Quantum reflection coefficients in a condensed matter interface

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Abstract. The problem of wave transmission across an interface between a quantum liquid and a solid is considered using many body theory. The model Hamiltonian operator considered, assumes a smooth interface with localized interaction on the surface and solid amplitudes within the linear phonon approximation. Expressions for the reflection coefficients for the waves incident from the liquid or the solid are obtained within the Hartree Fock approximation. An explicit result is given for the reflection coefficient in the solid as a function of temperature and frequency. A comparison to the classical theory and to experimental results are briefly discussed.

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1. Introduction

One of the areas of research in which Leopoldo has made significant contributions pertains to systems close to thermodynamic equilibrium. His treatments have been both macroscopic and microscopic [1]. For this reason I chose to write about a related problem in the context of quantum many body theory.

The problem to be discussed is motivated by a generic situation arising when two materials at different temperatures are put in contact with each other. From the laws of thermodynamics we know that the system will try to reach either thermal equilibrium, if the two materials are isolated from the rest of the universe, or they will establish a stationary state if there is a reservoir that makes sure that there is a constant heat flux $Q$ between the materials. It is found that very close to the interface, for distances on the order of tens of angstroms, there is a jump or discontinuity $\Delta T$ in the temperature profile so that the flow of heat from the cold to the warm material experiences a "surface thermal resistance" to the heat flow between them. The existence of this phenomenon was discovered by Kapitza in 1941 when he was trying to cool down helium [2]. It is clear that if one wants to cool a system the easiest way to do it is to put it in contact with a cooler one. Kapitza found that there was an inherent thermal resistance to the heat flow when liquid helium is put in contact with a solid. This surface thermal resistance is known as
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the "Kapitza resistance" and a significant body of work has been dedicated to its understanding. The Kapitza resistance per unit surface is defined as

\[ K_R = \lim_{\Delta T \to 0} \frac{\Delta T}{Q}. \]  

(1)

A few years later Khalatnikov produced an explanation as to why there is a resistance to the heat flow based on classical elasticity theory [3]. This theory is known as the acoustic mismatch theory or classical theory. I will briefly discuss the classical result for future comparison with the quantum treatment presented in this paper. It turns out that Khalatnikov's theory works quite well if the two materials that are in contact are "classical". In the case of $^4$He in contact with a solid the situation is different. It is found that both theoretically and experimentally, for temperatures between $T_\lambda$ and $1^\circ$K, $K_R \sim T^{-3}$. This means that the transfer of heat between $^4$He and a solid becomes increasingly difficult as the temperature is lowered and thus arises the difficulty in achieving lower $T$'s. I should emphasize that no anomalies were observed when the temperature was lowered passed $T_\lambda$ and thus the phenomenon has not appeared to be correlated with the onset of superfluidity in the liquid. At the beginning of the 1970's it was found experimentally that the classical theory fails whenever one of the systems is quantum. A solid is quantum whenever the DeBoer parameter $\Lambda^* > 1$. This parameter measures the importance of the zero point quantum fluctuations with respect to the potential energy of interaction in the system. The only materials that satisfy the DeBoer criteria to be quantum in increasing order are, D$_2$, HD, H$_2$, $^4$He and $^3$He.

The motivation for the work presented here is that of producing a quantum version of the Khalatnikov theory. Even to this day the properties of the surface, its degree of cleanliness, its faceted structure and other specific growth properties of the surface can influence the value of $K_R$. I would expect that the results obtained here will be good in the case where the surface is atomically smooth without imperfections.

The outline of the paper is the following: In Sect. 2 I review briefly the derivation of the results from the classical theory to point out its main characteristics and shortcomings. In Sect. 3 the model Hamiltonian is introduced and the corresponding Green function equations are derived. In Sect. 4 an approximate derivation of the general reflection coefficients for the energy transfer between the liquid and the solid are derived. In Sect. 5 an explicit result for the finite temperature and frequency reflection coefficient for the solid side is presented. Finally, in Sect. 6 a short discussion of the result and comparison to the classical theory is presented.

2. Classical Theory

I shall briefly discuss here the classical theory. The problem is that of finding out the main mechanisms for heat transfer between a solid and liquid $^4$He. In the classical theory, the Kapitza resistance is explained by the mismatch in the acoustic
properties of the two materials. The energy transfer between $^4$He and a solid can be
due to two sources: (i) The energy exchange resulting from the collisions between
the phonons and the rotons with the interface or (ii) by the radiation of the same
$^4$He excitations due to the solid's surface oscillations. $^4$He has properties that make
it very special, since it has a very low density as compared to that of the solid.
The effect of $^4$He on the solid is therefore quite weak. In the solid there are three
types of waves that can be excited in principle, transverse, longitudinal and surface
waves. The characteristics of these waves can be read off from any book on classical
elasticity theory since the effect of $^4$He on the solid is like that of the vacuum. In
fact, from the classical analysis it is clear that the transverse waves are not relevant
to the discussion and most of the contribution to the energy transfer comes from
the perpendicular component of the incident waves to the surface. We shall use this
fact to consider only perpendicular waves in the quantum treatment.

As the surface vibrates with frequency $\omega$ it will emit sound waves into the
surrounding liquid. Similarly, the phonons and rotons hitting the surface can in prin-
ciple exchange energy with the surface. Since the energy of the rotons is measured
by the roton gap $\Delta \gg k_B T$, with $k_B$ Boltzmann’s constant and $T$ the temperature, it
is clear that the probability that the surface will absorb or emit rotons is very low.
Therefore, the discussion will center about the energy exchange from the phonons
in the liquid and in the solid. These two types of phonons are however different. In
the $^4$He case, the phonons carry momentum and can only be longitudinal while
in the solid they do not carry momentum and they can be transversal as well as
longitudinal. The total energy exchanged between the liquid and the solid will then
be given by the energy coming from the solid to $^4$He minus the energy coming
from $^4$He to the solid. The total energy transferred across the interface is directly
proportional to the total phonon transmission coefficient. In the classical theory,
the transmission coefficient is calculated from elasticity theory together with the
Planck distribution to calculate the heat transfer.

The acoustic properties of a substance can be expressed in terms of its acoustic
impedance $Z = \rho C$, with $\rho$ its density and $C$ the speed of sound in the material.
In the case of $^4$He and, say, copper we have $Z_{^4\text{He}} = 10^{-3} Z_{\text{Cu}}$. This implies that the
majority of the phonons incident on the interface formed by Cu and $^4$He are reflected
specularly, independent of whether the phonon is incident from the solid or liquid
sides. To calculate the transmission coefficient in elasticity theory one assumes, as al-
ways, that there are incident, reflected and transmitted waves of frequency $\omega$. These
waves have amplitudes that are determined from the boundary conditions, in this
case by the continuity on the surface of the normal and tangential components of the
displacement vector and stresses, respectively. There can be also surface waves that
are excited by the incident phonons to the surface. However, the surface waves are
damped at relatively short distances in, for example, $^4$He and Cu so that these types
of waves make a small contribution to the total energy transfer and are therefore
also neglected [3]. Furthermore, most of the energy transferred is localized to the
cone of angles smaller than the critical angle for total internal reflection. In the case
of $^4$He and Cu this angle is $6^\circ$, quite small indeed. Therefore, one can concentrate
on the contributions due to waves incident perpendicular to the surface and forget
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about the angular dependence of the transmission and reflection coefficients. The continuity condition for the amplitudes in this case leads to \( A_i + A_r - A_t = 0 \), where \( i, r \), and \( t \) stand for incident, reflected and transmitted amplitudes, respectively. The continuity of the stresses yields the equation \( (A_i + A_r)C_L - C_S A_t (\rho_2/\rho_1) \). The reflection coefficient is defined by \( R = (A_r/A_i)^2 \) which, from the equations given above, leads to the result

\[
R = \left( \frac{Z_S - Z_L}{Z_S + Z_L} \right)^2
\]

In the case of \(^4\)He and Cu we have \( Z_L \ll Z_S \) so that \( R \sim 1 - 4(Z_L/Z_S) \). Assuming there is no energy loss in the transmission process, the transmission coefficient will then be simply given by

\[
\tau \sim 4 \frac{Z_L}{Z_S}.
\]

In the case of Cu and \(^4\)He, \( \tau \sim 10^{-3} \) so that very little energy is transmitted. This result is found to agree with experiment for temperatures in the range \( 1K \leq T \leq 100 K \), while it fails quantitatively in the range \( 10^{-3} K \leq T \leq 0.6 K \). Within the latter temperature range it is found that the classical theory is always off by one to two orders of magnitude. Furthermore, the classical result indicates that there is no frequency dependence for \( K_R \), while experimentally it is found otherwise. Since a strong disagreement between theory and experiment is found when the solid is in contact with a quantum substance. In the following sections I develop a quantum theory to calculate the transmission coefficient in a condensed matter system. In so doing I will use several of the simplifying assumptions made in the classical theory such as neglecting the roton contribution, surface and transverse waves, and consider only normal incidence.

3. Quantum Theory

Our goal here is to derive quantum expressions for the surface reflection coefficients for the system consisting of liquid \(^4\)He in contact with a solid. The treatment entails use of the temperature dependent Green function formalism. We need to derive the appropriate equations of motion for liquid \(^4\)He and the solid Green functions. In deriving the equations of motion we can either use the Heisenberg equations of motion or the Lagrangian operator formalism. Here I choose the former but both are conducive to the same equations.

3.1 The model

The model assumes that we have two gases, one of \(^4\)He atoms and the other of phonons, separated by an elastic surface (the solid’s surface). The surface can undergo small oscillations from its equilibrium position that are described by the surface displacement vector \( U_z(\vec{r}, t) \), where \( z \) denotes the axis perpendicular to the
surface, \( \vec{r} \) the three dimensional position vector, and \( t \) the time. The displacement \( U_z(\vec{r}, t) \) increases with temperature and its detailed time dependence is described in terms of the phonon modes of the semi-infinite solid. The surface equilibrium position is taken to be at \( U_z(\vec{r}, 0) = 0 \), and shall take \( U_z(\vec{r}, t) \), as the dynamic variable that describes the phonon modes in the solid.

The \(^4\)He liquid is described by the field operator \( \Psi(\vec{r}, t) \), obeying the usual commutation relations

\[
[\Psi(\vec{r}, t), \Psi(\vec{r}', t)]_- = [\Psi^\dagger(\vec{r}, t), \Psi^\dagger(\vec{r}', t)]_- = 0,
\]

and

\[
[\Psi(\vec{r}, t), \Psi^\dagger(\vec{r}', t)]_- = \delta(\vec{r} - \vec{r}').
\]

The Hamiltonian for the liquid is simply, \( (\hbar = 1 \text{ from now on}) \)

\[
\mathcal{H}_L = \frac{1}{2m} \int d\vec{r} \nabla \Psi^\dagger(\vec{r}, t) \cdot \nabla \Psi(\vec{r}', t) + \int d\vec{r} \int d\vec{r}' \Psi^\dagger(\vec{r}, t) \Psi^\dagger(\vec{r}', t) V(\vec{r} - \vec{r}') \Psi(\vec{r}', t) \Psi(\vec{r}, t). \tag{4}
\]

The first term is the kinetic energy of the \(^4\)He atoms with \( m \) their mass, the second their interactions. The \(^4\)He atoms interactions lead to an effective quasiparticle picture with appropriate renormalized effective mass. In our calculations we will replace the interaction by an effective renormalized single particle Bose field representing the phonon contribution in the energy spectrum of collective excitations in the fluid.

Considering the solid as an elastic medium its Hamiltonian is given by

\[
\mathcal{H}_s = \frac{1}{2} \int d\vec{r} \left\{ \frac{1}{\rho_s} \Pi^2_z + B(\nabla U_z)^2 \right\}, \tag{5}
\]

with \( \rho_s \) the density of the solid, \( B \) the adiabatic bulk modulus, and the dynamic variable

\[
\Pi_z = \rho_s \frac{\partial U_z}{\partial t},
\]

is the canonically conjugate variable to \( U_z \). The operators \( U_z \) and \( \Pi_z \) satisfy the commutation relations,

\[
[U_z(\vec{r}, t), U_{z'}(\vec{r}', t)]_- = [\Pi_z(\vec{r}, t), \Pi_{z'}(\vec{r}', t)]_- = 0,
\]

and

\[
[U_z(\vec{r}, t), \Pi_{z'}(\vec{r}', t)]_- = i\delta_{z, z'} \delta(\vec{r} - \vec{r}').
\]
To derive the Hamiltonian that describes the coupling between the two systems we proceed as follows. When the $^4$He atoms interact with the surface they exchange momentum. The work done by the $^4$He atoms on the surface can be expressed as

$$H_{SL} = \int d\vec{r} P(\vec{r}, t) \delta(z - U_z(\vec{r}, t)),$$

(6)

which has an easy physical explanation. $P(\vec{r}, t)$ stands for the $^4$He atom's microscopic pressure on the surface and the delta function guarantees that the interaction is localized on the surface. $P(\vec{r}, t)$ is, of course, related to the local momentum transport. The $k$th component of the momentum density operator $S_k$ is given as

$$S_k = \frac{1}{2i} \left[ \Psi^\dagger(\vec{r}, t) \partial_k \Psi(\vec{r}, t) - \partial_k \Psi^\dagger(\vec{r}, t) \Psi(\vec{r}, t) \right].$$

(7)

Using the Heisenberg equation of motion for $\Psi(\vec{r}, t)$

$$\frac{\partial \Psi}{\partial t} = [\Psi(t), H_L],$$

(8)

$S_k$ is shown to satisfy the continuity equation, $\partial_t S_k + \partial_j T_{jk}^L = 0$, where the stress tensor is given as

$$T_{jk}^L \equiv \frac{1}{2m} \left[ \partial_j \Psi^\dagger(\vec{r}, t) \partial_k \Psi(\vec{r}, t) + \partial_k \Psi^\dagger(\vec{r}, t) \partial_j \Psi(\vec{r}, t) - \frac{1}{2} \partial_j \partial_k (\Psi^\dagger(\vec{r}, t) \Psi(\vec{r}, t)) \right].$$

(9)

The local pressure is obtained from the trace of the stress tensor giving

$$P(\vec{r}, t) = \frac{1}{3m} \int d\vec{r} \nabla \Psi(\vec{r}, t)^\dagger \cdot \nabla \Psi(\vec{r}, t).$$

(10)

Here we neglected the laplacian terms because we assume that there is local uniformity in the liquid.

Since the discontinuity in the temperature between a solid and $^4$He takes place a few angstroms from the surface we can assume that the deviations from the single particle behavior is localized very near the surface. This is equivalent to requiring that the displacement of the surface from its equilibrium position is very small, which allows us to make the first order approximation

$$\delta(z - U_z(\vec{r}, t)) d\vec{r} \sim \delta(z) U_z(\vec{r}, t) dx dy.$$  

(11)

Here we replaced $dz$ for $U_z(\vec{r}, t)$ and expanded the Dirac $\delta$-function to lowest order. This implies that the coupling energy between the liquid and the solid becomes

$$H_{SL} = \frac{1}{3m} \int dx dy \int d\vec{r} \nabla \Psi(\vec{r}, t)^\dagger \cdot \nabla \Psi(\vec{r}', t) U_z(z).$$

(12)
As a convenient mathematical tool for generating the appropriate Green functions we include the source term
\[ \mathcal{H}_J = \int d\vec{r} J(\vec{r}, t) U_z(\vec{r}, t), \]
to the Hamiltonian, and \( J \) shall be taken to zero at the end of the calculation. Finally, the total model Hamiltonian describing the liquid solid interface problem is
\[ \mathcal{H} = \mathcal{H}_L + \mathcal{H}_S + \mathcal{H}_{SL} + \mathcal{H}_J. \] (13)

Using Heisenberg's equations of motion together with the commutation relations we obtain the equations of motion
\[ \hat{L} \Psi(2) = \frac{1}{3m} \int dx_1 dy_1 \delta(z_1) U_z(1) \nabla_x \cdot \nabla_{x'} [\Psi(1') \delta(\vec{r}_2 - \vec{r}_1)] \bigg|_{1 = 1'} \] (14)
\[ \rho_s \hat{S} U_z(1) = J(1) + \frac{1}{3m} \nabla \Psi(\vec{r}, t) \cdot \nabla \Psi(\vec{r}', t) \delta(z) \] (15)
where the differential operators \( \hat{L} \) and \( \hat{S} \) are defined as
\[ \hat{L} \equiv i \frac{\partial}{\partial t} + \frac{1}{2m} \nabla^2, \]
\[ \hat{S} \equiv \rho_s \left( \nabla^2 - \frac{1}{C_s^2} \frac{\partial^2}{\partial t^2} \right). \]

In writing the equations of motion we have used the notation \((\vec{r}_i, t_i) = (i)\) as well as the definition, \( C_s^2 = B/\rho_s \). Eqs. (14) and (15) form a set of coupled operator integro-differential equations from which we wish to determine \( \Psi \) and \( U_z \). Note that these equations have the feature that the coupling is entirely localized on the surface. As is usual, instead of trying to solve the equations for \( \Psi \) and \( U_z \) themselves, our procedure will be to solve their corresponding Green function equations. We derive the Green function equations in the following section.

### 3.2 Green function equations

The general properties of the temperature Green functions employed here can be found in the standard references [4]. In this particular case, the eigenstates of the composed system are constructed as direct products of the solid and liquid eigenstates, i.e., \(| \) = \(| L \otimes | S \rangle \), which are assumed to form a complete orthonormal set. The liquid and solid Green functions are then defined by
\[ g(1, 1') = -i \langle T (\Psi(1) \Psi(1')) \rangle \theta(-z) \theta(-z'), \] (16)
\[ D(1, 1') = -i \langle T (U_z(1) U_z(1')) \rangle \theta(z) \theta(z'). \] (17)

Here \( T \) stands for Wick's time ordering product and \( \theta \) is the standard step function, which will not be explicitly written from now on. The brackets denote the
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thermodynamic averages defined as usual, \( \langle A(t) \rangle = \langle e^{-\beta \mathcal{H}} A(t) \rangle / \langle e^{-\beta \mathcal{H}} \rangle \), with \( \beta^{-1} = k_B T \) and a sum over states is understood. The imaginary time variable in these Green functions is restricted to the interval \( 0 < it < \beta \). Because we assume that the solid and liquid systems are homogeneous in the plane parallel to the surface, both Green functions satisfy the rules \( g(\vec{r}, \vec{r}', t, t') = g(z, z', \vec{p} - \vec{p}', t - t') \), where \( \vec{p} \) is the two dimensional vector defined on the \( x-y \) plane. We shall use this property extensively in the following section.

Let us start with the liquid case. In Eq. (15) we can solve formally for \( U_z \) (setting \( J = 0 \)) in terms of the helium fields yielding

\[
U_z = \frac{1}{3 \rho_s} \int d\vec{r}' \nabla' \Psi(\vec{r}', t) \nabla' \Psi(\vec{r}', t) D_0(1, 1') \delta(z_1'), \tag{18}
\]

plus surface terms. Here \( D_0(1, 1') \) is defined as

\[
D_0(1, 1') \equiv \hat{S}^{-1} \delta(1, 1'), \tag{19}
\]

and satisfies the same boundary conditions as \( D(1, 1') \). The surface terms can be neglected requiring that the amplitude of the surface displacements are small enough with respect to the total dimensions of the surface. Substituting Eq. (18) back into Eq. (14), multiplying by \( \Psi^\dagger(3) \), time ordering and taking the thermodynamic average, we get the equation of motion for the one-particle liquid Green function

\[
\hat{L} g(2, 3) = \delta(2, 3) + i \epsilon \int dA \int dx_1 dy_1 D_0(1, 4) \delta(z_4) \delta(z_1) \\
\times \left[ \nabla_{\vec{r}_4} \nabla_{\vec{r}_4'} \nabla_{\vec{r}_1} \nabla_{\vec{r}_1'} g_2(1', 4'; 3, 4) \delta(\vec{r}_2 - \vec{r}_1) \right] \bigg|_{1=1', 4=4'} . \tag{20}
\]

Here we defined the coupling constant \( \epsilon = \rho_L / 3 \rho_s \). The two particle Green function \( g_2 \) is defined as

\[
g_2(1, 2; 3, 4) \equiv (-i)^2 \left\langle \mathcal{T} \left( \Psi(1) \Psi(2) \Psi^\dagger(3) \Psi^\dagger(4) \right) \right\rangle .
\]

Notice that the equation of motion is almost of the same form as the usual equations for a Bose field but with the differences that in this case the interactions are restricted to lie on the surface and we see extra gradients of \( g_2 \), which are due to the form of the pressure interaction and represent the transfer of energy between the two materials. As we shall see below, it will be useful to eliminate these gradients in favor of an energy Green function, of more relevance in this problem, rather than the single particle Green function.

To solve for \( g \) in Eq. (20) we need to know \( g_2 \). However, to get \( g_2 \) we need to solve another equation for \( g_2 \) itself. In fact the equation for \( g_2 \) will involve \( g_3 \) and the one for \( g_3 \) that of \( g_4 \) and so on and so forth. The first non trivial breaking of
this hierarchy involves the Hartree-Fock approximation which is

\[ g_2(4',1';4,3) = g(4',4)g(1',3) + g(1',4)g(4',3). \]

This approximation replaces the many body interaction between particles by an effective *mean field* interaction on each particle. Substituting this approximation for \( g_2 \) into Eq. (20) gives

\[
\dot{g}(2,3) = \delta(2,3) + i\epsilon \int d4 \int dx_1 dy_1 \ D_0(1,4) \delta(z_4) \delta(z_1) \\
\times \left[ \nabla_{\vec{r}_1} \nabla_{\vec{r}_1} (\delta(\vec{r}_2 - \vec{r}_1)g(1',3)G(4',4)) \right. \\
\left. - \nabla_{\vec{r}_1} \nabla_{\vec{r}_4} (\delta(\vec{r}_2 - \vec{r}_1)g(4',3)G(1',4)) \right] \bigg|_{1'=1',4'=4'}. \tag{21}
\]

Here is where the energy Green function is defined as

\[ G(1,1') = \nabla_{\vec{r}_1} \cdot \nabla_{\vec{r}_1} g(1,1'). \tag{22} \]

This function will play an important role in our future discussions. It satisfies many of the standard properties of the one particle Green function but not all, for example the sum rule for the weight function \( A(k_z, k_{z'}, k_{||}, \omega) \) instead of one in this case is

\[
- \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A = k_z k_{z'} + k_{||}^2,
\]

where \( k_z \) is the momentum vector along the perpendicular direction and \( k_{||} \) is the corresponding vector parallel to the surface. We obtain an equation for \( G \) itself by multiplying Eq. (21) by \( \hat{L}^{-1} \) and by \( \nabla_{\vec{r}_2} \cdot \nabla_{\vec{r}_3} \) on the left hand side, and using the definition \( g_0(1,1') \equiv \hat{L}^{-1}\delta(1,1') \) resulting in

\[
G(2,3) = G_0(2,3) + i\epsilon \int d4 \int dx_1 dy_1 dt_1 \delta(z_4) \delta(z_1) G_0(2,1) \\
\times \left[ G(4,4')G(1',3) + G(4',3)G(1',4) \right] D_0(1,4). \tag{23}
\]

We can rewrite this equation in a Dyson form

\[
G(2,3) = G_0(2,3) + i \int d4 \int dx_1 dy_1 dt_1 \ G_0(2,1) \Sigma(1,4) G(4,3), \tag{24}
\]

where the surface self energy \( \Sigma \) is defined as

\[
\Sigma(1,4) = \epsilon \delta(z_4) G(1,4) D_0(1,4) \delta(z_1). \tag{25}
\]
We now have transformed the problem of finding the single particle Green function $g$ from Eq. (21) to that of finding the energy Green function from Eq. (23), which satisfies formally a Dyson-like equation for a two particle interacting potential.

We move now to derive the Green function equation of motion for the solid. To find the equation of motion for $D(1,1')$ we take the average

$$
\langle A \rangle_J = -i \left< \frac{\mathcal{T} \left( A e^{-i \int_0^t dt \left[ \mathcal{H}_{SL} + \mathcal{H}_J \right] } \right)}{\mathcal{T} \left( e^{-i \int_0^t dt \left[ \mathcal{H}_{SL} + \mathcal{H}_J \right] } \right)} \right> 
$$

in Eq. (15) getting

$$
\rho_s \langle U_s(1) \rangle_J = \langle J(1) \rangle_J + \frac{1}{3m} \left< \nabla \Psi(\mathbf{r}, t)^\dagger \cdot \nabla \Psi(\mathbf{r}', t) \right> \delta(z) . \quad (26)
$$

Taking the variational derivative with respect to $J(1')$ and using the chain rule we get

$$
\hat{S} D(1,1') = \frac{1}{\rho_s} \delta(1,1') + \epsilon \int d^2 \delta(z_2) \delta(z_1) \times \left[ \nabla_{\mathbf{r}_1} \nabla_{\mathbf{r}'_1} + \nabla_{\mathbf{r}_2} \nabla_{\mathbf{r}'_2} + (g(1,1^+)g(2,2^+) - g(1,2;1^+,2^+)) \right] D(2,1'). \quad (27)
$$

Again we can rewrite this equation in terms of the energy Green function defined in Eq. (22)

$$
\hat{S} D(1,1') = \delta(1,1') + \int d^2 \Pi(1,2) D(2,1), \quad (28)
$$

where the phonon surface energy polarization is defined as

$$
\Pi(1,2) = \epsilon \delta(z_1) G(1,2^+) G(2,1^+) \delta(z_2). \quad (29)
$$

Multiplying Eq. (28) by the inverse operator $\hat{S}^{-1}$ we get the following Dyson-type equation

$$
D(1,1') = D_0(1,1') + \int \int d^2 d^2 D_0(1,3) \Pi(3,2) D(2,1'), \quad (30)
$$

where $D_0(1,2)$ is defined in Eq. (19). Note that although Eqs. (24) and (29) are formally equal to those of standard many body theory, their physical interpretation is quite different. Of course, these equations just express the mathematical fact that this type of integro-differential equation can be expressed in terms of an integral.
equation of the Volterra type. The advantage of writing the equations in this form is that we can obtain solutions to different orders of approximation systematically.

4. Liquid and Solid Reflectivity Coefficients

To find the solution to the integral equations (24) and (30) we use the translational invariance along the surface as well as the homogeneity in time to diagonalize the equations via the Fourier transform in the plane and in time. In the case of Eq. (24) we get

\[ G(z, z', k ||, \Omega_n) = G_0(z, z', k ||, \Omega_n) + i G_0(z, 0, k ||, \Omega_n) \Sigma(0, 0, k ||, \Omega_n) G(0, z', k ||, \Omega_n). \] (31)

Here the Matsubara frequency is given by \( \Omega_n = \frac{2 \pi n}{\beta} = i \beta_n \), and \( n \) is an integer. It is important to notice the order of the \( z \) variables in this equation. This is an algebraic functional equation which can be solved with the help of the auxiliary equation

\[ G(0, z', k ||, \Omega_n) = G_0(0, z', k ||, \Omega_n) + i G_0(0, 0, k ||, \Omega_n) \Sigma(0, 0, k ||, \Omega_n) G(0, z', k ||, \Omega_n). \] (32)

The solution for \( G(z, z', k ||, \Omega_n) \) is

\[ G(z, z', k ||, \Omega_n) = G_0(z, z', k ||, \Omega_n) + i G_0(z, 0, k ||, \Omega_n) \Gamma(0, 0, k ||, \Omega_n) G_0(0, z', k ||, \Omega_n), \] (33)

with

\[ \Gamma(0, 0, k ||, \Omega_n) = \left[ \Sigma^{-1}(0, 0, k ||, \Omega_n) - i G_0(0, 0, k ||, \Omega_n) \right]^{-1}. \] (34)

The solution to Eq. (33) has the interesting property that it depends only on knowing \( \Sigma(0, 0, k ||, \Omega_n) \) and \( G_0(0, 0, k ||, \Omega_n) \). The solution for the free particle Green function \( g_0 \) is obtained from solving the equation

\[ \left( k_n^2 + \frac{1}{2m} \frac{\partial^2}{\partial z^2} \right) g_0(z, z', k ||, \Omega_n) = \delta(z - z'). \] (35)

where

\[ b_n^2 = 2m \Omega_n - \frac{1}{2m} k ||^2 \] (36)
with boundary conditions

\[ g_0(0, z', k \parallel, \Omega_n) = 0, \quad \partial g_0(0, z', k \parallel, \Omega_n) \over \partial z = 0, \]  

(37)

that state the impossibility that the \(^4\)He atoms penetrate the surface. The solution for \( g_0 \) reads

\[ g_0(z, z', k \parallel, \Omega_n) = \frac{1}{2 \gamma_n} \left( e^{-\gamma_n |z-z'|} - e^{-\gamma_n (z+z')} \right), \]  

(38)

for \( z, z' \geq 0 \) and with \( \gamma_n^2 = 2mb_n^2 \). Therefore \( G_0 \) becomes,

\[ G_0(z, z', k \parallel, \Omega_n) = -\frac{\gamma_n}{2} \left( e^{-\gamma_n |z-z'|} + e^{-\gamma_n (z+z')} \right). \]  

(39)

Assuming for a moment that \( \Sigma \) is known, substituting this result back in Eq. (33) the solution for \( G \) becomes

\[ G(z, z', k \parallel, \Omega_n) = -\frac{\gamma_n}{2} \left( e^{-\gamma_n |z-z'|} + (1 - 2i\gamma_n \Gamma(0, 0, k \parallel, \Omega_n)) e^{-\gamma_n (z+z')} \right). \]  

(40)

This result has an immediate physical explanation. Consider, for example, the case \( z > z' \), then Eq. (40) is rewritten as

\[ G(z, z', k \parallel, \Omega_n) = -\gamma_n e^{-\gamma_n z} \left[ e^{-\gamma_n z'} + (1 - 2i\gamma_n \Gamma(0, 0, k \parallel, \Omega_n)) e^{-\gamma_n z'} \right]. \]  

(41)

The first term in the bracket can be interpreted as the energy transported by a plane wave of incident \(^4\)He atoms to the surface. The second term in the bracket then represents the amount energy carried away by the reflected wave. Therefore, we can identify the coefficient of the outgoing wave as the reflectivity and its modulus square gives the reflection coefficient. A nice way of rewriting the reflectivity in terms of \( \Sigma \) results in the suggestive expression

\[ r_L = \frac{1 - i\gamma_n \Sigma(0, 0, k \parallel, \Omega_n)}{1 + i\gamma_n \Sigma(0, 0, k \parallel, \Omega_n)}. \]  

(42)

This is one of the two main results of this paper.

Let us sketch a parallel analysis that leads to an equivalent result for the reflection coefficient in the solid side. Fourier diagonalizing Eq. (30) we get

\[ D(z, z', q \parallel, \omega_n) = D_0(z, z', q \parallel, \omega_n) \]

\[ + iD_0(z, 0, q \parallel, \omega_n)\Pi(0, 0, q \parallel, \omega_n)D(0, z', q \parallel, \omega_n), \]  

(43)
where \( \omega_\ell = \frac{2\pi}{l} \), with \( l \) an integer while \( q_\parallel \) is the solid phonon wave vector along the surface. We can solve this equation as before getting

\[
D(z, z', q_\parallel, \omega_n) = D_0(z, z', q_\parallel, \omega_n)
+ iD_0(z, 0, q_\parallel, \omega_n)W(0, 0, q_\parallel, \omega_n)D_0(0, z', q_\parallel, \omega_n),
\]

where we defined

\[
W(0, 0, q_\parallel, \omega_n) = \left[ \Pi^{-1}(0, 0, q_\parallel, \omega_n) - iD_0(0, 0, q_\parallel, \omega_n) \right]^{-1}.
\]

Again we first need to calculate the free phonon propagator which satisfies the equation

\[
\rho_s \left( \eta_n^2 + \frac{\partial^2}{\partial z'^2} \right) D_0(z, z', k_\parallel, \Omega_n) = \delta(z - z'),
\]

where

\[
\eta_n^2 = \frac{1}{C_3^2} \omega_n^2 - q_\parallel^2.
\]

The solution in this case reads

\[
D_0(z, z', q_\parallel, \omega_n) = \frac{1}{2\eta_n \rho_s} \left( e^{\eta_n |z - z'|} + e^{\eta_n (z + z')} \right),
\]

for \( z, z' \leq 0 \). The boundary conditions in this case are \( D_0(0, 0, q_\parallel, \omega_n) = 1/2\eta_n \) and \( \partial D_0(0, 0, q_\parallel, \omega_n)/\partial z = 0 \). Replacing Eq. (47) into Eq. (44) gives

\[
D(z, z', q_\parallel, \omega_n) = \frac{1}{2\eta_n \rho_s} \left[ e^{\eta_n |z - z'|} + \left( 1 + \frac{i}{\eta_n \rho_s} W(0, 0, q_\parallel, \omega_n) \right) e^{\eta_n (z + z')} \right].
\]

Again, using the specific value for \( D_0(0, 0, q_\parallel, \omega_n) \) in the definition of \( W \) we get the final expression for the reflection coefficient from the solid side

\[
r_s = \frac{1 + \frac{i}{2\eta_n \rho_s} \Pi(0, 0, k_\parallel, \Omega_n)}{1 - \frac{i}{2\eta_n \rho_s} \Pi(0, 0, k_\parallel, \Omega_n)}.
\]

This equation together with Eq. (42) are the main results of this paper.
5. Liquid Quantum Reflection Coefficient

To evaluate exactly expressions for the reflection coefficients is non-trivial, since both \( r_L \) and \( r_S \) depend on the unknown functions \( \Sigma \) and \( \Pi \). However, given that we are interested in understanding the energy transmission properties between \(^4\text{He} \) and a solid, preferably an insulator, the ratio between the densities of the two materials can serve as the smallness parameter about which we can calculate explicitly the reflection coefficients. To illustrate the approach we consider here the calculation of \( |r_L|^2 \) explicitly.

From Eq. (42) we see that to get \( r_L \) we need to know \( \Sigma(0,0,k,\Omega_n) \). From Eq. (25) and taking the Fourier transform in space and time we have

\[
\Sigma(1_n) = \epsilon \int d1' \eta D(1_n - 1'_n) D_0(1'_n).
\]

(50)

To simplify the notation here we defined the set \((k,\Omega_n) = 1_n\) and \((q,\omega) = 1\). The solution for \( G(1_n) \) follows from Eq. (41)

\[
G(1_n) = -2\gamma(1_n) \left[ 1 + i\gamma(1_n) \Sigma(1_n) \right]^{-1}.
\]

Substituting this result in Eq. (49) we get the integral equation

\[
\Sigma(1_n) = -2\epsilon \int d1' \left( \frac{\gamma(1_n - 1'_n)}{\eta(1'_n) \rho_S} \right) \left[ 1 + i\gamma(1_n - 1'_n) \Sigma(1_n - 1'_n) \right]^{-1}
\]

(51)

where we used the fact that \( D_0(0,0,q,\omega) = 1/2\eta_n \rho_S \). This is a continued fraction integral equation for \( \Sigma \). A general solution to this equation seems to be out of the question. However, since \( \epsilon \ll 1 \) we can solve this equation to zeroth order obtaining

\[
\Sigma(1_n) = -2\epsilon \int d1' \left( \frac{\gamma(1_n - 1'_n)}{\eta(1'_n) \rho_S} \right),
\]

(52)

which should give a good approximation to the answer. To the same order of approximation the energy reflection coefficient obtained from Eq. (42) becomes, \( R_L \sim 1 - T_L + O(\epsilon^2) \), where the transmission coefficient is given by

\[
T_L = -4 \text{Im} \gamma(1_n) \Sigma(1_n).
\]

(53)

To evaluate the integrals implied in Eq. (52) we proceed as usual by replacing the frequency sum by an integral in the complex plane with the weight function \( f(z) = [e^{iz} - 1]^{-1}, \) i.e. the Bose distribution in the complex plane, so that Eq. (52)
reads

\[ 
\Sigma(q, \omega_n) = -2 \frac{e}{\rho_s} \int d\vec{k}_\parallel \oint \frac{dz}{2\pi} f(z) \left[ \frac{2m(\omega_n - z) - (\vec{k}_\parallel - q||)^2}{1/C_s^2 z^2 - k_\parallel^2} \right]^{1/2} .
\]  

To evaluate the frequency integral we use the identity

\[ 
\int_{-\infty}^{\infty} \frac{dx}{A + x^2} = \frac{\pi}{\sqrt{A}}
\]

in each one of the square roots in the numerator and denominator to get

\[ 
\Sigma(q, \omega_n) = -2 \frac{1}{\pi^2} \frac{e}{\rho_s} \int d\vec{k}_\parallel \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \oint \frac{dz}{2\pi} f(z)
\times \left[ \frac{2m(\omega_n - z) - (\vec{k}_\parallel - q||)^2}{x_1^2 + 2m(\omega_n - z) - (\vec{k}_\parallel - q||)^2} \right] \left[ \frac{1}{x_2^2 + 1/C_s^2 z^2 - k_\parallel^2} \right].
\]

The calculation of this fivefold integral is direct but involved. Here I just mention some of the results used in the evaluation and present the final result of the calculation. First we need to analytically continue \( z \) from the upper half of the complex plane to the real axis by \( z \to \omega + i\delta \), where \( \delta \) is a positive infinitesimal quantity. To get the imaginary part of \( \Sigma \) we use the identity \([x + i\delta]^{-1} = \frac{P}{x} \pm i\pi \delta(x)\), where \( P \) stands for the Cauchy principal value. The Dirac \( \delta \) functions lead to energy conservation conditions. In doing the remaining integrals over \( x_1 \) and \( x_2 \) one uses the identity for Bose integrals, \( \int_0^\infty x^{\nu-1} [e^{\beta x} - 1]^{-1} dx = \frac{1}{\beta} \Gamma(\nu) \xi(\nu) \), valid for \( \text{Re} \beta > 0 \) and \( \text{Re} \nu > 1 \), and with \( \Gamma \) and \( \xi \) the standard gamma and zeta functions, respectively. Since we know that the probability to excite surface modes by the \(^4\)He atoms is small we set \( q|| = 0 \) at the end of the calculation. The result for \( \beta \omega = \Omega < 1 \) finally reads, (we have now set \( h = h/2\pi \))

\[ 
T_L = \frac{32\pi^3}{3} \left( \frac{Z_L}{Z_s} \right) \frac{k_B^4 T^3}{\hbar^3 C_s^2} \left( 4.808 + 11.73\tilde{\Omega} - \frac{1}{2}\tilde{\Omega}^2 + 2.08\tilde{\Omega}^3 - 6\tilde{\Omega}^2 \ln \tilde{\Omega} \right).
\]

We discuss this result in what follows.

6. Conclusion

Although I have called \( T_L \) the transmission coefficient, it is in fact the inverse of the thermal resistance per unit area of the problem. Whereas in the classical calculation one evaluates the transmission coefficient at \( T = 0 \) and then carries out a frequency integral in convolution with Planck's distribution, here both operations are done at
once. To compare the result given in Eq. (57) to the classical theory I list now the temperature dependent result obtained from the classical theory [4]

\[
T_L = \frac{16\pi^5 k_B^4 T^3 Z_L}{15 \frac{h^3 C_s^2}{Z_S}}.
\]

We notice immediately that, just as is found in the experiments, the temperature dependence is the same, i.e. the transmission decreases as \( T^3 \). Both results depend on the ratio of the impedances of both materials, however, in the limit of zero frequency, the quantum answer is about five times larger. This is good indeed although experimentally the differences between the classical theory and the experiment are found to be five to ten times larger than the classical theory prediction. More important is the fact that by doing the calculation quantum mechanically we have found an important frequency dependent contribution to \( T_L \) as is found experimentally. For the regime for which Eq. (57) is valid, \( \Omega < 1 \), \( T_L \) increases monotonically with \( \Omega \) for fixed \( \beta \). The curvature is qualitatively like that found experimentally [4].

We conclude by noting that although the quantum calculation leads to a better quantitative agreement with experiment the orders of magnitude are still in some cases off. The alternatives are either to do more accurate experiments in cleaner surfaces or modify the theory by adding extra mechanisms like a solid helium layer in the interface, or roughness in the surface. In any of this cases the formalism developed here can be adapted to obtain the thermal boundary resistance between two quantum materials and further applications of the formalism will appear elsewhere [6].

Dedicatory

I dedicate this paper to Professor L. García-Colín on the occasion of his sixtieth birthday as a humble testimony of my deep appreciation for his support and guidance during my formative years as a scientist.

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References


Resumen. En este artículo se considera el problema de transmisión de calor a través de una interface que separa un líquido cuántico de un sólido en términos de la entropía de muchos cuerpos. Se estudia un modelo en términos de un operador hamiltoniano que supone una interface continua con interacciones localizadas en ella y pequeñas oscilaciones del sólido dentro del contexto de la aproximación lineal fonónica. Se derivan expresiones explícitas para los coeficientes de reflexión de ondas provenientes del líquido o del sólido dentro de la aproximación de Hartree-Fock. Se exhibe el resultado explícito para el coeficiente de reflexión en el sólido como función de la temperatura y la frecuencia. Se compara brevemente el resultado obtenido con la teoría clásica así como con los resultados experimentales.