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

P K Torongey$^1$, K M Khanna$^1$, Y K Ayodo$^2$, W T Sakwa$^2$, F G Kanyeki$^1$, R T Ekai$^1$, R N Kimengichi$^1$ & S Rotich

$^1$Department of Physics, Moi University, Box 1125-Eldoret-Kenya
$^2$Department of Physics, Masinde Muliro University, Box 190-Kakamega-Kenya

E-mail: yudah2000@yahoo.com

Received 23 April 2010; accepted 11 August 2010

Elastic scattering of $^4$He atoms when they approach the surface of $^4$He 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 $^4$He atom will interact with a large number of $^4$He atoms in the liquid near the surface of liquid $^4$He. 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 $^4$He for the various values of $\chi$. 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, $^4$He atoms, t-matrix, Potential energy

1 Introduction

The free surface of liquid $^4$He is very simple, clean and amenable to theoretical and experimental investigations$^1$. The density profile of the surface has been measured with increased accuracy$^2$ and it has been found to extend unusually because of the quantum nature of liquid helium. The surface supports quantized capillary waves called ripplons, which are thermally excited$^3$ whereas elementary excitations at solid surface are rather well understood, relatively little is known about the elementary excitations at fluid surface (i.e. ripplons). 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 $^4$He below the lambda temperature and, in fact, the existence of a large wave-vector ripplons both on bulk $^4$He and in films has been predicted by theory and has indirectly been confirmed experimentally$^4$.

Theorists interested in the properties of inhomogenous quantum many-body systems investigated on the subject$^4,5$ and detailed calculations for the free surface of bulk $^4$He 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 ripplons. Attempts at obtaining reflectivity $R(k_z)$ have been made by considering the creation of ripplons 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 ripplons such that ripplon production by the reflecting atom is not important.

Edwards and co-workers$^8-11$ have measured the reflectivity of $^3$He from the surface at low temperature ($T<40$ mK) where thermal ripplons are unimportant. Edward and Fatouros$^{12}$ 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 Edwards$^{15}$ 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 ripplons 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 $k \to 0$. This is due to the surface potential profile appearing more abrupt and more reflecting for the incident atoms with longer wavelengths. Edwards and Fatouros\textsuperscript{12} obtained the following equation relating the static effective potential $U(z)$ to the superfluid density. This can be obtained as follows:

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

where $U(z)$ is the static effective potential, $m$ is the mass of the $^4$He 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 $\psi$ 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 $R(k_s)$ so as to compare with the measured reflectivity.

In a variation upon this model, Edward and Fatouros\textsuperscript{12} 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 $R(k_s)$. We have calculated the energy of interaction $V_B$ and the binding energy $E_B$. Previous studies\textsuperscript{1} have been carried out under the assumption that when $^4$He atom approaches the surface of $^4$He 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 other\textsuperscript{13}.

In liquid helium, the higher order correlations increase the binding energy over that calculated one only using pair potentials\textsuperscript{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 $^4$He atom approaches the surface of $^4$He liquid, the incident atom is likely to interact with a large number of $^4$He atoms in the liquid near the surface of $^4$He liquid. In a more realistic sense, the effective interaction of the incident particle will be due to many-body forces. Hence, there is no 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 $^4$He atom interacts with a large number of $^4$He atoms in the liquid near the surface of the liquid $^4$He. 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 $^4$He Atom Scattering at the Liquid $^4$He Surface

When $^4$He atom approaches the surface of $^4$He 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 $^4$He atom interacts with a large number of $^4$He atoms in the liquid near the surface of liquid $^4$He. 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 $r_k$. In the equations for the potential energy per atom in the bulk liquid, the pair potential is replaced by the reaction matrix:

$$t_k = V(r) + V(r)G_0V(r) + V(r)G_0V(r)G_0V(r) + \ldots \quad \text{(2)}$$

where $V(r)$ is the two-body interaction potential and $G_0$ is the Green’s function. The Gaussian form of the potential\textsuperscript{15} 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 $^4$He using the t-matrix formalism, the expectation value of the $t$-matrix can be written as:

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

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

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

Using Eqs (1 and 2), $t_k$ becomes:

$$\langle t_k \rangle = \int e^{ikr} V r e^{-ikr} r^2 \sin \theta d\theta d\phi dr + \int e^{ikr} V G_0 V e^{-ikr} r^2 \sin \theta d\theta d\phi d\tau + \ldots \quad \text{(5)}$$
\[ \langle t_k \rangle = \frac{1}{\sin \theta d\theta} \int_0^{2\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \]
\[ + \int V G_0 V r^2 dr \int_0^{2\pi} \sin \theta d\theta \int_0^{2\pi} d\phi + \text{other terms} \]
\[ \langle t_k \rangle = \int V r^2 dr \left[ -\cos \theta \right]_0^\theta \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi + \text{other terms} \]
\[ \langle t_k \rangle = 4 \int V r^2 dr + \int V G_0 V r^2 dr + \text{other terms} \]
\[ \langle t_k \rangle = \frac{2}{\sin \theta} \int_0^{2\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \]
\[ + \int V G_0 V r^2 dr \int_0^{2\pi} \sin \theta d\theta \int_0^{2\pi} d\phi + \text{other terms} \]
\[ \langle t_k \rangle = \frac{2}{\sin \theta} \int_0^{2\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi + \text{other terms} \]

The two body interaction potential \( V(r) \) can be expressed as:
\[ V(r) = \begin{cases} \frac{2\pi}{\sin \theta} \int_0^{2\pi} \sin \theta d\theta \int_0^{2\pi} d\phi & r < a \\ \frac{a}{r} G_0(a,a) - \frac{2a^3 m \rho}{\chi^2 \eta^2 r} & r \geq a \end{cases} \]

where \( 2a \) is the hard-core diameter, \( \mu_r \) is the repulsive range of the Gaussian potential, \( \mu_a \) the attractive range of the Gaussian potential and \( \xi \) is the energy in erg.

The values of \( G_0(a,r), G_0(a,a) \) can be expressed as:
\[ G_0(a,r) = \frac{a}{r} G_0(a,a) = -\frac{2a^3 m \rho}{\chi^2 \eta^2 r} \]

The general expression for the zero-point kinetic energy is:
\[ \langle t_k \rangle = 4\pi \zeta \left[ \frac{1}{4} \mu_r^3 \sqrt{\pi + \mu_a^2 a + \frac{a^2 \mu_r}{2}} \right] \]
\[ -16\pi \zeta \left[ \frac{1}{4} \mu_r^3 \sqrt{\pi + \mu_a^2 a + \frac{a^2 \mu_a}{2}} \right] \]
\[ -128\pi \zeta^2 a^3 m \rho \left[ \frac{1}{4} \mu_r^2 + \mu_a a \sqrt{\frac{\pi}{2} + \frac{1}{4} \mu_a^2 + \mu_a \sqrt{\frac{\pi}{2}}} \right] \]
\[ + 256\pi \zeta^2 a^3 m \rho \left[ \frac{\mu_r^2 \mu_a}{2 \left( \mu_a^2 + \mu_r^2 \right)} + \frac{a \mu_a \mu_r}{2 \left( \mu_r^2 + \mu_a^2 \right)} \sqrt{\frac{\pi}{\mu_r^2 + \mu_a^2}} \right] \]
where $\Delta q$ 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 $^4$He particles from the surface of $^4$He 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 $^4$He atom at the surface of $^4$He liquid is many-body interaction and not a two-body interaction. When a $^4$He atom approaches the surface of $^4$He liquid, it will interact with a large number of $^4$He atoms near the surface of the liquid $^4$He. 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 Das$^{15}$ 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 $\chi^2$ was varied between 10 and 58 for each value of the reaction matrix. Tucker and Wyatt$^6$ obtained potential energy per atom in the bulk liquid $^4$He as $V_B=-20.81$ K whereas the measured binding energy$^{17}$ 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 measurements$^{18}$ of $K=0=13.33\pm1.3371$ 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 $\chi^2$ approaches 58, expected values of $-6.457$ K and $-8.535$ K are obtained, which are close to the measured binding energy$^{17}$ of $E_B=-7.16$ K. This value corresponds to the large values of the hard-core radius. We can similarly locate values of $\langle t_k \rangle$, which are close to $E_B$ for some definite values of $\chi^2$. 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 $\chi^2$ were computed and tabulated for each potential width. The values of the core radii used include 2.05, 2.10, 2.56 and 2.84Å. For a core radius of 2.05Å, the gradient of the graph changed sharply when the energy of interaction was reduced to about $-120$ K. As the value of $\chi^2$ 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 2.10Å, the gradient of the graph changed sharply when the energy of interaction was about $-125$ K. As the value of $\epsilon^2$ is increased, the energy of interaction reduced to about $-20$ K and, before the gradient becomes insignificantly small. For the radii of 2.56Å and 2.84Å, the graphs changed sharply when the energy of interaction was about $-120$ K and $-300$ K, respectively. Once again as the value of $\chi^2$ 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 $\chi^2$ 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
work done, it was noted that the following pairs of the \( \chi^2 \) 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 \( V_B = \langle t_k \rangle = -20.130 \) K which is in agreement with the value obtained by Tucker and Wyatt\(^1\), 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 experiment\(^1\), \( K_0 = 13.3 \pm 1.3 \) 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.

**Acknowledgement**

The authors are very grateful to Moi and Masinde Muliro Universities for availing the necessary texts and journals that were useful in the preparation of this manuscript.

**References**


---

**Table 1** — Relation between the expectation value of the reaction matrix \( \langle t_k \rangle \) and \( \chi^2 \)

<table>
<thead>
<tr>
<th>( \chi^2 )</th>
<th>( \langle t_k \rangle ) for Hard-core diameter ( 'a' )</th>
<th>Potential ( V_B )</th>
<th>Binding energy ( E_B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a=2.05A )</td>
<td>10 −112.874</td>
<td>−21.337</td>
<td>−20.81</td>
</tr>
<tr>
<td></td>
<td>12 −78.385</td>
<td>−21.047</td>
<td>−20.81</td>
</tr>
<tr>
<td></td>
<td>14 −57.589</td>
<td>−11.839</td>
<td>−11.423</td>
</tr>
<tr>
<td></td>
<td>16 −44.091</td>
<td>−8.396</td>
<td>−10.577</td>
</tr>
<tr>
<td></td>
<td>18 −34.818</td>
<td>−7.421</td>
<td>−9.472</td>
</tr>
<tr>
<td></td>
<td>20 −19.600</td>
<td>−6.715</td>
<td>−8.832</td>
</tr>
<tr>
<td></td>
<td>22 −14.899</td>
<td>−5.329</td>
<td>−8.184</td>
</tr>
<tr>
<td></td>
<td>24 −11.023</td>
<td>−3.846</td>
<td>−7.181</td>
</tr>
<tr>
<td></td>
<td>26 −8.245</td>
<td>−2.371</td>
<td>−6.214</td>
</tr>
<tr>
<td></td>
<td>28 −6.105</td>
<td>−1.576</td>
<td>−5.247</td>
</tr>
</tbody>
</table>

---

**Table 2** — Summary of important results obtained from the calculations

<table>
<thead>
<tr>
<th>Core radius ( a ) ( \chi^2 )</th>
<th>Chi-square ( \chi^2 )</th>
<th>Expectation value, ( \langle t_k \rangle )</th>
<th>Potential ( V_B )</th>
<th>Binding energy, ( E_B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.050</td>
<td>23</td>
<td>−21.337</td>
<td>−20.81</td>
<td>−3.355</td>
</tr>
<tr>
<td>2.100</td>
<td>24</td>
<td>−21.047</td>
<td>−20.81</td>
<td>−3.866</td>
</tr>
<tr>
<td>2.556</td>
<td>32</td>
<td>−21.213</td>
<td>−20.81</td>
<td>−7.181</td>
</tr>
<tr>
<td>2.840</td>
<td>38</td>
<td>−21.576</td>
<td>−20.81</td>
<td>−9.474</td>
</tr>
</tbody>
</table>

---

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 \( \chi^2 \). Unlike previous studies that analyzed \( ^4 \)He 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 \( ^4 \)He atom interacts with a large number of \( ^4 \)He atoms in the liquid near the surface of liquid \( ^4 \)He. 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 \( \langle t_k \rangle \) 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 \( \chi^2 \) 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 \( \chi^2 \) 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 Wyatt\(^1\), 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 experiment\(^1\), \( K_0 = 13.3 \pm 1.3 \) 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.