frac{\hbar^2}{2M} \sum_{q_1 \neq 0, q_2 \neq 0} (q_1 q_2) b_{q_1}^\dagger b_{q_2}^\dagger b_{q_1} b_{q_2},$$

(normal ordering of operators of creation-annihilation is suggested). But, by using an arbitrariness of this separation, we introduce an additional parameter $\phi(q)$, with the help of which we try to improve the approach of the perturbations theory outcome to an exact solution. In other words, let’s assume

$$H_* = \widetilde{H}_0^* + \widetilde{H}_{int}^*,$$

where

$$\widetilde{H}_0^* = H_0^* + \sum_{q \neq 0} \phi(q) b_q^\dagger b_q,$$

$$\widetilde{H}_{int}^* = H_{int}^* - \sum_{q \neq 0} \phi(q) b_q^\dagger b_q.$$

In support of such a step it is possible to mention also the argument that the small parameter of natural origin does not exist in the input Hamiltonian $H$.

We further develop the usual perturbation theory for an energy of the ground state $H_*:

$$E = E^{(0)} + E^{(1)} + E^{(2)} + ...$$

In a zero approximation the system under consideration is a set of harmonic oscillators in an inhomogeneous external field, therefore, without the assumption of the smallness of the liquid - impurity interaction, we obtain

$$E^{(0)} = E_0 + \frac{N}{V} w_0 + \frac{P^2}{2M} -$$

$$\frac{N}{V^2} \sum_{q \neq 0} \frac{w_q^2}{\alpha_q} \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} qP \right) + \phi(q).$$
The first and the second correction to $E^{(0)}$ have the following expression

$$E^{(1)} = -\frac{N}{V^2} \sum_{q \neq 0} \phi(q) \frac{w_q^2}{\alpha_q \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} (qP) + \phi(q) \right)^2} +$$

$$+ \frac{\hbar^2}{2M} \left( \frac{N}{V^2} \sum_{q \neq 0} q \frac{w_q^2}{\alpha_q \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} (qP) + \phi(q) \right)^2} \right)^2,$$

$$E^{(2)} = -\frac{N}{V^2} \sum_{q \neq 0} \frac{w_q^2}{\alpha_q \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} (qP) + \phi(q) \right)^3} \times$$

$$\times \left( \phi(q) - \frac{\hbar^2}{M V^2} \sum_{k \neq 0} (qk) \frac{w_k^2}{\alpha_k \left( E_k + \frac{\hbar^2 k^2}{2M} - \frac{\hbar}{M} (kP) + \phi(k) \right)^2} \right)^2 +$$

$$+ \frac{N^2}{V^4} \sum_{q \neq 0} \alpha_q^2 \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} (qP) + \phi(q) \right)^5 -$$

$$- \frac{N^2}{V^4} \sum_{q_1 \neq 0} \sum_{q_2 \neq 0} \left( \frac{\hbar^2}{M} (q_1 q_2) \right)^2 \alpha_{q_1} \left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} - \frac{\hbar}{M} (q_1 P) + \phi(q_1) \right)^2 \times$$

$$\times \alpha_{q_2} \left( E_{q_2} + \frac{\hbar^2 q_2^2}{2M} - \frac{\hbar}{M} (q_2 P) + \phi(q_2) \right)^2 \times$$

$$\times \frac{1}{E_{q_1} + \frac{\hbar^2 q_1^2}{2M} - \frac{\hbar}{M} (q_1 P) + \phi(q_1) + E_{q_2} + \frac{\hbar^2 q_2^2}{2M} - \frac{\hbar}{M} (q_2 P) + \phi(q_2)}.$$

In order to fix the arbitrary function $\phi(q)$ it is possible to use the demand of the minimization of energy as a functional of $\phi(q)$, but we did not manage to solve the equations appearing in such an approach. We propose to require vanishing the first correction to $E^{(0)}$, that is to determine $\phi(q)$ from the condition $E^{(1)} = 0$. Explicitly we have the equation:

$$-\frac{N}{V^2} \sum_{q \neq 0} \phi(q) \frac{w_q^2}{\alpha_q \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} (qP) + \phi(q) \right)^2} +$$

$$+ \frac{\hbar^2}{2M} \left( \frac{N}{V^2} \sum_{q \neq 0} q \frac{w_q^2}{\alpha_q \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} (qP) + \phi(q) \right)^2} \right)^2 = 0.$$
The equation will be satisfied identically, if one puts

\[ \phi(q) = \frac{\hbar}{M} (qx) \]

and imposes on the vector \( x \) a condition

\[ x = \frac{\hbar N}{2 V^2} \sum_{q \neq 0} q \frac{w_q^2}{\alpha_q \left( E_q + \frac{\hbar^2 q^2}{2M} - \frac{\hbar}{M} (q, P - x) \right)^2}. \] (4)

At \( P = 0 \) we herefrom find \( x = 0 \). For small \( P \) let us assume that \( x = \lambda P \), then, expanding the right-hand side (4) in the powers of \( P \) we obtain the following relation for the definition of \( \lambda \)

\[ \lambda = (1 - \lambda) \frac{\sigma_1}{2} + o(P^2). \]

Here for the some of simplicity we introduce

\[ \sigma_1 = \frac{4 N}{3 V^2} \sum_{q \neq 0} \frac{w_q^2 \hbar^2 q^2}{\alpha_q \left( E_q + \frac{\hbar^2 q^2}{2M} \right)^3}. \]

Hence, within the accuracy of the square and higher powers of impulse of the impurity, we have

\[ \lambda = \frac{\sigma_1}{2 + \sigma_1}. \]

The usual theory of perturbations for \( H_{int}^* \) corresponds to the value \( \lambda = 0 \).

4 Effective mass of the impurity

The spectrum obtained above is in the region of small impulses, as it should be, looks like

\[ E(P) = \varepsilon_0 + \frac{P^2}{2M_*}, \]
where $M^*$ is the so-called effective mass of the impurity atom, and the constant independent of impulse equals

$$
\varepsilon_0 = E_0 + \frac{N}{V} w_0 - \frac{N}{V^2} \sum_{q \neq 0} \alpha_q \left( E_q + \frac{\hbar^2 q^2}{2M} \right) + \frac{N^2}{V^4} \sum_{q \neq 0} \alpha_q^2 \left( E_q + \frac{\hbar^2 q^2}{2M} \right)^2 - \frac{N^2}{V^4} \sum_{q_1 \neq 0} \sum_{q_2 \neq 0} \left( \frac{\hbar^2}{M} \langle q_1, q_2 \rangle \right)^2 \times \frac{w_{q_1}^2 w_{q_2}^2}{\alpha_{q_1} \left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} \right) \alpha_{q_2} \left( E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right) \left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} + E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2}.
$$

The outcome of our calculations is such an expression for $M^*$

$$
\frac{M}{M^*} = 1 - \sigma_1 + \sigma_1^2 - \sigma_1^3 - \sigma_2 + 2\lambda \left( \sigma_1^3 + \sigma_2 \right) - \lambda^2 \left( \sigma_1^2 + \sigma_1^3 + \sigma_2 \right), \quad (5)
$$

where one more notation is introduced

$$
\sigma_2 = \left( \frac{4N}{3V^2} \right)^2 \sum_{q_1 \neq 0} \sum_{q_2 \neq 0} \frac{\hbar^2 q_1^2 \hbar^2 q_2^2}{2M} \frac{w_{q_1}^2 w_{q_2}^2}{\alpha_{q_1} \left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} \right)^2 \left( E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2}
$$

$$
\times \frac{1}{\left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} + E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \left\{ 2 \left( \frac{3}{\left( E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \right) + \frac{1}{\left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} + E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \right\}
$$

$$
+ \left( \frac{1}{\left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} + E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \right) \left( \frac{3}{\left( E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \right) + \left( \frac{1}{\left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} + E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \right) \left( \frac{3}{\left( E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \right) + \left( \frac{1}{\left( E_{q_1} + \frac{\hbar^2 q_1^2}{2M} + E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \right) \left( \frac{3}{\left( E_{q_2} + \frac{\hbar^2 q_2^2}{2M} \right)^2} \right) \right\}.
$$
5 Numerical calculations

We provide numerical computations of the effective mass of the $^3\text{He}$ impurity in $^4\text{He}$ at $T = 0$ K. We assumed that the potentials of interatomic interactions $^3\text{He} - ^4\text{He}$ and $^4\text{He} - ^4\text{He}$ are identical, that is $\nu_q = w_q$, and further we expressed $\nu_q$ through the $^4\text{He}$ structure factor with the help of relations [1]

$$ S_q = \frac{1}{\alpha_q}. $$

For evaluations we made use of measurements $S_q$ [3] continued to the point $T = 0$ K by means of equalities [1]

$$ S_q(T = 0) = S_q(T) \tanh \left[ \frac{E_q}{2T} \right]. $$

The density of $^4\text{He}$ was considered to be equal to $\rho_{^4\text{He}} = 0.02185\text{Å}^{-3}$. The following values are obtained:

$$ \sigma_1 = 0.416 \quad (6) $$

$$ \sigma_2 = 0.222 \quad (7) $$

And, accordingly,

$$ \frac{M^*}{M} = 1.82. $$

The usual theory of perturbations ($\lambda = 0$) gives

$$ \frac{M^*}{M} = 2.15. $$

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