

Elastic scattering of ^4He atoms at the surface of liquid helium

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Elastic scattering of ^4He atoms when they approach the surface of ^4He liquid, has been studied. The liquid surface is assumed to be uniform and the density profile is the same along and perpendicular to the surface. The incident ^4He atom will interact with a large number of ^4He atoms in the liquid near the surface of liquid ^4He . Hence, the effective interaction of the incident particle will be due to many-body forces. The many-body forces are represented by the t -matrix. In the equation for potential energy per atom in the bulk liquid, the pair potential was replaced by the t -matrix. The Gaussian potential used in calculating the expectation value of the t -matrix is equivalent to the Lennard-Jones potential. The results give quantitative agreement with the corresponding experimental values for ^4He for the various values of χ^2 . The potential energy per atom in the bulk liquid obtained in this calculation is -20.130 K. The experimental energy of interaction is -20.81K, which implies that the formula derived by us for the potential energy per atom in the bulk liquid works well.

Keywords: Elastic scattering, ^4He atoms, t -matrix, Potential energy

1 Introduction

The free surface of liquid ^4He is very simple, clean and amenable to theoretical and experimental investigations¹. The density profile of the surface has been measured with increased accuracy² and it has been found to extend unusually because of the quantum nature of liquid helium. The surface supports quantized capillary waves called ripples, which are thermally excited² whereas elementary excitations at solid surface are rather well understood, relatively little is known about the elementary excitations at fluid surface (i.e. ripples). In a normal fluid, these excitations are overdamped at large wave vectors due to the effect of viscosity. In a superfluid, the damping is expected to be much lower, hence, the observation of well-defined excitation with wavelengths down to inter-atomic distances should be possible. An obvious system for this purpose is ^4He below the lambda temperature and, in fact, the existence of a large wave-vector ripples both on bulk ^4He and in films has been predicted by theory and has indirectly been confirmed experimentally³.

Theorists interested in the properties of inhomogeneous quantum many-body systems investigated on the subject^{4,5} and detailed calculations for the free surface of bulk ^4He and films of atomic thickness absorbed on a solid substrate at coverage have yielded the dispersion relation and the dynamic structure factor of the elementary excitations in the

microscopic regime, i.e., for large wave vectors. The theories above do not involve ripples. Attempts at obtaining reflectivity $R(k_z)$ have been made by considering the creation of ripples on the liquid surface by the incoming atom^{6,7}. The measured reflectivity could only be reproduced by such models in the limit of very low energy ripples such that ripplon production by the reflecting atom is not important.

Edwards and co-workers⁸⁻¹¹ have measured the reflectivity of ^4He from the surface at low temperature ($T < 40$ mK) where thermal ripples are unimportant. Edward and Fatouros¹² developed a theory for the reflectivity at a translationally invariant liquid helium surface ($T = 0$ K), which shows that reflectivity depends upon the density profile, especially in the low-density region. They obtained a density profile for the surface by fitting this model to the measurements. The extensive measurements of Edwards¹² have shown that the reflectivity $R(k_z)$ is a function of the incident angle. These parameters are independent and so reflectivity $R(k_z)$ can be expressed as a function of the wave vector component k_z that is perpendicular to the plane of the surface. This arises because the surface is translationally invariant when there are no ripples or other defects present, then, the Schrödinger equation for the atomic wavefunctions can be resolved into independent components parallel and perpendicular to the surface. It is found that $R(k_z)$

tends to unity as $k \rightarrow 0$. This is due to the surface potential profile appearing more abrupt and more reflecting for the incident atoms with longer wavelengths. Edwards and Fatouros¹² obtained the following equation relating the static effective potential $U(z)$ to the superfluid density. This can be obtained as follows:

$$\frac{-\eta^2}{2m} \left(\frac{\partial^2 \psi}{\partial z^2} \right) + V(z) \psi = -E_B \psi \quad \dots(1)$$

where $U(z)$ is the static effective potential, m is the mass of the ^4He atom and E_B is the binding energy of the atom in the bulk. The z -dependence of the potential $U(z)$ is defined by the local curvature of the superfluid density. A functional form for ψ was chosen, which gave the asymptotic behaviour $U(z) = -Cz^{-3}$ for large z , i.e., consistent with the long range Van der Waals attraction. The magnitude of C was determined from an interatomic potential. The Schrödinger equation for the scattered atom was numerically integrated through the surface to obtain $R(k_z)$ so as to compare with the measured reflectivity.

In a variation upon this model, Edward and Fatouros¹² also used the different approach of integrating over all the interatomic potentials to get $U(z)$. However, they found that the density $n(z)$ could not be determined uniquely. In the present study, we have not calculated $R(k_z)$. We have calculated the energy of interaction V_B and the binding energy E_B . Previous studies¹ have been carried out under the assumption that when ^4He atom approaches the surface of ^4He liquid, it will interact with one atom in the liquid. Hence, the effective interaction used in the previous studies is a two-body interaction. When calculating the potential above the liquid surface, the correction to the sum of their pair potentials due to the many-body correlations becomes important because of the close proximity of the condensed atoms to each other¹³.

In liquid helium, the higher order correlations increase the binding energy over that calculated one only using pair potentials^{14,15}. Consequently, this would give an apparent increase in the strength of the r^{-6} term in the pair potential over the dilute gas value. When a ^4He atom approaches the surface of ^4He liquid, the incident atom is likely to interact with a large number of ^4He atoms in the liquid near the surface of ^4He liquid. In a more realistic sense, the effective interaction of the incident particle will be due to many-body forces. Hence, there is need to take into account multi-particle interactions.

In this study, since the density profile cannot be uniquely determined, the liquid surface will be assumed to be uniform and the density profile is the same along and perpendicular to the surface. The incident ^4He atom interacts with a large number of ^4He atoms in the liquid near the surface of the liquid ^4He . Therefore, the effective interaction that the incident particle will have is due to the many-body forces. Hence, we intend to pursue the following objectives in this study to derive the expression for potential energy per atom in the bulk liquid, and to calculate its numerical value.

2 Theory of ^4He Atom Scattering at the Liquid ^4He Surface

When ^4He atom approaches the surface of ^4He liquid, it will be scattered. The liquid surface will be assumed to be uniform and the density profile is the same along and perpendicular to the surface. The incident ^4He atom interacts with a large number of ^4He atoms in the liquid near the surface of liquid ^4He . Hence, the effective interaction of the incident particle will be due to the many-body forces. The many-body interaction is represented by the reactive matrix t_k . In the equations for the potential energy per atom in the bulk liquid, the pair potential is replaced by the reaction matrix:

$$t_k = V(r) + V(r)G_0V(r) + V(r)G_0V(r)G_0V(r) + \dots \dots(2)$$

where $V(r)$ is the two-body interaction potential and G_0 the Green's function. The Gaussian form of the potential¹⁵ was used instead of the Lennard-Jones potential since integrations cannot be done using Lennard-Jones potential.

To derive the expression for the potential energy per atom in the bulk liquid ^4He using the t-matrix formalism, the expectation value of the t-matrix can be written as:

$$\langle t_k \rangle = \int e^{ikr} t_k e^{-ikr} d\tau \quad \dots(3)$$

where t_k is given by Eq. (2) and $d\tau$ is expressed in spherical co-ordinates as:

$$d\tau = r^2 \sin \theta d\theta d\phi dr \quad \dots(4)$$

Using Eqs (1 and 2), t_k becomes:

$$\begin{aligned} \langle t_k \rangle = & \int e^{ikr} V e^{-ikr} r^2 \sin \theta d\theta d\phi dr \\ & + \int e^{ikr} V G_0 V e^{-ikr} r^2 \sin \theta d\theta dr + \dots \end{aligned} \quad \dots(5)$$

$$\begin{aligned} \langle t_k \rangle = & \int_0^\infty V r^2 dr \int_0^{2\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \\ & + \int_0^\infty V G_0 V r^2 dr \int_0^{2\pi} \sin \theta d\theta \int_0^{2\pi} d\phi + \text{other terms} \end{aligned} \quad \dots(6)$$

$$\begin{aligned} \langle t_k \rangle = & \int_0^\infty V r^2 dr [-\cos \theta]_0^\pi [-\phi]_0^{2\pi} \\ & + \int_0^\infty V G_0 V r^2 dr [-\cos \theta]_0^\pi [-\phi]_0^{2\pi} + \text{other terms} \end{aligned}$$

$$\langle t_k \rangle = 4 \int_0^\infty V r^2 dr + \int_0^\infty V G_0 V r^2 dr + \text{other terms} \quad \dots(7)$$

The two body interaction potential $V(r)$ can be expressed as :

$$V(r) = \begin{cases} \infty & r < a \\ 4\xi \left[e^{-\left(\frac{r-a}{\mu_r}\right)^2} - e^{-\left(\frac{r-a}{\mu_a}\right)^2} \right] & r \geq a \end{cases} \quad \dots(8)$$

where $2a$ is the hard-core diameter, μ_r is the repulsive range of the Gaussian potential, μ_a the attractive range of the Gaussian potential and ξ is the energy in erg. The values of $G_0(a, r)$, $G_0(a, a)$ can be expressed as^{15,16}:

$$G_0(a, r) = \frac{a}{r} G_0(a, a) = -2 \frac{a^3 m \rho}{-\chi^2 \eta^2 r} \quad \dots(9)$$

where $\chi^2 = 2 \frac{Na^2 m}{\eta^2 G_0(a, a)}$ and $G_0(a, a) = -\frac{m}{4\pi a}$

Since the rest of the quantities in Eq. (9) are constants, χ^2 depends on the variable a (hard-core radius). The potential energy per atom in the bulk liquid can be calculated using the t-matrix formalism expressed in Eq. (7). Substituting Eq. (9) into (7), we get:

$$\begin{aligned} \langle t_k \rangle = & 16\pi\xi \int_a^\infty e^{-\left(\frac{r-a}{\mu_r}\right)^2} r^2 dr - \int_a^\infty e^{-\left(\frac{r-a}{\mu_a}\right)^2} r^2 dr \\ & - \frac{128\pi\xi^2 a^3 m \rho}{\chi^2 \eta^2} \int_a^\infty e^{-2\left(\frac{r-a}{\mu_r}\right)^2} r dr \end{aligned}$$

$$\begin{aligned} & - \frac{128\pi\xi^2 a^3 m \rho}{\chi^2 \eta^2} \int_a^\infty e^{-2\left(\frac{r-a}{\mu_a}\right)^2} r dr \\ & + \frac{256\pi\xi^2 a^3 m \rho}{\chi^2 \eta^2} \int_a^\infty e^{-\left(\frac{r-a}{\mu_r}\right)^2} e^{-\left(\frac{r-a}{\mu_a}\right)^2} r dr \end{aligned} \quad \dots(10)$$

Upon integration of Eq. (10) and using the substitution $r-a=x$ and therefore, $dr=dx$, the following equations are obtained:

$$\int_a^\infty e^{-\left(\frac{r-a}{\mu_r}\right)^2} r^2 dr = \frac{1}{4} \mu_r^3 \sqrt{\pi} + \mu_r^2 a + \frac{a^2 \mu_r}{2} \sqrt{\pi} \quad \dots(11)$$

$$\int_a^\infty e^{-\left(\frac{r-a}{\mu_a}\right)^2} r^2 dr = \frac{1}{4} \mu_a^3 \sqrt{\pi} + \mu_a^2 a + \frac{a^2 \mu_a}{2} \sqrt{\pi} \quad \dots(12)$$

$$\int_a^\infty e^{-\left(\frac{r-a}{\mu_r}\right)^2} r dr = \frac{1}{4} \mu_r^2 + \mu_r a \sqrt{\frac{\pi}{2}} \quad \dots(13)$$

$$\int_a^\infty e^{-2\left(\frac{r-a}{\mu_a}\right)^2} r dr = \frac{1}{4} \mu_a^2 + \mu_a a \sqrt{\frac{\pi}{2}} \quad \dots(14)$$

$$\int_a^\infty e^{-\left(\frac{r-a}{\mu_r}\right)^2} e^{-\left(\frac{r-a}{\mu_a}\right)^2} r dr = \frac{\mu_a^2 \mu_r^2}{2(\mu_a^2 + \mu_r^2)} + \frac{a \mu_a \mu_r}{2} \sqrt{\frac{\pi}{\mu_a^2 + \mu_r^2}} \quad \dots(15)$$

Substituting Eqs (11-15) into Eq. (10), we get the expression for the potential energy per atom in the bulk liquid as:

$$\begin{aligned} \langle t_k \rangle = & 16\pi\xi \left[\frac{1}{4} \mu_r^3 \sqrt{\pi} + \mu_r^2 a + \frac{a^2 \mu_r}{2} \sqrt{\pi} \right] \\ & - 16\pi\xi \left[\frac{1}{4} \mu_a^3 \sqrt{\pi} + \mu_a^2 a + \frac{a^2 \mu_a}{2} \sqrt{\pi} \right] \\ & - \frac{128\pi\xi^2 a^3 m \rho}{\chi^2 \eta^2} \left[\frac{1}{4} \mu_r^2 + \mu_r a \sqrt{\frac{\pi}{2}} + \frac{1}{4} \mu_a^2 + \mu_a a \sqrt{\frac{\pi}{2}} \right] \\ & + \frac{256\pi\xi^2 a^3 m \rho}{\chi^2 \eta^2} \left[\frac{\mu_a^2 \mu_r^2}{2(\mu_a^2 + \mu_r^2)} + \frac{a \mu_a \mu_r}{2} \sqrt{\frac{\pi}{\mu_a^2 + \mu_r^2}} \right] \end{aligned} \quad \dots(16)$$

The general expression for the zero-point kinetic energy is:

$$K_0 = \frac{\eta^2}{2m(\Delta q)^2} \quad \dots(17)$$

where Δq is the distance between two helium atoms at the time of elastic scattering of the incident helium atom from the surface of the liquid helium.

3 Results

Since the scattering of ^4He particles from the surface of ^4He liquid is assumed to be elastic, the kinetic energy is conserved. The potential energy per atom in the bulk liquid was found by integrating over the expectation value of a reaction matrix from the hard-core radius to infinity. The formula for $\langle t_k \rangle$ takes into account the many body interaction since the scattering of a ^4He atom at the surface of ^4He liquid is many-body interaction and not a two-body interaction. When a ^4He atom approaches the surface of ^4He liquid, it will interact with a large number of ^4He atoms near the surface of the liquid ^4He . The effective interaction of the incident particle will be due to the many-body forces. The many-body interaction is represented by the reaction matrix t_k .

The Gaussian potential was used and not the Lennard-Jones potential. Khanna and Das¹⁵ fitted the experimental curve with the potential, which was used in this study. The Gaussian potential used is equivalent of the Lennard-Jones potential. The potential energy per atom in the bulk liquid was obtained. The value of χ^2 was varied between 10 and 58 for each value of the reaction matrix. Tucker and Wyatt¹ obtained potential energy per atom in the bulk liquid ^4He as $V_B = -20.81$ K whereas the measured binding energy¹⁷ has a value $E_B = -7.16$ K. The contribution to the kinetic energy from the superfluid density gradients is zero in the bulk liquid. This fixes the zero-point kinetic energy in the bulk liquid at $K_0 = 13.65$ K, which is close to the value obtained using neutron scattering measurements¹⁸ of $K_0 = 13.3 \pm 1.3371$ K.

Figure 1 shows the graph of expectation value of the reaction matrix against chi-square for various values of the hard-core radius of the atoms. Increasing the values of hard-core radii and at the chi-square values of $\chi^2 = 23, 24, 32$ and 38 give Van der Waals potentials of $V_B = \langle k \rangle = -21.337, -21.047, -21.213$ and -20.576 K, respectively. It can be seen in Fig. 1 that as χ^2 approaches 58, expected values of -6.457 K and -8.535 K are obtained, which are close to the measured binding energy¹⁷ of $E_B = -7.16$ K. This value corresponds to the large values of the hard-core

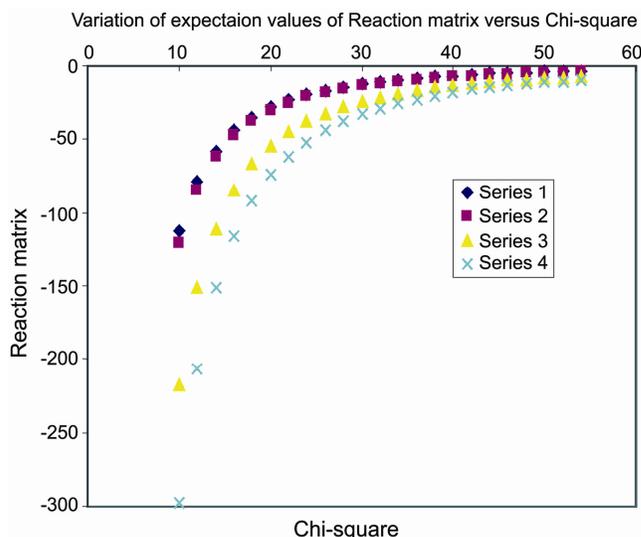


Fig. 1 — Relation between the expectation value of the reaction matrix $\langle t_k \rangle$ and the Chi-square. Series 1: $a = 2.05 \text{ \AA}$, Series 2: $a = 2.10 \text{ \AA}$, Series 3: $a = 2.556 \text{ \AA}$, Series 4: $a = 2.84 \text{ \AA}$

radius. We can similarly locate values of $\langle t_k \rangle$, which are close to E_B for some definite values of χ^2 . The zero-point kinetic energy somehow does not appear in the final value of $\langle t_k \rangle$.

The values of $\langle t_k \rangle$ for the various values of χ^2 were computed and tabulated for each potential width. The values of the core radii used include $2.05, 2.10, 2.56$ and 2.84 \AA . For a core radius of 2.05 \AA , the gradient of the graph changed sharply when the energy of interaction was reduced to about -120 K. As the value of χ^2 was increased, the energy of interaction was reduced to about -20 K and, hence, the changes in the gradient become insignificantly small. With a core radius of 2.10 \AA , the gradient of the graph changed sharply when the energy of interaction was about -125 K. As the value of c_2 is increased, the energy of interaction reduced to about -20 K, before the gradient becomes insignificantly small. For the radii of 2.56 \AA and 2.84 \AA , the graphs changed sharply when the energy of interaction was about -120 K and -300 K, respectively. Once again as the value of χ^2 was increased, the energy of interaction reduced to about -20 K.

At the point where there is insignificant change in the gradient of the graph as the value of χ^2 was increased, all the atoms are assumed to have equal potential energy in the bulk liquid. It was noted that this point (-20 K) was the same for all potential widths used in this calculation and, therefore, gives the potential energy per atom in the bulk liquid. This value is irrespective of the potential used. From the

Table 1 — Relation between the expectation value of the reaction matrix $\langle t_k \rangle$ and χ^2

| χ^2 | $\langle t_k \rangle$ for Hard-core diameter 'a' | | | |
|----------|--------------------------------------------------|----------|----------|----------|
| | a=2.05Å | a=2.10Å | a=2.556Å | a=2.840Å |
| 10 | -112.874 | -121.232 | -217.225 | -297.111 |
| 12 | -78.385 | -84.189 | -150.854 | -206.327 |
| 14 | -57.589 | -61.853 | -110.829 | -151.587 |
| 16 | -44.091 | -47.356 | -84.854 | -116.059 |
| 18 | -34.818 | -37.417 | -67.045 | -91.701 |
| 20 | -28.218 | -30.308 | -54.306 | -74.278 |
| 22 | -23.321 | -25.048 | -44.881 | -61.387 |
| 24 | -19.600 | -21.047 | -37.713 | -51.582 |
| 26 | -16.697 | -17.934 | -32.134 | -43.951 |
| 28 | -14.397 | -15.463 | -27.707 | -37.897 |
| 30 | -12.542 | -13.470 | -24.136 | -33.012 |
| 32 | -11.023 | -11.839 | -21.213 | -29.015 |
| 34 | -9.764 | -10.487 | -18.791 | -25.702 |
| 36 | -8.245 | -9.354 | -16.761 | -22.925 |
| 38 | -7.421 | -8.396 | -15.043 | -20.576 |
| 40 | -6.715 | -7.577 | -13.577 | -18.569 |
| 42 | -6.105 | -6.873 | -12.314 | -16.069 |
| 44 | -5.334 | -6.262 | -11.220 | -14.672 |
| 46 | -4.899 | -5.729 | -10.266 | -13.450 |
| 48 | -4.515 | -5.262 | -9.428 | -12.374 |
| 50 | -4.174 | -4.661 | -8.689 | -11.423 |
| 52 | -3.871 | -4.316 | -8.033 | -10.577 |
| 54 | -3.474 | -4.008 | -7.449 | -9.822 |

Table 2 — Summary of important results obtained from the calculations

| Core radius a Å | Chi-square χ^2 | Expectation value, $\langle t_k \rangle$ | Potential V_B | Binding energy, E_B |
|--------------------|------------------------|---------------------------------------------|--------------------|--------------------------|
| 2.050 | 23 | -21.337 | -20.81 | -3.355 |
| 2.100 | 24 | -21.047 | -20.81 | -3.866 |
| 2.556 | 32 | -21.213 | -20.81 | -7.181 |
| 2.840 | 38 | -21.576 | -20.81 | -9.474 |

work done, it was noted that the following pairs of the χ^2 and hard-core radius, respectively, gave the value of the expectation values that agree with the measured data as presented in Table 2. From the data, the average value of the Van der Waals $V_B = \langle t_k \rangle = -20.30$ K. This is with agreement with the value obtained by Tucker and Wyatt¹, who obtained $V_B = -20.81$ K.

4 Discussion and Conclusions

The question of interaction between particles is a matter of probability, whose function follows a chi-square distribution with various values of χ^2 . Unlike previous studies that analyzed ^4He scattering at the liquid helium in terms of the two-body interaction,

this study has taken a more realistic approach of the many-body interactions due to the close proximity of the condensed atoms to each other. The incident ^4He atom interacts with a large number of ^4He atoms in the liquid near the surface of liquid ^4He . To sum up the repeated scattering of particles, the *t-matrix* has been used. Using the Gaussian potential with the Green function, the expectation value of the reaction matrix t_k is calculated. Results show a general increase in the expectation value of the reaction matrix $\langle t_k \rangle$ as the hard-core radius of the atom decreases. As the value of χ^2 and the core radii increase, the energy of interaction reduced to about -20 K, before the gradients became insignificantly small. At the point where there is insignificant change in the gradient of the graph as the value of χ^2 increases, all the atoms are assumed to have equal potential energy in the bulk liquid. The point of -20 K shared by all the potential widths used in this study gives the potential energy per atom in the bulk liquid. Results show the average value of Van der Waals $V_B = \langle t_k \rangle = -20.130$ K which is in agreement with the value obtained by Tucker and Wyatt¹, their value being $V_B = -20.81$ K. Now, the measured value of binding energy is $E_B = -7.16$ K; hence, the zero point kinetic energy in the bulk liquid according to our calculations is $K_0 = 12.97$ K, which is close to the value obtained by neutron scattering experiment¹⁸, $K_0 = 13.3 \pm 1.3$ K. The distance between the helium atoms at the time of elastic scattering of the incident helium atom from the surface of liquid helium is $\Delta q = 2.17 \times 10^{-20}$ m.

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