MATSCIENCE REPORT 99

Lectures on
SOME SURFACE PHENOMENA IN SUPERFLUID HELIUM

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Introduction

This report is the outcome of a series of lectures given by me at Matscience on some surface phenomena in superfluid Helium-4.

The topics covered and the work surveyed are those which have attracted my attention and the analysis presented here is by no means exhaustive. The idea is mainly to give an introduction and point out a few unsolved problems in some surface phenomena.

I thank Professor Alladi Ramakrishnan for his constant encouragement and Professors R.Vasudevan, N.R.Ranganathan and V.Radhakrishnan for their valuable comments and criticisms.

R.Sridhar

EVAPORATION FROM SUPERFLUID HELIUM

1. Initial speculation regarding the role of density of states:

Interest in the theory of evaporation from superfluid helium started growing after the experimental measurements by Johnston and King (1966) of the velocity distribution of atoms evaporating from the surface of liquid helium in the temperature range 0.59 to 0.7°K. These measurements were made in an atomic beam apparatus using a chopped beam and time-of-flight method. It was found that the energy distribution of evaporated atoms shifted towards higher energies-to be precise the distributions were characteristic of a source approximately 1.1°K hotter than the liquid and that they could be fitted well with a Maxwellian distribution at an effective temperature $T_{eff} = 1.55$ to 1.6°K.

These experimental observations (and the theories supporting these findings) were disputed later by more refined, careful and hence reliable measurements which will be discussed subsequently. We shall however discuss the initial theoretical attempts as a necessary background for future theoretical refinements.

The experimental results of Johnston and King led to some very interesting developments in the theory of evaporation from superfluid Helium. Hyman, Scully and Widom (1969) and Anderson (1969) have suggested that the process of evaporation at low temperatures can be regarded as a quasi-particle tunneling process: decay of quasi-particles of appropriate energies near the liquid surface leading to the emission of free atoms above the liquid surface.

Standard methods of tunneling theory could be applied to derive a general expression for the total evaporation rate as a function of temperature.

A. Tunneling approach:

Following the work of Hyman et al (1969) one can write the tunneling hamiltonian as

$$H = H_L + H_V + H_T \tag{1}$$

where H_L, H_V and H_T denote respectively the hamiltonians for the liquid, the evaporated free atoms (in the Vapour) and the tunneling mechanism .

While H_L need not be explicitly specified

$$H_V = \sum_p T_p a_p^\dagger a_p \quad \text{with} \quad T_p = p^2/2m \tag{2}$$

$$H_T = \sum_p \left(\ell_p a_p^\dagger + \ell_p^\dagger a_p \right) \tag{3}$$

where a_p, $a_p^\dagger$ denote the destruction and creation of the atoms in the vapour while ℓ_p and $\ell_p^\dagger$ denote the removal and addition of atoms to the liquid. The index p denotes the momentum of the concerned particle.

The probability of evaporation of an atom from the liquid into the vapour state can be readily written down using Fermi's "Golden rule" as

$$W_{i\to f}(\vec{p}, n_{\vec{p}}) = 2\pi \left| \langle n_p+1, f | H_T | n_p, i \rangle \right|^2 \delta(T_p + \epsilon_f - \epsilon_i) \tag{4}$$

where $|n_p, i\rangle$ denotes the combined initial state of the vapour-liquid system with n_p particles of momentum $\vec{p}$ in the vapour with the liquid being in the state $|i\rangle$.. Similarly $|n_p+1, f\rangle$ denotes the final state of the system with (n_p+1) particles in the vapour and the liquid being in the state $|f\rangle$. ϵ_f and ϵ_i denote respectively the final and initial liquid energies.

Using the explicit form of H_T equation (4) can be rewritten as

$$W_{i\to f}(\vec{p}, n_{\vec{p}}) = (2\pi)(n_p+1)\,|\langle f|\ell_p|i\rangle|^2\,\delta(T_p+\epsilon_f-\epsilon_i) \tag{5}$$

The evaporation rate can be obtained on averaging eq.(5) with the canonical occupation probability P_i of the state $|i\rangle$

$$W_e = \sum_{i,f} P_i\, W_{i\to f}(\vec{p}, n_{\vec{p}}) \tag{6}$$

with $\quad P_i = \exp[\beta(F_n - \epsilon_i)]$

$\beta = (k_B T)^{-1}, \qquad k_B$ = Baltzmann's constant.

Let

$$D^<(\vec{p}, E) = \sum_{i,f} P_i\,|\langle f|\ell_p|i\rangle|^2\,\delta(E+\epsilon_f-\epsilon_i) \tag{7}$$

so that (6) can be rewritten as

$$W_e(\vec{p}, n_p) = 2\pi(n_p+1)\,D^<(\vec{p}, E_p) \tag{8}$$

and $D^{<}(\vec{p},E_p)$ can be shown to be a thermodynamic Green's function.

$$\int D^{<}(\vec{p},E)\exp(iEt)\,dE$$
$$=\sum_{i,f} P_i\,|\langle f|\ell_p|i\rangle|^2\exp[-i(\epsilon_i-\epsilon_f)t]$$
$$=\sum_{i,f} P_i\langle f|\ell_p^{\dagger}(0)\,\ell_p(t)|i\rangle = \langle\langle \ell_p^{\dagger}(0)\,\ell_p(t)\rangle\rangle \qquad (9)$$

where $\langle\langle \cdots\cdot \rangle\rangle$ denotes the usual thermal average. Proceeding in a similar manner one can evaluate the total absorption rate for an atom. In this case $D^{>}(\vec{p},E)$ has to be used where

$$\int D^{>}(\vec{p},E)\exp(-iEt)\,dE = \langle\langle \ell_p(t)\,\ell_p^{\dagger}(0)\rangle\rangle \qquad (10)$$

so that

$$W_{abs}(\vec{p},n_p) = 2\pi\;n_p\;D^{>}(\vec{p},E) \qquad (11)$$

Using standard procedures one can establish now

$$D^{<}(\vec{p},E) = \exp[\beta(\mu-E)]\,D^{>}(\vec{p},E) \qquad (12)$$

Experimentally one is interested in the case of evaporation into vacuum so that on using (8), (10) along with (12)

$$W_e(\vec{p},0) = \exp[\beta(\mu-E_p)]\,W_{abs}(\vec{p},1) \qquad (13)$$

The total rate can be obtained by summing this over all the states.

$$\text{Total rate} = R = \sum_p W_e(\vec{p},0)$$

$$= e^{\beta\mu} \sum_p e^{-\beta E_p} W_{abs}(\vec{p},1)$$

$$= \exp(\mu\beta)\ \eta(T) \qquad (14)$$

where it is supposed that $\eta(T)$ is a slowly varying function of T compared to $\exp(\beta\mu)$.

B. Anderson-Widom assumption:

It is known from experimental results of Henshaw and Woods (1961) on HeII that a considerable fraction of inelastic scattering is accounted for by the production of single excitations in the liquid. Also Miller, Pines and Nozieres (1962) have estimated that in the region of roton minimum nearly 60% of the scattering is due to the production of rotons. Thus instead of neutrons if cold 4He atoms are used as projectiles one can presume that a similar fraction of absorbed atoms would create single excitations. Since scattering and evaporation are complementary to each other.

Following Anderson (1969) and Widom (1969) it can be assumed that the dominant rocess in the evaporation phenomenon is a single particle process-conversion of a high energy phonon or roton into an atom of the vapour (or vice versa). It should be noted that it takes a finite amount of energy to remove an atom from the liquid (the so called heat of evaporation) which is equal to 7.15°K at low temperatures.

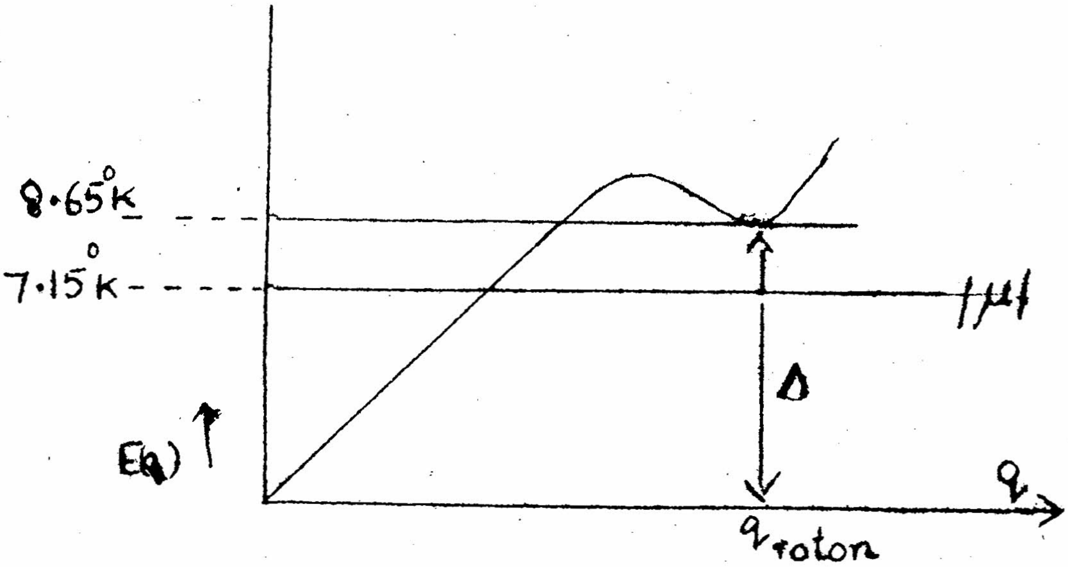


Fig.1

The operators ℓ_p introduced in eq.(3) can be constructed as superposition of liquid ^{4}He creation and annihilation operators $b_k^\dagger$ and b_k with an amplitude λ_{pk} .

$$\ell_p(t) = \sum_k \lambda_{pk}\, b_k(t)\, \exp(-i\mu t) \qquad (15)$$

The factor $\exp(-i\mu t)$ is due to the fact that ℓ_p removes an atom from the liquid and connects the initial n particle liquid state to (n-1) particle final liquid state. The operators b_k's obey the usual Bose commutation rules

$$[b_p, b_q^\dagger] = \delta_{p,q} \;, \quad [b_p, b_q] = 0 = [b_p^\dagger, b_q^\dagger]$$

If we define

$$G^>(q,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t} \langle\langle b_q(t)\, b_q^\dagger(0)\rangle\rangle\, dt \qquad (16)$$

we can write

$$\overset{>}{D}(p,E) = \sum_{q} |\lambda_{pq}|^2 G^{>}(\vec{q}, E-\mu) \tag{17}$$

and

$$\langle\langle \ell_p(t)\, \ell_p^{\dagger}(0) \rangle\rangle = \sum_{q} |\lambda_{pq}|^2 e^{-i\mu t} \langle\langle b_q(t) b_q^{\dagger}(0) \rangle\rangle \tag{18}$$

The principle of detailed balance (equation (12)) yields

$$W_e(\vec{P},0) = 2\pi \exp[\beta(\mu-E_p)] \sum_{k} |\lambda_{pk}|^2 \overset{>}{G}(\vec{k}, E_p-\mu) \tag{19}$$

The contribution of rotons and phonons t W_e can be discussed from phase-space considerations.

C. Phonons:

Let the phonons be regarded as stable quasi-particle excitations with

$$\overset{>}{G}_{ph}(\vec{k},\omega) = 2\pi \left\{ 1 + [\exp(\beta\omega)-1]^{-1} \right\} \delta(\omega - ck)$$

ck being the energy of the phonon. From the previous discussion it is clear that $\omega > |\mu| = 7.15^{\circ}k$ (see Fig.1). For his ω, $\exp(\beta\omega) \gg 1$ at low temperatures T where $\beta = 1/k_B T$.

Therefore

$$G_{ph}^{>}(\vec{k},\omega) \sim (2\pi)\, \delta(\omega - ck) \tag{20}$$

Replacing the quantities λ_{pk} by a constant λ and using eq.(20) and (19) one can write down the contribution of phonons W_e in the following manner;

$$W_e^{ph}(\vec{p},0) = 2\pi \exp(\beta(\mu-E_p)) \cdot \lambda \sum_k 2\pi\,\delta(E_p-\mu-ck)$$

$$= 2\pi\, e^{\beta(\mu-E_p)} \frac{\Omega}{(2\pi)^3} \cdot 4\pi \int_0^\infty dk\, k^2\, \delta(E_p-\mu-ck)$$

$$= K \exp[\beta(\mu-E_p)] \cdot (E_p-\mu)^2$$

K being a constant. On multiplying the above results by free particle density of states $N(E_p)$ one obtains the emission rate into an energy interval dE_p around E_p .

$$W_e(\vec{p},0)\, N(E_p)\, dE_p \sim e^{\beta(\mu-E_p)} (E_p-\mu)^2 \sqrt{E_p}\, dE_p \qquad (21)$$

The energy dependent part of this expression (on the right) is shown in figure 2. Note that this contribution (marked as phonon in figure) is similar to a Maxwellian peaked approximately at an energy 0.4°K. Still this is not consistent with the findings of Johnston and King. To improve this result one can include the roton contribution as well.

D. Rotons:

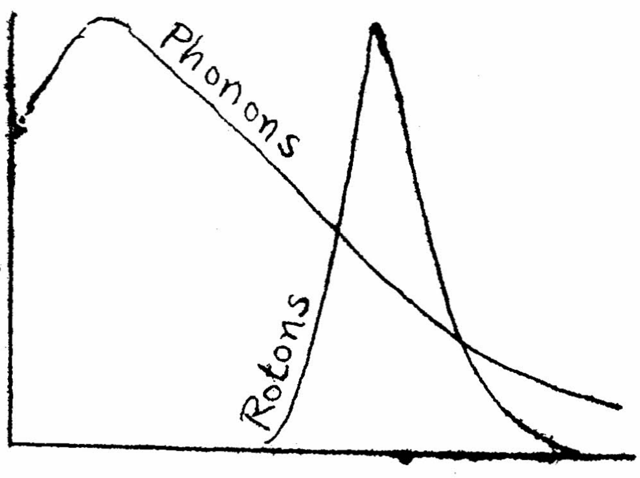


Fig.2
Relative contributions of phonons and rotons

From fig.1 it is evident that at the roton minimum, E_p is a constant Δ which leads to an infinite density of states. Consequently W_e^{rot} is also divergent. However, if the roton life time is taken into account by including a small average line width γ in the Green's function the divergence could be avoided.

$$G^{>}_{rot} = \left\{1 + \left[\exp(\beta\omega) - 1\right]^{-1}\right\} \gamma \Big/ \left\{(\omega - E_p)^2 + \gamma/4\right\}$$

$$\approx \gamma \Big/ \left\{(\omega - E_p)^2 + \gamma/4\right\} \tag{22}$$

The procedure outlined in the case of phonons is to be followed:

$$W_e \sim e^{\beta(\mu - E)} \int_{q_{rot}}^{\infty} dp\, p^2\, \gamma \Big/ \left\{(E - \mu - E_p^2) + \gamma^2/4\right\}$$

$$\sim \exp(\beta(\mu - E)) . p_0^2 \int_{\Delta}^{\infty} d\epsilon \; \frac{(\epsilon - \Delta)^{-\frac{1}{2}}\, \gamma}{(E - \mu - \epsilon)^2 + \gamma^2/4} \tag{23}$$

The integral in (23) can be evaluated by standard methods. For this consider

$$I(E) = \int_{\Delta}^{\infty} d\epsilon\, (\epsilon - \Delta)^{-\frac{1}{2}} \; \frac{A}{A^2 + (\omega - \epsilon)^2}$$

Put

$$(\epsilon - \Delta) = t^2$$

Then $$I(E) = A\int_{-\infty}^{\infty} \frac{dt}{A^2 - (\varpi - t^2)^2} \quad \text{where } \varpi = \omega - \Delta$$

$$= A\int_{-\infty}^{\infty} \frac{dt}{(t-\sqrt{t_1})(t+\sqrt{t_1})(t-\sqrt{t_2})(t+\sqrt{t_2})}$$

with $t_1 = \varpi + iA$ and $t_2 = \varpi - iA$.

This integral is evaluated as a contour integral in which the path encloses the upper half of the complex τ -plane.

ϖ	Poles in the upper half plane		
$\varpi > 0$	$\sqrt{t_1}$	and	$-\sqrt{t_2}$
$\varpi < 0$	$\sqrt{t_1}$	and	$\sqrt{t_2}$

so that

$$I(E) = \begin{cases} \frac{\pi}{\sqrt{2}} \sqrt{A^2 + 2\varpi^2}\ (A^2+\varpi^2)^{-3/4} & (\varpi > 0) \\ \frac{\pi}{\sqrt{2}} A\,(A^2+\varpi^2)^{-3/4} & (\varpi < 0) \end{cases} \tag{24}$$

so that when $\varpi = 0$, $I(E)$ takes the value $\pi/\sqrt{2A}$.

Using (24) in (23) we have

$$W_e = (\text{Const}) \times \exp(\beta(\mu - E))\left\{(E-\mu-\Delta)^2 + \frac{\gamma^2}{4}\right\}^{-3/4} F(E) \tag{25}$$

where

$$F(E) = \gamma/2 \qquad \text{for } (E-\mu-\Delta) < 0$$

$$= \left\{2(E-\mu-\Delta)^2 + \frac{\gamma^2}{4}\right\}^{\frac{1}{2}}, \text{ for } (E-\mu-\Delta) > 0 \qquad (26)$$

Following Hyman et al if γ/k_B is chosen to be 0.001°K for $T = 0.6^{\circ}$K, it is readily seen from (25) that the roton contribution to emission rate is sharply peaked at an energy approximately equal to 1.5°K. Thus it was believed that the apparent existence of the peak in the experimentally measured velocity distribution of Johnston and King might be due to the direct conversion of rotons into evaporated atoms.

E. To conclude:

Adding the contributions due to rotons and phonons and comparing with the Maxwellian distribution

$$W(E) = E \exp(-\beta E)$$

at a temperature $T = 1.5^{\circ}$K, it is found that the single particle processes account for only 35% of the evaporation rate. It was conjectured that the remaining contribution may be due to multi-excitation processes.

The outcome of the above discussions may be summarised as follows:

a) The anomalously high density of states in HeII at the roton minimum might influence the evaporation spectrum.

b) The role of multiexcitations remains to be studied.

c) From the point of view of fitting the results with a Boltzmann type of distribution, a shift in the peak exists at an energy $E = \Delta - \mu$.

These conclusions had to be revised in view of the later developments discussed below.

2. The controversy-consequent theoretical attempts:

A. The disappearence of the earlier observed (?) shift.

When King, McWave and Tinker (1972) with an improved set up made a more careful measurement of the velocity distribution of the evaporated atoms both from superfluid films and bulk helium, at temperatures from 0.53 K to 0.61K, they found that there is no significant shift towards higher energies. Thus the data contradicts theories (as well as the earlier experiment) predicting signficant warming of the evaporated atoms.

Andres, Dynaes and Narayanamurthy (1973) have also studied the properties of helium atoms evaporating from the surface of a liquid (^{3}He and ^{4}He) film using the heat pulse technique. The time of flight measurements were done with sensitive superconducting bolometers with submicrosecond response times. The experiment was performed in the temperature range 0.1 to 3.4°K. In the ballistic region (single non-interacting particle flow) at low temperatures the evaporated spectrum was found to be Maxwell-Boltzmann in nature. No effects that could be ascribed to the quasiparticle nature of the liquid was observed.

B. A Kinetic Theory description:

A kinetic theoretic approach was used by Cole (1972) to calculate the angular and spectral distributions of evaporated atoms. In this approach use is made of the hypothesis due to Anderson and Widom (1969) that

(i) inelastic processes are not important

(ii) only single particle processes are dominant.

Let $(\vec{q_i}, \omega_i)$ and $(\vec{q_e}, \omega_e)$ denote respectively the momentum and energy of the incident and emergent particles. Translational invariance is obtained parallel to the liquid surface resulting in the conservation of momentum parallel to the surface

$$q_{i\parallel} = q_{e\parallel} \tag{27}$$

As has already been pointed out an energy $|\mu|$ has to be spent to liberate an atom from the liquid surface into the vacuum so that

$$\omega_e = \frac{p^2}{2m} = \omega - |\mu| \tag{28}$$

Consider a quasiparticle of momentum $q_i < q_{roton}$ hitting the surface from below. In this region of momentum the group velocity is opposite to $\vec{q_i}$. Further the surface force also acts in the direction of the group velocity. Consequently it is not possible for a He atom (with its momentum in this region) to escape to the vapour state. Thus the region of anomalous despersion where the emitted atoms have approximately the energy $(\Delta - |\mu|) k_B^{-1} = 1.5K$ can be ignored. Similarly phonons having momenta $q_i > q_o = m\{c - \sqrt{c^2 - 2|\mu|/m}\}$ cannot contribute to evaporation since the evaporated atoms would have momenta $\vec{q_e} > \vec{q_i}$. This region starts with an energy $(q_o c - |\mu|) k_B^{-1} = 1.36$ k.

The general formula for the rate of arrival at unit surface area from solid angle $d\Omega$ of quasiparticles in the energy interval $(\omega, \omega + d\omega)$ is

$$\frac{d^2 \dot{N}_{oP}}{d\omega_i \, d\Omega_i} = f(\omega_i)\, \eta(\omega_i) \cos\theta \; d\omega_i \, d\Omega_i \tag{29}$$

where

θ = angle of incidence with respect to surface normal

$f(\omega) = [\exp(\beta\omega) - 1]^{-1}$

$\omega(q)$ = quasi particle energy corresponding to momentum $\vec{q}$

$\eta(\omega)$ = density of states per unit solid angle in the liquid

$$= q^2 \left[8\pi^2 \left| \frac{d\omega}{dq} \right| \right]^{-1}$$

We can now write

$$d\Omega_i \; p_i^2 \cos\theta_i = d\Omega_e \; p_e^2 \cos\theta_e \tag{30}$$

so that

$$\frac{d^2 \dot{N}_e}{dE\, d\Omega_e} = \frac{d^2 \dot{N}_{OP}}{d\omega_i\, d\Omega_i} \; T_{p_i, p_e} \; \frac{d\Omega_i}{d\Omega_e}$$

$$= \exp[-\beta(E + |\mu|)] \, mE \cos\theta_e \, \frac{T_{p_i, p_e}}{(4\pi)^3} \tag{31}$$

where T_{p_i, p_e} = Fraction of quasi particles incident upon the surface which are transferred to the vapour state

and $f(\omega) \cong \exp(-\beta\omega)$

Due to the kinematical considerations discussed above, a gap will occur in the spectrum between the energies 1.36 K to 1.5 K. Thus there is an effective cancellation of the bulk quasiparticle density of states.

Equations (27) and (28) allow to escape only those quasi particles incident from within a cone $\theta_i < \theta_{max}$ centered about the surface normal. θ_{max} is given by

$$\sin^2 \theta_{max} = 2m\,(\omega - |\mu|)\,/\,q^2 \tag{32}$$

Corresponding to the value $q = q_{roton}$, θ assumes the value of 15^o. If $\theta_i > \theta_{max}$ total internal reflection occurs.

Let P be the saturated vapour pressure given by

$$P = e^{-\beta|\mu|}\left(\frac{m}{2\pi}\right)^{3/2}\beta^{-5/2} \tag{33}$$

so that angular distribution of atoms incident on the surface from the vapour side is written as

$$\frac{d^2 \dot{N}_{inc}}{dE\, d\Omega'} = P\,\beta^{5/2}(2m\pi^3)^{-1/2} E \cos\theta' \, e^{-\beta E} \tag{34}$$

which along with (31) readily yields

$$\frac{d^2 \dot{N}_e}{dE\, d\Omega_e} = \frac{d^2 \dot{N}_{inc}}{dE\, d\Omega'}\; T_{p_i, p_e} \tag{35}$$

T_{p_i, p_e} is invariant under time reversal. The time reversed process can be described by the quantities $(p_e, E-p_i, \omega)$.

Because of this, right side of (35) can be interpreted as the number of atoms impinging on the surface which 'condense' into the quasi-particles of the liquid.

$$\frac{d^2 \dot{N}_{cond}}{dE\, d\Omega'} = \frac{d^2 \dot{N}_e}{dE\, d\Omega_e} \tag{36}$$

which is the principle of detailed balance (Widom, 1969). An interesting feature of the formula (35) is that it does not involve the density of states near the anomalous region of the spectrum.

C. Bogoliubov Model

A modified treatment of the tunnelling hamiltonian technique using the Bogoliubov model for HeII with a delta shell potential has been given by Salinas and Turski (1974). In this model the hamiltonian H_L for the liquid is explicitly taken into consideration (compare this with the tunnelling approach in 1A)

$$H_L = \sum_p (T_p - \eta)\, b_p^\dagger b_p + N_0 \sum_p V(p) \left\{ b_p^\dagger b_{-p}^\dagger + b_p b_{-p} \right\}$$

$$T_p = p^2/2m \tag{37}$$

where No is the condensate density and $V(p)$ is the Fourier transform of the two particle interaction potential. Now make the well known Bogoliubov transformation

$$b_p = u_p \ell_p + v_p \ell^\dagger_{-p}$$

$$b_p^\dagger = u_p \ell_p^\dagger + v_p \ell_{-p}$$

with

$$u_p^2 - v_p^2 = 1$$

and the diagonalisation requirements lead to

$$u_p^2 = \tfrac{1}{2}\left\{-1 + (T_p + N_0 V(p))/\epsilon_p\right\}$$

and the Bogoliubov excitation spectrum ϵ_p is given by

$$\epsilon_p = \left[T_p^2 + 2N_0 V(p) T_p \right]^{1/2} \tag{38}$$

In (38) V(p) is taken as the Fourier transform of the delta shell potential

$$V(p) = V_0 \frac{\sin(p\sigma)}{p\sigma} \tag{39}$$

V_0 is decided by the velocity of sound c by the relation

$$c^2 = N_0 V_0 / m$$

and σ which is related to the scattering length is taken to be 2.5A. The tunnelling Hamiltonian H_T (see eq.(3)) is taken to be

$$H_T = \sum_{p,q} \mathcal{A}_{pq} \left(a_p^\dagger \ell_q + \ell_q^\dagger a_p \right) \tag{40}$$

with a transition amplitude $\mathcal{A}_{pq}$ for the liquid-vapour (and vice versa) single particle transfer process. The probability of evaporation is given by equation (4) and substituting (40) in (4) we have

$$W_{i\to f}(\vec{p}, n_p) = 2\pi\, \delta(T_p + \epsilon_f - \epsilon_i)\, (n_p + 1)$$

$$\times \sum_{k,q} T_{kp} T_{qp} \langle f | \ell_k | i \rangle \langle i | \ell_q | f \rangle \tag{41}$$

The evaporation rate $W_e(\vec{p}, n_p)$ can be obtained on using equation (6) so that

$$W_e(\vec{p}, n_p) = 2\pi\,(n_p+1) \times \sum_{k,q} T_{kp}\, T_{qp} \int \frac{dt}{2\pi}\, e^{it\epsilon_p} \ll \ell_p^{\dagger}(0)\, \ell_p(t) \gg \tag{42}$$

If Greens functions $D^{<}(pE)$ and $D^{>}(p,E)$ are defined as in equations (9) and (10) we can obtain the spectral function $A(\vec{p}, \epsilon)$

$$G^{<}(p,\epsilon) = f(\epsilon)\; A(p,\epsilon) \tag{43}$$

where

$$f(\epsilon) = \left[\exp(\beta\epsilon) - 1\right]^{-1}$$

Then

$$W_e(\vec{p}, n_p) = (n_p+1)\, f(\epsilon_p) \sum_{k,q} T_{kp}\, T_{k+q,\,p}\, A(q, \epsilon_q) \tag{44}$$

Since k summation can be independently done, let

$$\sum_{k} T_{k,p}\; T_{k+q,\,p} = M(q,p) \tag{45}$$

Hence

$$W_e(\vec{p}, n_p) = (n_p+1)\, f(\epsilon_p) \sum_{q} M(q,p)\, A(q, \epsilon_p) \tag{46}$$

According to experimental set up, one is interested only in the rate in which the initial vapour states are not occupied so that

$$n_p = 0 \tag{4\&}$$

Further nothing is known about the amplitude $\mathcal{A}_{pq}$ for the liquid vapour single particle transition process. As a matter of fact $\mathcal{A}_{pq}$ contains all the information obtained from a microscopic theory (if one such theory is proposed) about the mechanism of "evaporation" Since very little is known about the structure of $\mathcal{A}_{pq}$ Salinas and Turski assume that it can be taken to be a constant M.

$$\mathcal{A}_{pq} = M \qquad \text{for all } p, q. \tag{48}$$

Equation (46) can now be simplified on account of (47) and (48)

$$W_e(\vec{p}, 0) = M\, f(\epsilon_p) \sum_q A(\vec{q}, \epsilon_p) \tag{49}$$

The spectral function A (q, ϵ_p) can be computed easily for the Bogoliubov model by standard procedutres.

$$A(\vec{p}, \omega) = 2\pi\, u_p^2\, \delta(\omega - \epsilon_p) - 2\pi\, v_p^2\, \delta(\omega + \epsilon_p) \tag{50}$$

Substitute this in (49).

$$W_e(\vec{p}, 0) = M\, f(\epsilon_p) \frac{\Omega}{(2\pi)^3} \times 4\pi \int_0^\infty dq\, q^2 \left\{ 2\pi\, u_q^2\, \delta(\epsilon_p - \epsilon_q) \right\}$$

q integration can be converted into an energy integration by introducing the density of states. Thus

$$W_e(\vec{p}, 0) = (\text{Const}) \sqrt{\epsilon_p}\, f_B(\epsilon_p) \sum_{p_0} \left\{ p^2 u_p^2 \left| \frac{d\epsilon_p}{dp} \right|^{-1} \right\}_{p=p_0} \tag{51}$$

where p_o is the root of the equation $\epsilon_p = \epsilon$. This rate is plotted in fig.3.

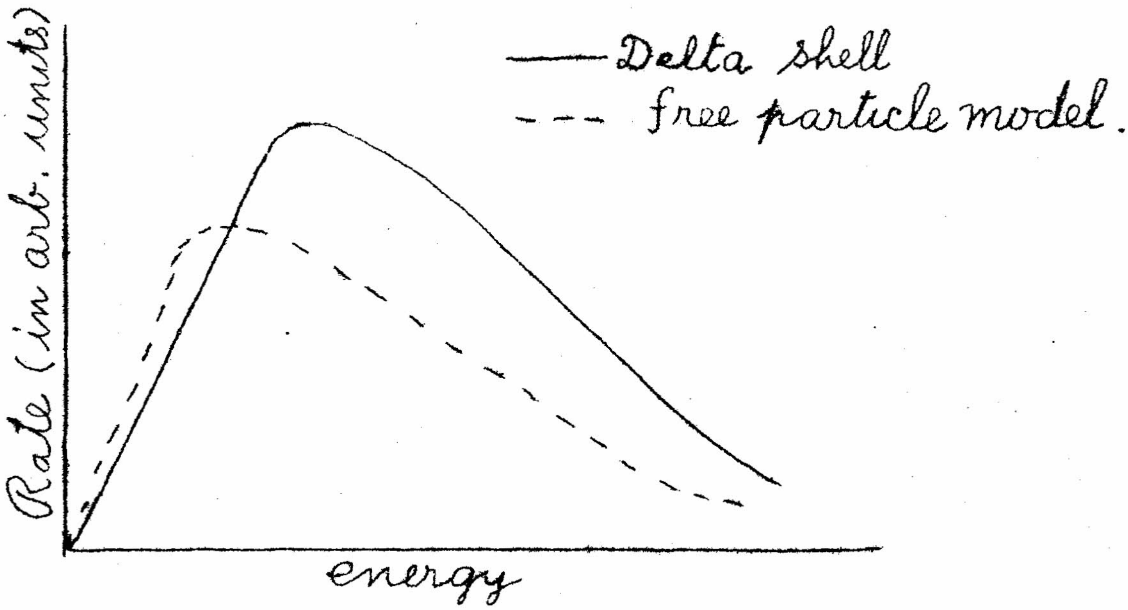


Fig.3. Rate of evaporation in the Bogoliubov model of HeII at $T = 0.6^oK$.

The outcome of this attempt is that

(i) The evaporation rate is a Maxwellian. But the maximum rate is shifted toward higher energies by about 0.35^oK. This feature, though an improvement over the previous theories, still does not confirm to the revised experimental measurements.

(ii) Still there are two peaks due to infinity in the density of states $\left(\frac{d}{dp}E_p = 0\right)$ associated with high energy phonons and the roton minimum. These peaks, however, occur in the tail of the plotted distribution function (not shown in fig.3) but are greatly suppressed compared to the maximum rate shown in the figure (They occur in the order of magnitude rate x 10^{-2})

(iii) The small shift in the rate is quite stable and is almost independent of the type of potential used.

This model may be improved provided

(i) a realistic form for $\mathcal{A}_{pq}$ is fed in instead of (48). It is more physical to suppose high energy atoms would have a greater contribution to the evaporation rate than the low energy ones. In this context the phase space considerations due to cole would be of importance.

(ii) This model does not take into account the threshold energy required to lift an atom from the liquid state and transfer it to the vapour. This energy has been calculated to be 7.15°K. (Anderson 1969). Thus ϵ, the energy of the evaporated atoms, should be measured from this $|\mu| = 7.15$ and not from zero.

Suggestion (ii) has been proposed and used in the evaluation of W_e by Salinas and Turski themselves. Surprisingly this suggestion instead of improving the situation drastically alters the very evaporation rate curve itself to a shape far from a Maxwellian! Again rotons dominate the emission. If the role of rotons is to be suppressed $|\mu|$ has to be chosen to be 0.3°K in order to get the experimental peak. This again contradicts the well known value of 7.15°K for $|\mu|$!

D. Estimation of the condensate density

Since the transfer process can occur only when the excitation is in the bare particle configuration (Appelbaum and Brinkman, 1969) following Griffin (1970) and Cole (1972) one can consider the transfer amplitude $\mathcal{A}_{pq}$ in equation (40) as proportional to the single particle spectral weight functions of the subsystems which are written as

$$A_V(\vec{p}, E) = 2\pi\ \delta(E - T_p - |\mu|) \quad (52)$$

$$A_L(\vec{p}, E) = 2\pi\ Z_p\ \delta(\omega - \omega(p)) \quad (53)$$

for the vapour and liquid respectively. It is presumed that for smaller values of momentum $(p < 2\ \mathring{A}^{-1})$ resonances in $A_L(p, \omega)$ are identical to those found in $S(p, \omega)$ the dynamic correlation function. The strength of the pole Z_p is expected to be fairly dependent on the number N_0 of atoms in the condensate. For small p and low temperatures $Z_p \sim N_0$. Thus evaporation mechanism may estimate N_0 in an indirect fashion. The total evaporation rate is the quantity of interest

$$\dot{N}_e = \sum_{q, \theta < \pi/2} W_q\, Z_q\, \frac{d\omega}{dq}\, f(\omega) \cos\theta\ \delta_{p_{\parallel}, q_{\parallel}} \quad (54)$$

W_q being the bare atom transfer coefficient (a part of the transfer rate $|A_{pq}|^2$). Consequently $T_{p_i p_e}$ occurring in (31) is identified, with $W_q Z_q$.

In the case of electron tunnelling problems in solids W_q is of the order 10^{-8} since the wave functions are required to decay exponentially in the classically forbidden barrier region. However, no such requirement is imposed in evaporation processes as a result of which one may take $T_{p,q}$ to be roughly of the order of unity.

3. Discussion

A major problem in all the tunnelling models is the microscopic evaluation of the transfer amplitudes. It has been reported that in an unpublished work A.Griffin and J.Demers have attempted to evaluate this quantity by using Bogoliubov's theory. In this approach it seems that that the liquid-vapour interface has been represented by a discontinuity in both real and off-diagonal potentials. As reported by Cole (1972) this indicates that T increases monotonically from zero for evaporation energy to a value of the order of unity for $(E/k_B) \gtrsim 1\,^{\circ}K$.

One has to incorporate many body effects in a suitable way. For instance, local selfenergy effects have been neglected in choosing the spectral functions (52) and (53) by taking them as the bulk liquid values.

In these calculations quantized surface excitations have not been taken into account. Such quantized surface waves called ripplons may affect the evaporation spectrum in a significant way. (These waves will be discussed subsequently). Also in all these theories structure of the free surface of HeII (the density profile) has not been considered.

Evaporation and scattering are very intimately related phenomena and an experiment in which ^4He atoms are scattered from the free surface of ^4He would yield information about the elastic and inelastic processes occurring at the surface. Such an experiment has indeed been performed by Edwards and his group (1978). These results are also to be discussed subsequently.

To conclude it should be noted that no microscopic theory is available to date to explain the experimental results on evaporation which show no significant shift in the rate of evaporation.

II. ATOMIC SCATTERING FROM THE FREE SURFACE OF HELIUM II.

1. Relation to evaporation.

Edwards et al (1975) have studied the free surface of pure ^4He by measuring the probability of elastic scattering $\mathcal{R}(k,\theta)$ for ^4He atoms striking the surface of the liquid as a function of their momentum k and angle of incidence θ. During the scattering experiment the temperature of the liquid was varied between 0.025K and 0.125K. At such low temperatures the ^4He target may be considered to be in its ground state.

When a free ^4He atom strikes the surface of liquid HeII three possibilities exist:

(A) Elastic scattering (specular reflection). In this process no energy is transferred to the liquid. The probability for such a scattering is denoted by $R(k,\theta)$.

(B) Inelastic scattering - In this process part of the kinetic energy of the atom is converted into excitations; either phonons or ripplons (quantized surface waves) or both. The probability of such a process is denoted by $\mathcal{D}(k,\theta)$.

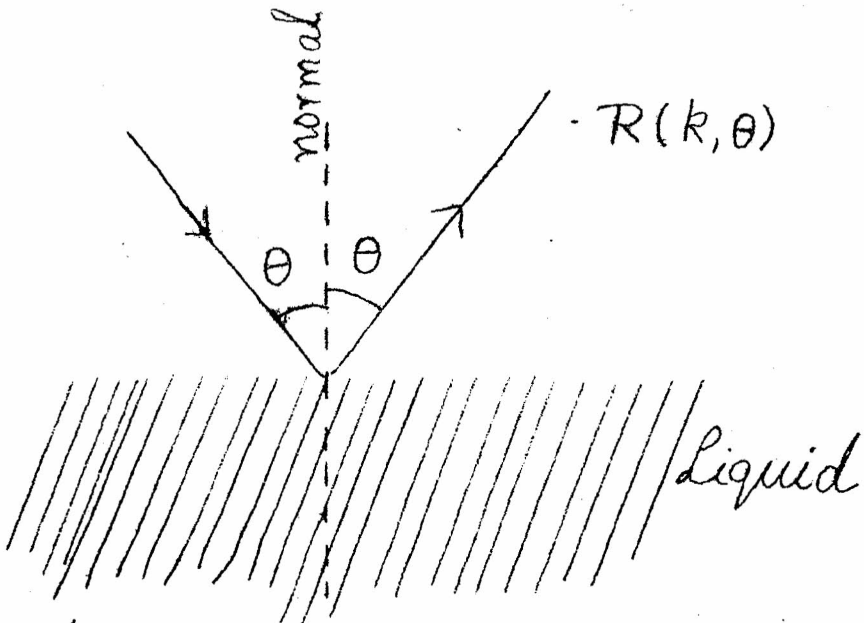
(c) Absorption - In this case the kinetic energy of the atom plus the binding energy L_0 is fully used to create excitations of the liquid $(L_0/k_B = 7.16°K)$. The probability of such a process is denoted by $F(k,\theta)$ The excitations which may be produced can be either phonons or ripplons. If the incident particle is ^3He, then the energy of the ^3He quasi-particle must be considered.

Since no other possibility exists we should have

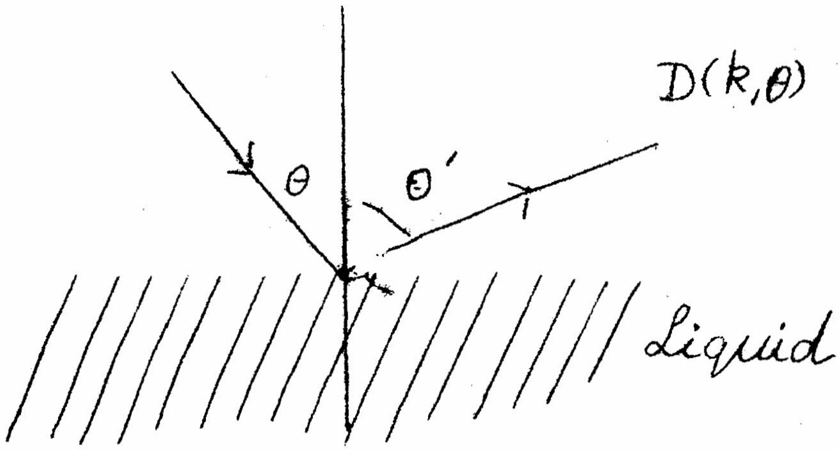
$$R(k,\theta) + D(k,\theta) + F(k,\theta) = 1 \qquad (1)$$

Invoking the principle of detailed balance the probability for absorption can be related to evaporation. According to this principle the flux of evaporated atoms with momentum k and emerging out making an angle θ with the normal to the surface is exactly balanced by the flux of vapour atoms condensing with the same momentum and direction. The condensing flux is obtained by multiplying $F(k,\theta)$ by appropriate ideal gas distribution (Maxwell-Boltzmann). The accommodation coefficient $\bar{F}(T)$ which is the average probability of condensation is given by

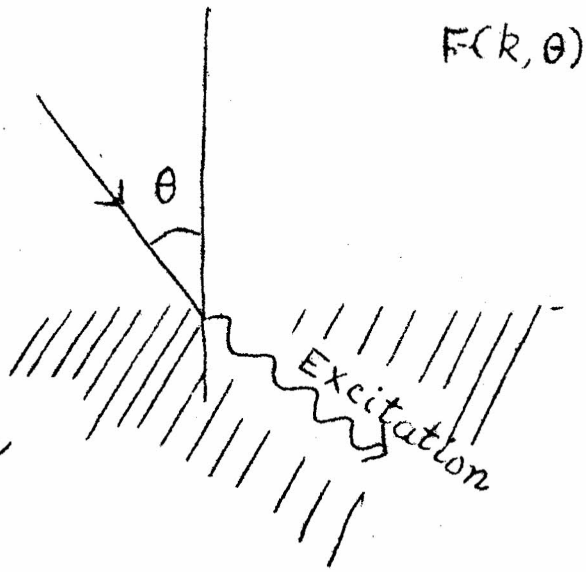
$$\bar{F}(T) = \frac{\iint F(k,\theta)\exp[-k^2/2m\beta]\,k^3\,dk\,\sin\theta\,\cos\theta\,d\theta}{\iint \exp[-k^2/2m\beta]\,k^3\,dk\,\sin\theta\,\cos\theta\,d\theta} \qquad (2)$$



a) Elastic Scattering



b) Inelastic Scattering



c) absorption

The experimental results of Edwards et al can be summarised as:

(i) The probability of elastic scattering depends only upon the vertical component ($k \cos\theta$) of the momentum.

(ii) The probability of inelastic scattering is very small. Within experimental error it is estimated that $D(k,\theta) < 2\times10^{-3}$

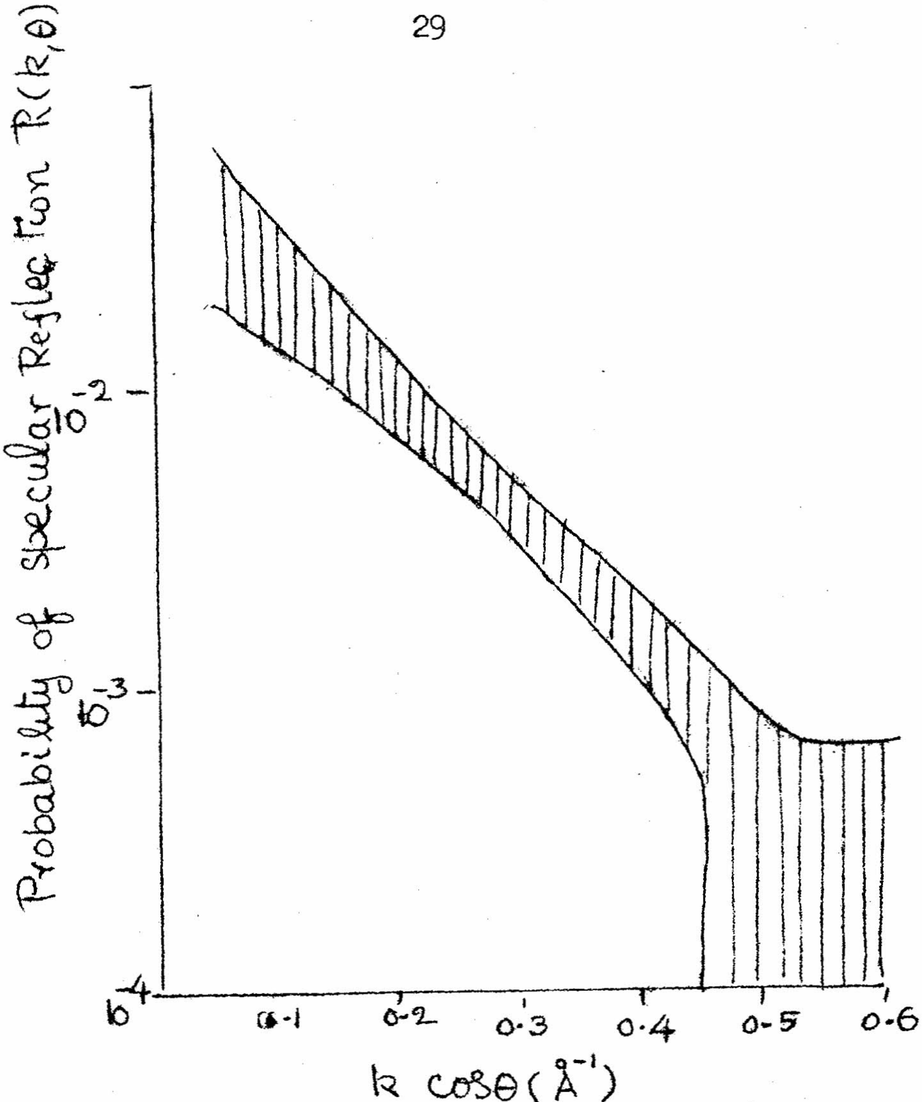
(iii) $k \cos\theta$ was varied from 0.05 to 0.5 $\mathring{A}^{-1}$. From (i) and (ii) it follows that the probability of absorption $F(k,\theta)$ is almost unity.

(iv) As $k\cos\theta \rightarrow 0$ it is expected that the elastic scattering probability tends to unity. However experimentally it has been observed that $R(k\cos\theta)$ tends to some value in the neighbourhood of 0.05.

(v) No dip or edge was observed in $R(k,\theta)$ at the roton threshold. (Compare the similarity of the corresponding results in the case of improved experiments on evaporation.)

(vi) The above mentioned results were found to be unaffected by variations in temperature in the range 0.03 to 0.12°K. Thus the results apply to the scattering by liquid ^{4}He in its ground state.

(Vii) Corollary to (vi) is that thermally excited ripplons or phonons have no effect or surface scattering.



▥ encloses the experimental points (Edwards et al)

Fig.4

To conclude this section we note that the observation $F(k,\theta) \sim 1$ for most k and θ implies that the accommodation coefficient is also very close to unity. Consequently the spectrum of evaporated atoms is very close to a Maxwellian when the liquid is in equilibrium with the vapour.

When $k = 0.5A^{-1}$ the combined kinetic energy and the binding energy L_o of the incident atom equals the roton energy 8.65^oK. (see fig.1). According to the shift predicting theories of evaporation as well as the theory of Cole (1972) there would be a discontinuity in the spectrum of evaporated atoms as well as in the probability of elastic scattering in this region of momentum. This prediction has not been confirmed by the experiment on surface scattering. (see (v) and (vii).

2. The limiting behaviour of $R(k\cos\theta)$

Consider the limit $k\cos\theta \to 0$ in $R(k\cos\theta)$. By analogy with the simple quantum mechanical problem of a very slow particle approaching a stepped attractive potential it is expected that $R \to 1$ as $k\cos\theta \to 0$. However, this does not happen (see (iv)). Edwards et al (1975) have explained this as due to the effect of attractive van der Waals potential outside the liquid. To a good degree of accuracy this potential is approximated by the behaviour z^{-3}, where z denotes the distance in the direction of the normal (In this discussion only normal incidence is discussed). Accordingly Schrodinger's equation is written as

$$\frac{\partial^2 \psi}{\partial z^2} + \left[(k\cos\theta)^2 + \lambda z^{-3} \right] \psi = 0 \qquad (3)$$

Considering the potential between two helium atoms in the super-fluid λ has been estimated to be 20 °A. Equation (3) can be rewritten on making the substitution $x = (k\cos\theta)\, z$

$$\frac{\partial^2 \psi}{\partial x^2} + \left\{ 1 + (\lambda k \cos\theta)\, x^{-3} \right\} \psi = 0 \qquad (4)$$

$R(k,\theta)$ would approach unity when $\lambda k\cos\theta \to 0$ since the potential in the limit will act like a step function. Thus we expect that the probability for elastic scattering will tend to unity in the limit of vanishing $k\cos\theta$ provided

$$\lambda k \cos\theta << 1$$

i.e., when $k << \lambda^{-1}$ which leads to an upper bound for k as

$$k \ll 0 \cdot 05 \ \mathring{A}^{-1}$$

This explains the observation (iv). Edwards et al (1972) have also made a detailed calculation to support this estimate.

3. Theory due to Echenique and Pendry

Echenique and Pendry (1976) have proposed a theory to explain the above mentioned results on the reflectivity of liquid ^4He surface to an externally incident atom. The main features of this theory are the following.:

(i) It is supposed that the interaction with the surface is via the van der Waals potential and extends beyond the mass density cut off. Accordingly the potential energy between an element of liquid at $\vec{r}$ and the particle at $\vec{R}$ is given by

$$- \frac{\alpha}{|\vec{r} - \vec{R}|^6} \ d^3r \tag{5}$$

with $\alpha = 3 \cdot 232 \times 10^{-38}$ cgs units. If the liquid is supposed to be incompressible then the surface tension waves are much 'softer' than the sound waves and in this case the surface tension waves are neglected. Consequently the particle moves in a potential

$$- \frac{\lambda}{|z|^3} \qquad \text{with} \quad \lambda = \pi\alpha/6$$

(ii) If the surface wave exists, it results in a coupling between the particle and the surface mode. The quantised surface tension waves (the so called ripplons) have the following classical dispersion relationship

$$\omega^2 = q^3 T/\rho \tag{6}$$

where T is the surface tension and ρ is the density of the liquid.

$$T = 0\cdot 35 \text{ dyn cm}^{-1} \text{ at } 0^\circ \text{K}$$

$$\rho = 0\cdot 14 \text{ gm cm}^{-3}$$

The coupling to a ripplon extends beyond the density limit but not so far into the vacuum as the van der Waals potential does.

(iii) The thickness of the surface region itself has to be taken into account.

In this model, the incident atom first interacts with the weak tail of the Van der Waals potential. At this stage (elastic) reflection and coupling to ripplons are possible. Reflection is small because of the weakness of the tail whereas coupling to the ripplons increases very rapidly from a negligible to a very large value. An atom as it penetrates beyond this region loses considerable energy as a result of which it is eventually caught in the attractive well of the liquid. Inelastic reflectivity is also small due to this reason. These phenomena happen well above the physical surface of liquid Helium.

The reason why rotons have no influence on the elastically scattered flux is given as follows: To excite a roton the atom must tunnell into the liquid and still have a large amount of energy to excite a roton. This is possible only when the incident atom is very close to the surface. But when the atom is very close to the surface it had already lost most of its energy to the ripplons.

Due to surface waves there is a displacement ζ of the surface given by

$$\zeta = \Omega^{-\frac{1}{2}} A_q \cos(\vec{q} \cdot \vec{r}) \tag{7}$$

Ω being the surface area and A_q is the amplitude of the surface wave in the z direction. The Lagrangien for the system is written down as

$$\mathcal{L} = \sum_q \frac{\rho}{4|\vec{q}|} \left[\dot{A}_{\vec{q}}^2 - \omega^2 A_{\vec{q}}^2 \right] + \frac{1}{2} m \dot{R}^2 + \lambda z^{-3} - \sum_q \Phi_{\vec{q}}(\vec{R}) A_{\vec{q}} \tag{8}$$

In the above $\vec{R}$ denotes the position vector of the incident atom. The first term in (8) is the surface wave, the second term is due to the incident atom and the last term represents coupling of the two.

$$\Phi_q(\vec{R}) = -\frac{6\lambda}{\pi} \int d^3 r_{\parallel} \, \Omega^{-\frac{1}{2}} \cos(\vec{q} \cdot \vec{r}) \left\{ (\vec{R}_{\parallel} - \vec{r}_{\parallel})^2 + z^2 \right\}^{-3} \tag{9}$$

Information regarding the probability for the particle to be reflected without having lost energy to a surface wave has been obtained using the path integral formalism due to Feynman and Hibbs (1965). Referring the reader to the paper of Echenique and Pendry (1976) for more details, we write down the attenuating factor γ as

$$\gamma(\vec{R}) = \exp\left\{-\frac{\Omega}{2\pi}\int \frac{\bar{\Phi}_q^2}{2\rho\omega\hbar}\, q^2\, dq\right\} \tag{10}$$

where $\bar{\Phi}_q$ gives the impulse

$$\sum_q \int_{-\infty}^{\infty} \phi_q(\mathbb{R}(t))\, A_q\, dt = \sum_q \bar{\Phi}_q A_q$$

The impulse is conveyed by the trajectory $\mathbb{R}(t)$. $\mathbb{R}$ and A_q are suitably chosen coordinates.

It is assumed that only cos like ripplons are excited and a first order estimate for particle ripplon interaction V_{PR} becomes

$$V_{PR}(\vec{R}) = -\alpha \int \frac{d^2 r_{\parallel}\; u(r_{\parallel})}{\left[\,|R_{\parallel} - r_{\parallel}|^2 + z^2\,\right]^3}$$

$u(r_{\parallel})$ can be expanded in terms of normal modes to obtain

$$u(\vec{r}_{\parallel}) = \Omega^{-\frac{1}{2}} \sum_q \phi_q(\vec{R})\, A_q \cos(\vec{q}\cdot r_{\parallel})$$

so that

$$V_{PR}(\vec{R}) = \sum_q \phi_q(\vec{R})\, A_q \tag{11}$$

where

$$\Phi_q(\vec{R}) = \frac{-\pi\alpha}{4\Omega^{1/2}} \cos(\vec{q}\cdot\vec{R}_{\parallel}) \frac{q^2}{Z^2} K_2(qZ) \tag{12}$$

In this K_2 denotes the second order modified Bessel function of the second kind.

The dominant trajectories in the Feynman formalism have been assumed to be those in which the particle travels in a straight line to the point of reflection, with uniform velocity $\vec{v}$. (see Fig.3A). For such a trajectory the impulse to the q^{th} mode has been calculated to be

$$\bar{\Phi}_q = \int_{-\infty}^{\infty} \phi_q(\vec{R}(t))\, dt$$

$$= \frac{-\pi\alpha}{2\sqrt{\Omega}} \frac{1}{V\cos\theta} \int_{z_0}^{\infty} \left[\cos\left\{ \frac{\vec{q}\cdot\vec{V}(r - Z_0)}{V\cos\theta} \right\} \times \frac{q^2}{r^2} K_2(qr) \right] dr \tag{13}$$

With increasing argument the function K_2 decays with increasing rapidity so much so the integral gets a very significant contribution from the region of $\vec{R}$ near the point of reflection. Consequently we can treat the argument of Cosine function in (13) as nearly equal to zero and replace the Cosine function by unity. This approximation is actually exact for normal incidence. Then

$$\gamma = \exp\left[- \delta\epsilon / k_z^2 Z_0^{15/2} \right] \tag{14}$$

with

$$\left.\begin{aligned} \delta &= \pi \alpha^2 m^2 / 16 \hbar^3 \, (\rho T)^{\frac{1}{2}} \\ \epsilon &= \int_0^\infty dx \; x^{13/2} \int_x^\infty dy \; \frac{k_2(y)}{y^2} \end{aligned}\right\} \qquad (15)$$

is evaluated numerically to obtain

$$\gamma = \exp\left[-1.075 \times 10^{-3} / K_Z^2 \, Z_0^{15/2} \right] \qquad (16)$$

The graph of $|\gamma_1(Z_0)|^2$ is given below:

FIG 5

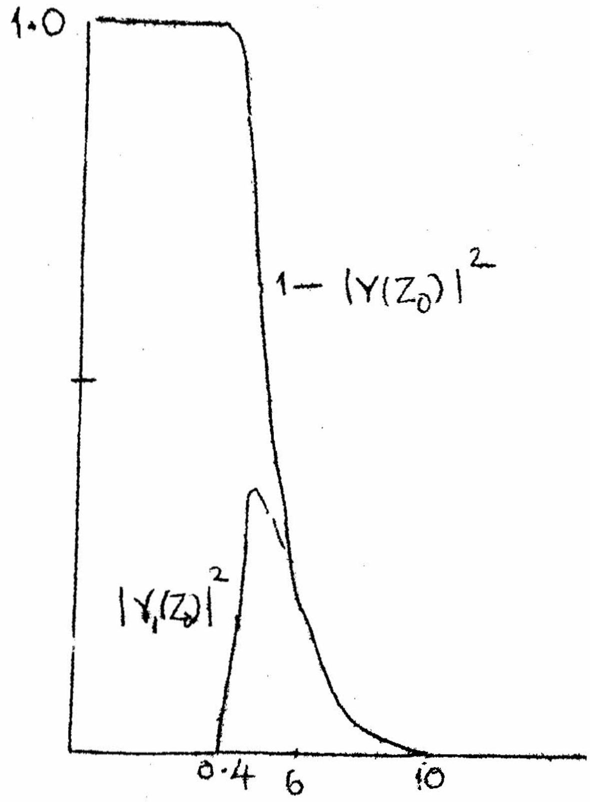


FIG 6

Echenique and Pendry have also calculated the reflectivity of the Van der Waals potential corrected for the attenuation of elastic flux caused by ripplon interaction. To solve this they simply integrate the Schrodinger equation by including the corrections from the ripplon interactions as absorptive self energy in the Schrodinger equation. Thus the following equation is considered

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2} + \left(-\frac{\lambda}{|z|^3} + i\,\Sigma_i(z)\right)\psi = \frac{\hbar^2 k_z^2}{2m}\,\psi \quad (17)$$

where the imaginary term

$$i\,\Sigma_i(z_0) = -i\,\frac{\hbar k_z}{2m}\;\frac{15}{2}\;\frac{\delta\epsilon}{k_z^2\,|z_0|^{17/2}}$$

$$= -i\,\frac{15}{4}\;\frac{\hbar\,\delta\epsilon}{m k_z\,|z_0|^{17/2}} \quad (18)$$

when included along with the Lagrangian increases the probability of the dominant paths by an amount

$$\Delta Y = Y(z_0)\;\frac{15}{2}\;\frac{\delta\epsilon}{k_z^2\,z_0^{17/2}}\;\Delta z_0 \quad (19)$$

For some suitably chosen positive value Z_c of Z, Σ_i becomes so large that little elastic flux reaches the region $Z<Z_c$. For all

$Z<Z_c$ the potential term is chosen to be a constant

$$-\frac{\lambda}{|z_c|^3} + i\,\Sigma_i\,(Z_c) \qquad \text{for } Z<Z_c \tag{20}$$

Then for $Z<Z_c$ the wave field is purely a decaying wave . Let Z_f be a sufficiently large value where the potential and self energy can be taken to be zero. In this scheme the singularity at $z=0$ has been avoided.

Wave field is then integrated from a value $z<z_0$ to the value Z_f and the wave function is matched to incident and reflected plane waves.

The results clearly depend on $k\cos\theta$, the normal component of momentum. This is in confirmity with the experimental observations. However, the magnitudes of the reflectivities, as obtained from this theory do not match well with the experimentally observed magnitudes.

This theory explains why experiments mainly observe elastic flux reflected from the surface. To explain this consider the graph for $|\gamma_1(z_0)|^2$ (figure 5) which gives the probability of completing a trajectory with the loss of one and only one ripplon. The graph $|1-\gamma_0|^2$ gives the probability of losing at least one ripplon. A comparison of these two graphs clearly indicates that there is only a very narrow domain $4 \leq Z(\text{Å}) \leq 8$ in which one-ripplon-loss reflection process can take place. It thus follows that as soon as the particle enters the absorption zone the probability that it loses its energy to many ripplons (and ultimately gets assimilated with the liquid) is very dominant. Hence the inelastic spectrum is insignificant when compared to the elastic spectrum.

The outcome of this attempt clearly indicates that

(i) the classical relationship for the surface waves as given by equation (6) has to be reexamined. Different calculations by several authors have yielded different relationships.

(ii) The diffuse nature of helium surface is very important. This will significantly alter the dispersion relation for the ripplons as well as the coupling of the incident particle to the ripplons. Following the Monte Carlo calculation of Lieu et al (1975) who have observed that the diffuseness of the surface of ^4He spreads over a region of the size 5Å, Echenique and Pendry approximated the diffuse surface with a linear increase of density from the surface/and redid the calculation of the reflectivities to obtain a better agreement with experiments.

4. Variational Approach.

Let Φ denote the ground state of N ^4He atoms. Φ is real and positive and if H is Hamiltonian for the ^4He system

$$H \Phi = 0 \tag{21}$$

provided the energies are measured from the ground state of the pure ^4He system. Consider the situation where one of the ^4He atoms has been replaced by an 'impurity' helium atom. If one uses the variational method due to Feynman (1954) to study this system the trial wave function for the system (in which an 'impurity' has been added) can be written as

$$\Psi = f(\vec{r}_1)\ \Phi\ (\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \tag{21}$$

Assuming that the impurity interacts with the background in the same way as a ^4He atom would do the modified Hamiltonian H' can be written as

$$\left.\begin{aligned} H' &= \left[-\frac{\hbar^2}{2m_1} + \frac{\hbar^2}{2m}\right] \nabla_1^2 + H \\ &\text{where} \\ H &= -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V(r_{ij}) - E_0 \end{aligned}\right\} \qquad (23)$$

m_1 being the mass of the 'impurity' atom. E_0 is the ground state energy relative to vacuum. The expectation value for the energy E is

$$E = \frac{\int \psi^* H \psi \, d\vec{r}_1 \ldots d\vec{r}_N}{\int \psi^* \psi \, d\vec{r}_1 \ldots d\vec{r}_N} \qquad (24)$$

Following Feynman it is easy to show that E is minimum for a state (in bulk helium) with momentum $\hbar k$ if

$$f(r_1) = \exp(i\vec{k}\cdot\vec{r}_1)$$

with energy $E = \frac{\hbar^2 k^2}{2m_1} + \left[\frac{m}{m_1} - 1\right] \nu_0/\rho_0$

where (ν_0/ρ_0) is the kinetic energy per atom in the bulk ^{4}He ground state. To apply this theory to the case of helium with a free surface f is rewritten as

$$f(\vec{r}_1) = \psi(\vec{r}_1) \Big/ \left(\rho(r_1)/\rho_0\right)^{1/2} \tag{25}$$

$\rho(\vec{r}_1)$ being the number density at a point $\vec{r}_1$ in the bulk liquid in the ground state Φ ; that is

$$\rho(\vec{r}_1) = N \int \Phi^2 \, d\vec{r}_2 \ldots d\vec{r}_N$$

while ρ_0 is the average number density in the bulk liquid. The probability density for atom 1 in the state ψ is then constant $\times\, |\psi(\vec{r}_1)|^2$. Minimising the energy leads to the following equation (which is actually a Schrodinger equation with an effective potential $\frac{\hbar^2}{2m_1} U(\vec{r})$) for $\psi(\vec{r}_1)$.

$$\nabla_1^2 \psi(\vec{r}_1) + \left[\frac{2m_1 E}{\hbar^2} - U(\vec{r}_1) \right] \psi(\vec{r}_1) = 0 \tag{26}$$

(See also Lekner (1970)). For the surface scattering experiments using ^{4}He beams, $m_1 = m$, in which case the effective potential can be written down as

$$U(r) = a''/a \quad \text{where} \quad a(\vec{r}) = \sqrt{\rho(\vec{r})/\rho_0} \tag{27}$$

so that $a''(\vec{r}) = d^2a/dz^2$. Since $\psi^*\psi$ is the probability density for the scattered atom and ψ obeys the Schrodinger equation (26) it follows that the current of the scattered atom is conserved. Thus one has to find only the single particle reflection coefficient for the one dimensional potential function $U(z) = a''/a$. In this case the probability for elastic scattering is directly related to the density profile of the liquid $\rho(z) = [a(z)]^2/\rho_0$.

This model explains the experimental observation that there is no inelastic scattering and that the reflection coefficient depends only on the perpendicular component of the incident momentum i.e. $\hbar k \cos\theta$.

In calculating the reflection coefficient the proper asymptotic behaviour of a(z) has to be taken into account.

Far above the surface, where the liquid density decreases exponentially with z, the effective potential must be identical to the Van der Waals potential for pure ^{4}He so that in this limit

$$U \rightarrow \beta^2 - \lambda/z^3 \qquad (28)$$

where

$\frac{\hbar^2\beta^2}{2m} = L_0 =$ Binding energy or latent heat of ^{4}He at 0°K.

$L_0/k_B = 1.087\ \text{A}^{\circ -1}$, $\beta = 1.087\ \mathring{A}^{-1}$

Consequently from (27) we have

$$a \longrightarrow \exp\left\{-\beta z - \text{const} - \frac{\lambda}{4\beta z^2} - \cdots\right\} \tag{29}$$

This implies that $\rho(z) = a^2/\rho_0$ that is, for larg z the density decreases as $\exp(-2\beta z)$. This is in confirmity with the observation of Regge (1972) and Saam (1971).

Deep inside the liquid

$$a \rightarrow 1 \quad \text{and} \quad U \rightarrow 0 \tag{30}$$

The following choice of a(z) interpolates between the asymptotic behaviour far from the liquid (eq.28) and deep inside the liquid (eq.30):

$$a(z) = \left\{\exp p(z) + 1\right\}^{-1}$$

with

$$p(z) = \beta(z) - g_1 + \frac{\lambda}{4\beta(z^2 + g_2)} \tag{31}$$

g_1 and g_2 being adjustable constants. g_2 has to be restricted only to positive (>0) values in order to give regular behaviour for p(z). Then

$$U = \frac{a''}{a} = (1-a)\left[p'^2(1-2a) - p''\right] \tag{32}$$

where $p' = \dfrac{dp}{dz}$, $p'' = \dfrac{d^2p}{dz^2}$

Edwards et al (1978) have solved the Schrodinger equation for $\psi(r_1)$ (eq.26) for the potential given by (32). With $m_1 = m$ and $\psi = e^{ik_x x}\,\zeta(z)$ and $k_x = k\sin\theta$, $k_z = k\cos\theta$ eq.(26) can be rewritten as

$$\frac{d^2\zeta(z)}{dz^2} + \left\{ k_z^2 + \beta^2 - U(z) \right\} \zeta(z) = 0 \tag{33}$$

Starting from several angstroms below the surface where the conditions (30) apply so that

$$\zeta(z) = \exp\left\{-i(k_z^2+\beta^2)^{\frac{1}{2}} z\right\} \tag{34}$$

We integrate out upto $z = 200$ Å where $U = \beta^2$ and

$$\zeta(z) = A\exp(-ik_z z) + B\exp(ik_z z)$$

The reflection coefficient is obtained from $|B/A|^2$. The choice $g_1 = 2.5$ and $g_2 = 8.5$Å^2 gives a good fit with the experimental data as indicated in fig. 7. These values of g_1 and g_2 when

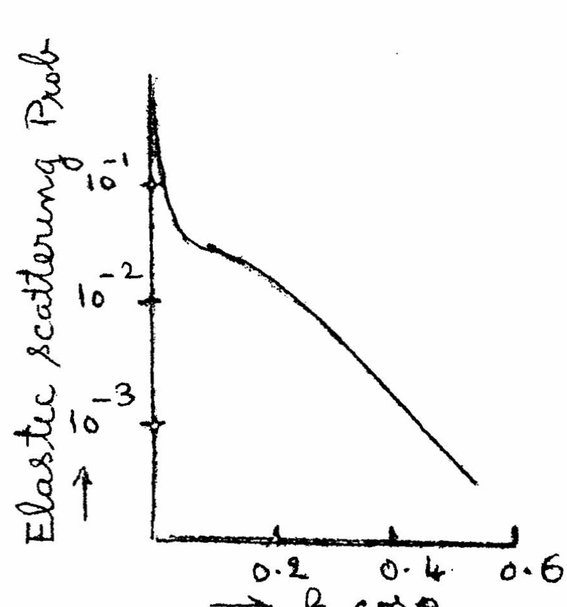


Fig. 7

substituted in (31) and (32) yield the model potential $U_M(z)$ and the 'model profile' $a(z)^2$:

(A) Even though the fit with experimental data is quite good there is a rather unsatisfactory feature - viz the reflection coefficient is not sensitive to the potential U(z) in the region where $\rho(z)$ is considerably greater than zero (i.e. in the 'liquid' region' where the density profile is really to be learnt). Edwards et al modified U_M in two ways

$$U_{IM} = U(z) + \frac{1}{2}\beta^2 a^2 \tag{35}$$

$$U_{IIM} = U(z) - i\gamma^2 a^2 \tag{36}$$

U_{IM} differs from $U(z)$ only in the region $a^2 = \frac{\rho}{\rho_0} \gg 0$. $R_I(k,\theta)$ corresponding to U_{IM} is not significantly altered by this modification. U_{IIM} contains an imaginary term proportional tothe density of the liquid and the imaginary part of U_{IIM} produces a strong absorption inside the liquid region. U_{IIM} does not also alter $R(k,\theta)$ significantly.

(B) Another point to be rectified is the lack of symmetry in the variational wave function (22). If the trial wave function is thus symmetrised, the theory then can describe the conversion of an incident atom into a single high energy excitation with the same energy and transverse momentum. Even here the assumption that only single particle processes dominate (Anderson-Widom hypothesis) is employed.

The symmetrised form of (22) would be

$$\Psi_{Sym} = \sum_{i=1}^{N} f(\vec{r}_i)\ \Phi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \tag{37}$$

When the energy E (see (24)) is minimised for the inhomogeneous liquid with a free surface, the resulting Euler-Lagrange equation is

$$\nabla_1 [\rho_1 \nabla_1 f_1] + \frac{2mE}{\hbar^2} f_1 \rho_1$$

$$+ \int d\vec{r}_2 \left\{ \nabla_2(\rho_{12} \nabla_2 f_2) + \frac{2mE}{\hbar^2} f_2 \rho_{12} \right\} = 0 \tag{38}$$

where

$$f_i = f(\vec{r}_i)\ , \quad i = 1,2$$

$$\rho_1 = \rho(\vec{r}_1) = N \int \Phi^2 d\vec{r}_2 \dots d\vec{r}_N$$

$$\rho_{12} = \rho(\vec{r}_1, \vec{r}_2) = N(N-1) \int \Phi^2 d\vec{r}_3 \dots d\vec{r}_N$$

$$= \rho_1 \ \rho_2 \ g(\vec{r}_1, \vec{r}_2)$$

For a homogeneous liquid the two particle correlation function $g(\vec{r}_1, \vec{r}_2)$ is a function of $r = |\vec{r}_1 - \vec{r}_2|$. Defining $f(r)$ as in (25) one can reformulate (38) as

$$\nabla_1^2 \psi(\vec{r}_1) + \left[\frac{2mE}{\hbar^2} - U_1\right] \psi(\vec{r}_1)$$

$$= \frac{2mE}{\hbar^2} \int d\vec{r}_2 \sqrt{\rho(\vec{r}_1)\, \rho(\vec{r}_2)}\, \left[1 - g(\vec{r}_1, \vec{r}_2)\right] \psi(\vec{r}_2) \tag{39}$$

where $U_1 = U(\vec{r}_1)$ is obtained from (27). It is convenient to define $1 - g(\vec{r}_1, \vec{r}_2) = c_{12}$ so that

$$c_{12} = 1 \quad \text{for} \quad \vec{r}_1 = \vec{r}_2$$

$$= 0 \quad \text{for} \quad |\vec{r}_1 - \vec{r}_2| >> 1$$

In general c_{12} can be written as $c(z_1, z_2; h)$ where z_i are the vertical components of $\vec{r}_i$ $(i=1,2)$ and h equals the magnitude of the horizontal component of $(\vec{r}_1 - \vec{r}_2)$.

Let $\psi(\vec{r}) = \exp(ik_x x)\,\zeta(z)$ and $a(z) = \sqrt{\rho(z)/\rho_0}$ equation (39) can be r~~a~~ewritten as

$$\zeta''(z_1) + \left[\frac{2mE}{\hbar^2} - k_x^2 - U_1\right]\zeta(z_1)$$

$$= 2\pi\rho_0 \frac{2mE}{\hbar^2} a(z_1) \int dz_2\, a(z_2)\, \zeta(z_2) \tag{40}$$

$$\times \int dh\, h\, J_0(k_x h)\, c(z_1, z_2; h)$$

This integro-differential equation was first obtained by Saam (1971). Note that when $a(z_1)$ is negligibly small (i.e. in the region outside the liquid) the integro-differential equation (40) reduces to the Schrodinger equation (26). Thus both the symmetrised and the unsymmetrized theories are expected to lead to identical results in the vacuum region above the liquid.

The solution of the integral equation (40) are of several types.

Corresponding to a phonon in the bulk liquid or an evaporated atom in the vacuum region;

solutions which are localised in the surface region (corresponding to ripplon excitations),

solutions which decrease exponentially in the liquid region (corresponding to totally reflected atoms)

The symmetrised theory however is in contradiction with experimental evidence, particularly in the prediction of complete or almost complete reflection for certain k and θ .

(c) It is also found that it is quite difficult to determine the density profile $\rho(z)$ unambiguously by this theory.

To conclude, it looks as though the specular reflection coefficient is mainly determined by the static van der Waals potential outside the liquid. An atom which penetrates this region starts producing low energy excitations and is incoherently scattered. This point has been emphasised by Echenique and Pendry also.

Also it has been shown that $R(k,\theta)$ is insensitive to in the region where a^2 is appreciable. Even the addition of a large imaginary component does not alter $R(k,\theta)$ in the region where a^2 is significantly different from zero.. Thus an incident atom which has penetrated a critical distance in the surface region (which according to Echenique and Pendry is about 5Å) has a negligible probability of reflection.

III. HEAT FLOW ACROSS A BOUNDARY BETWEEN SOLID AND LIQUID HELIUM

1. Kapitza conductance.

Let us briefly consider the problem of heat flow across a boundary between solid and liquid helium. In this case a discontinuity in temperature appears between the two materials which for small temperatures $(\delta T << T)$ is proportional to heat current density $\dot{Q}/A$. This discontinuity which was first observed by Kapitza in 1941 enables one define a resistance R_k and a conductance h_k by the following equation:

$$(1/R_K) = \dot{Q}/A\delta T = h_K \qquad (1)$$

generally thermal boundary resistances are smaller, less well defined and more difficult to measure. But in the case of liquid helium this turns out to be an interesting one both experimentally and theoretically. The interface between a solid and HeII is experimentally interesting because intimate thermal contact may be established without strain and the temperature of the liquid may be conveniently measured. Also a hydrodynamic pressure may be applied at the interface since Kapitza resistance depends on the pressure also. Also Kapitza resistance has an important role to play in reaching temperatures lower than 1^{o}k. (see for instance the excellent review by Pollack (1969)).

Kapitza resistance is supposed to be due to the large impedence to the passage of thermal phonons across the interface. The acoustic impedences of the two sides, i.e. the product of the density and the sound velocity, play a vital part in determining the reflection and transmission of phonons at the interface. Generally the acoustic impedense of the solid may be more than two or three orders of magnitude greater than that of liquid He. This acoustic mismatch prevents a large fraction of the phonons impinging on the interface from both sides from penetrating the interface.

Contribution to the energy flux across the interface may arise from the following:

(a) Consider the solid and liquid HeII in thermal equilibrium Then there is no net flow of heat. However, if the solid is heated the distribution of phonons in the entire solid changes. Consequently there is a significant change in the thermal oscillations of the surface. The energy flux $\dot{Q}/A$ transferred across the boundary depends on the efficiency with which the component of surface oscillations in the direction normal to the interface transmits energy to liquid helium. The normal surface oscillations in turn are made up of logitudinal lattice waves, transverse lattice waves and surface waves (Rayleigh waves).

(b) The energy flux may also be transmitted due to the collision of excitations of liquid helium with the oscillating wall.

(c) The theory of Kapitza resistance in metals involves an added feature which is interesting: the role of electrons in transferring thermal energy across the interface. Electron-phonon interactions, for instance may increase the energy transport from surface waves into the bulk solid.

Theories of Kapitza resistance can be generally classified as those based on the two-fluid model of HeII and those based on the acoustic mismatch.

The two-fluid model proposed by Landau is a remarkably accurate model which has successfully explained several interesting properties of HeII such as the fountain effect, the first and the second sound. The observation of Kapitza resistance between solids and liquid ^{3}He by Fairbank and Lee (1958, 1959) has demonstrated that the two fluid properties of HeII play only a small or insignificant part in Kapitza resistance in HeII (at least in the temperature region 0.1^{o}k and 0.6^{o}k where ^{3}He is not a superfluid).

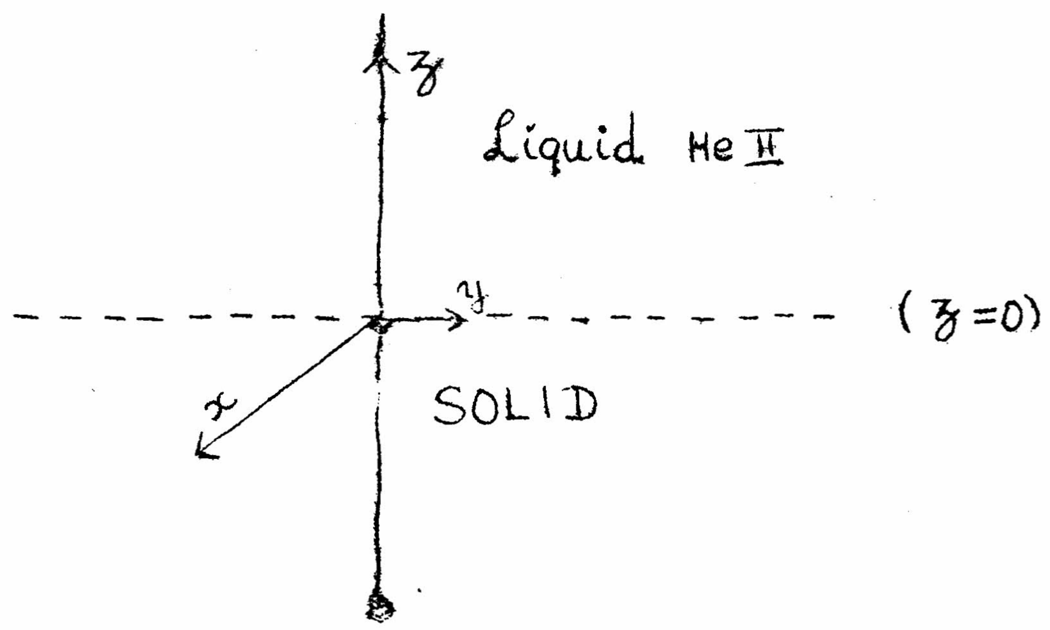
The acoustic impedance theory proposed by Khalatnikov (1952) and independently by Mazo and Onsager (1955) comes closest to quantitatively explaining the experimental measurements. Even in this approach the calculated values of R_K are higher than the experimental R_K's generally by anoorder of magnitude.

2. The acoustic mismatch theory.

This theory is based on the fact that the velocity of sound in a solid is an order of magnitude higher than in liquid He. Thus the phonon momenta in solids are very much different from the phonon momentum in liquid HeII. Therefore phonons impinging on the interface cannot pass freely across since energy and momentum cannot be conserved for arbitrary angles of incidence . This results in the impedence of the transfer of phonon energy across the interface which in turn leads to a jump in temperature at the interface.

Consider a solid at temperature T_1 in contact with liquid HeII at a slightly lower temperature T_2. Heat exchange between the two phases occur in one of the two ways: lattice vibrations from the surface of the solid can emit energy (radiation of phonons and rotons) or phonons and rotons in liquid HeII on colliding with solid wall can transfer energy.

Consider a liquid HeII solid interface (fig.8)



Let $u_z(\omega)$ denote the displacements of the small oscillations of the solid surface perpendicular to the interface, ω denoting the frequency of the oscillations. If A denotes the interface area the rate at which energy will be radiated into liquid HeII is given by

$$W(\omega, T_2) \sim \rho \int |\dot{u}_z(\omega)|^2 \, dA \tag{2}$$

The integration is over the interface area. This formula is true if the wavelength of the emitted excitation is small compared to the dimension of the solid. Then

$$\frac{W(\omega, T_2)}{A} = \rho C_1 \, |\dot{u}_z(\omega)|^2 \tag{3}$$

The net energy flux from the solid to the liquid radiated over all frequencies, $\dot{Q}/A$ is calculated as

$$\frac{\dot{Q}}{A} = \frac{W(T_1) - W(T_2)}{A} = \int \frac{W(\omega, T_2)}{A} \left[n(T_1) - n(T_2) \right] dT_\omega \tag{4}$$

and $n^{-1}(T) = \left[\exp(\beta\omega) - 1 \right]$ is the Bose-Einstein distribution of the phonons. The net energy flux is written as the difference of the energy flux radiated over all frequencies from the solid into liquid minus the energy flux radiated from the liquid to the solid.

As discussed before the normal oscillations of the solid surface has three components:

(i) longitudinal waves impinging on the surface from the solid (denoted by displacements $u_{z\ell}$)

(ii) transverse waves with displacements u_{zt}

(iii) surface waves with displacement u_{zs}.

Consider a longitudinal displacement plane wave impinging on the solid surface from below. Upon reflection from the surface both longitudinal and transverse waves will be produced. We shall consider the xz plane as the plane of incidence. Then reflection as well as longitudinal and transverse oscillations take place in the same plane. We shall use the following notation.

	amplitude	unit vector in the direction of propagation	unit wave vector	associated angle of incidence (or reflection)
incident wave	a_o	$\hat{n}_o$	$\hat{k}_o$	θ_o
reflected longitudinal wave	a_ℓ	$\hat{n}_\ell$	$\hat{k}_\ell$	θ_ℓ
reflected transverse wave	a_t	$\hat{n}_t$	$\hat{k}_t$	θ_t

If c_ℓ and c_t are defined as the velocities of the longitudinal and transverse waves respectively

$$k_o = k_\ell = \omega / c_\ell \quad , \quad k_t = \omega / c_t \tag{5}$$

and

$$\theta_o = \theta_\ell \quad , \quad c_t \sin\theta_o = c_\ell \sin\theta_t \tag{6}$$

Also

$$c_t < c_\ell \tag{7}$$

It is assumed that the normal component of displacement and the normal component of the stress are continuous at the interface. If π_{ik} denotes the stress tensor, the stress boundary conditions are

$$\pi_{ik}\, n_k = 0 \tag{8}$$

Since xz plane has been considered as the plane of incidence and reflection these reduce to

$$\pi_{zz} = 0 = \pi_{xz} \tag{9}$$

One can write down the full displacement vector as

$$\begin{aligned} u(\vec{r},t) = \Big\{ & a_0\, \hat{n}_0 \exp(i k_0 \cdot r) \\ & + a_\ell\, \hat{n}_\ell \exp(i k_\ell \cdot r) \\ & + a_t\, \hat{n}_t \exp(i k_t \cdot r) \Big\} \exp(-i\omega t) \end{aligned} \tag{10}$$

for which the boundary conditions of the displacement canbe applied. Ultimately these determine the ratio a_ℓ/a_0 and a_t/a_0, as

$$\frac{a_\ell}{a_0} = \frac{c_t^2 \sin 2\theta_t \sin 2\theta_0 - c_\ell^2 \cos^2 2\theta_t}{c_t^2 \sin 2\theta_t \sin 2\theta_0 + c_\ell^2 \cos^2 2\theta_t} \tag{11}$$

$$\frac{a_t}{a_0} = -\frac{2c_\ell c_t \sin 2\theta_0 \cos 2\theta_t}{c_t^2 \sin 2\theta_t \sin 2\theta_0 + c_\ell^2 \cos^2 2\theta_t} \tag{12}$$

These equations substituted back into (10) leads to

$$u_{z\ell}(\omega) = a_0 \frac{2c_\ell^2 \cos\theta_0 \cos 2\theta_t}{c_t^2 \sin 2\theta_t \sin 2\theta_0 + c_\ell^2 \cos^2 2\theta_t} e^{-i\omega t} \tag{13}$$

To determine $|a_0|$ one uses the prescription of Khaltnikov that the total energy of the incoming plane wave (twice the kinetic energy) equals the phonon energy $\hbar\omega$ $(\hbar = 1)$

$$\int \rho_S |\dot{u}_\ell|^2 dV_S = \rho_S |A_0|^2 \omega^2 V_S = \omega \tag{14}$$

so that

$$|a_0| = (\rho_S \omega V_S)^{-1/2} \tag{15}$$

V_S being the solid volume. Thus we are led to the following expression for the absolute magnitude of the normal surface velocity due to longitudinal waves.

$$|\dot{u}_{z\ell}(\omega)| = \left(\frac{\omega}{\rho_S V_S}\right)^{\frac{1}{2}} \left| \frac{2c_\ell^2 \cos\theta_0 \cos 2\theta_t}{c_t^2 \sin 2\theta_t \sin 2\theta_0 + c_\ell^2 \cos^2 2\theta_t} \right| \tag{16}$$

From this the contribution to W can be easily calculated on using (3). Transverse displacement plane waves in the solid may be treated in an analogous way. The incident transverse wave upon reflection will generate a longitudinal wave and a transverse wave. The connection between the angles of the incident and reflected waves are

$$\theta_0 = \theta_t \,, \quad c_t \sin\theta_\ell = c_\ell \sin\theta_0 \tag{17}$$

and

$$|\dot{u}_{zt}(\omega)| = \sqrt{\frac{\omega}{\rho_s V_s}} \left| \frac{2c_t^2 \cos\theta_0 \sin 2\theta_\ell}{c_t^2 \sin 2\theta_t \sin 2\theta_0 + c_\ell^2 \sin^2 2\theta_0} \right| \tag{18}$$

To calculate the contribution from surface displacement waves let u_{zs} and u_{xs} be the surface displacements in the longitudinal and transverse directions. The velocity of the displacement is

$$c_s = \xi\,(c_t/c_\ell)\, c_t \tag{19}$$

and wave number $k_s = \omega/c_s$. Then

$$\int_0^\infty \rho_s \left(|\dot{u}_{xs}|^2 + |\dot{u}_{zs}|^2 \right) A\, dz = \omega \tag{20}$$

with the stress boundary condition being identical to (8). Then

$$|\dot{u}_{zs}(\omega)| = \frac{(k_s^2 - k_t^2)}{2k_s} \left(\omega/\rho_s A f \right)^{1/2} \tag{21}$$

with

$$K_t = \omega \left(c_s^{-2} - c_t^{-2} \right)^{\frac{1}{2}} . \tag{22}$$

and f is a known function of k_s, c_ℓ and c_t .

The net thermal flux from the solid to the liquid may be calculated from equations (16), (18) and (21). This requires an integration over solid angles to account for all possible angles of incidence θ_0 of longitudinal and transverse waves

$$\begin{aligned}
\frac{W(T)}{A} &= \int \frac{W(\omega,T)}{A} \, n(T) \, d\tau_\omega \, d\Omega \\
&= \int \rho c_1 \left\{ \exp\left(\frac{\hbar\omega}{kT}\right) - 1 \right\}^{-1} d\omega \\
&\qquad \times \int |\dot{u}_{z\ell}|^2 \frac{\omega^2 V_s \, d\Omega}{2(2\pi c_\ell)^3} \\
&\quad + \int \left[|\dot{u}_{zt}|^2 \frac{\omega^2 V_s \, d\Omega}{2(2\pi c_t)^3} + |\dot{u}_{zs}|^2 \frac{2\pi\omega A}{(2\pi c_s)^2} \right] \\
&= \frac{4\pi^5 \rho c_1 (kT)^4}{15 \rho_s (h c_t)^3} \, F(c_\ell/c_t)
\end{aligned} \tag{23}$$

$F(c_\ell/c_t)$ is a known but rather complicated integral which is of order unity.

Note that (23) has brought forth an important fact - viz the energy radiated from one body to the other is proportional to the fourth power of T. When the temperature difference $(T_1 - T_2)$ is small, using equation (23) we can write

$$(\dot{Q}/A) = (W(T_1)/A) - (W(T_2)/A)$$

$$= \frac{16\pi^5 \rho c_1 k (kT)^3}{15 \rho_s (hc_t)^3} F(c_\ell/c_t)\ (T_1 - T_2) \qquad (24)$$

Note that on interchanging T_1 and T_2, $(\dot{Q}/A)$ remains the same. On using (1) and (24) we can write

$$R_K^{rad} = \frac{15 h^3 \rho_s c_t^3}{16 \pi^5 k^4 \rho c_1\ F(c_\ell/c_t)\ T^3} \qquad (25)$$

which is the Kapitza resistance due to radiation of phonons.

Thus to summarise:

(1) the energy radiated from one body to the other is proportional to the fourth power of the absolute temperature.

(2) $(\dot{Q}/A)$ does not change when the direction of energy flow is reversed. Thus in this model Kapitza resistance is quantitatively reversible.

(3) R_K^{rad} as given by equation (25) is insensitive to the properties of the liquid. Note that the only quantity in eqn. (25) that depends upon the liquid properties is ρc_1 and this quantity is not a strongly temperature dependent one.

(4) In the above radiation of rotons has been neglected. Because to excite a roton a minimum energy of 8.65°K is required At the range of temperatures in which we are interested phonons are not energetic enough to excite a significent number of rotons.

3. A Collective variable approach.

Surakawa and co-workers (1969) have put forth a collective variable approach to study the excitation spectrum and other properties of liquid He II. This approach has been employed by Sheard et al to formulate a microscopic theory of the Kapitza resistance at a solid-liquid ^{4}He interface

If $\rho(\vec{r})$ and $\vec{j}(\vec{r})$ represent the number density and momentum density respectively then

$$\rho(\vec{r}) = \psi^{\dagger}(\vec{r})\,\psi(\vec{r})$$

$$\vec{j}(\vec{r}) = -\frac{i\hbar}{2}\left[\psi^{\dagger}(\vec{r})\,\nabla\psi(\vec{r}) - (\nabla\psi^{\dagger}(\vec{r}))\,\psi(\vec{r})\right] \qquad (26)$$

$\psi(\vec{r})$ and $\psi^{\dagger}(\vec{r})$ being the Boson annihilation and creation operators. If Ω represents the volume, then these can be fourier analysed as

$$\rho(\vec{r}) = \frac{N}{\Omega} + \frac{\sqrt{N}}{\Omega}\sum_{k\neq 0}\rho_k\, e^{-ik\cdot r}$$

$$\vec{j}(\vec{r}) = \frac{\sqrt{N}}{\Omega}\sum_{k\neq 0} j_k\, e^{-ik\cdot r} \qquad (27)$$

The velocity operator $\vec{v}(\vec{r})$ may be defined through the relation

$$\vec{j}(\vec{r}) = m\,\rho(\vec{r})\,\vec{v}(\vec{r}) \quad \circ \qquad \vec{v}(\vec{r}) = \frac{1}{m\sqrt{N}}\sum_k \vec{v}_k$$

which will lead to the following integral equation for the fourier component v_k of the velocity field.

$$\vec{v}_k = \vec{J}_k - \sqrt{N} \sum_{p \neq k} \rho_{p-k} \vec{v}_p \tag{28}$$

This integral equation for $\vec{v}_k$ has been obtained under the assumption that $\rho^{-1}(\vec{r})$ can be expanded as a power series around its ground state expectation value (N/Ω):

$$\rho^{-1}(\vec{r}) = \left(\frac{N}{\Omega}\right)^{-1} \left\{ 1 - \left(\frac{N}{\Omega}\right)^{-1} \rho'(\vec{r}) + \left(\frac{N}{\Omega}\right)^{-2} (\rho'(\vec{r}))^2 - \cdots \right\} \tag{29}$$

where $\rho'(\vec{r}) = \frac{\sqrt{N}}{\Omega} \sum_{p \neq 0} \rho_{\vec{p}}\, e^{-i\vec{p}\cdot\vec{r}}$ being the fluctuation about the mean density. The usual second quantized form of the hamultonian for the liquid viz

$$\frac{1}{2m}\int d^3r\, \nabla\psi^{+}(\vec{r}) \nabla\psi(\vec{r}) + \frac{1}{2}\iint d^3r\, d^3r'\, \psi^{+}(r)\psi^{+}(r')\, V(|r-r'|)\, \psi(r)\psi(r')$$

can now be transformed as

$$H_{liq} = \int d^3r \left[\frac{m}{2} \rho(\vec{r})\, \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}) + \frac{1}{8m} \nabla\rho(\vec{r}) \cdot \rho^{-1}(\vec{r}) \nabla\rho(\vec{r}) \right]$$
$$+ \frac{1}{2}\int d^3r \int d^3r'\, \rho(\vec{r})\rho(\vec{r}')\, V(|r-r'|)$$
$$- \sum_k (k^2/4m) - \frac{1}{2} N\, V(r=0) \tag{30}$$

One can now substitute the infinite series expansion (29) for $\rho^{-1}(\vec{r})$. Restricting our attention to

(i) only the phonon excitations - neglecting higher order terms and

(ii) irrotational flow i.e. curl $\vec{v}(\vec{r})\,|0\rangle = 0$ and

making the Bogoliubov transformation to new set of Boson creation and annihilation operators as

$$\rho_k = -(B_{-k} - B_k^{\dagger})\,\lambda_k^{1/2}$$
$$\vec{v}_k = -\tfrac{1}{2} i\vec{k}\,(B_k + B_{-k}^{\dagger})\,\lambda_k^{-1/2} \qquad (31)$$

with

$$\lambda_k^{-2} = 1 + 4mN\,U(k)/k^2\Omega$$

where $U(k) = \int d^3r\, U(r)\, e^{-ik\cdot r}$ the hamiltonean can be diagonalised as

$$H^d_{liq} = E_0 + \Sigma \quad \omega_k B_k^{\dagger} B_k \qquad (32)$$

with $\omega_k = k^2/2m\lambda_k$

The solid-liquid interaction hamiltonian is obtained by the following argument: Let $U_a(\vec{R}_n - \vec{r})$ denote the interatomic potential between an atom of the solid at lattice site $\vec{R}_n = (X_n, Y_n, Z_n)$ and a liquid atom at $\vec{r} = (x, y, z)$. Let $\vec{u}_n$ denote the atomic displacement at site $\vec{R}_n$. Then the total interaction energy between the vibrating solid and liquid helium is

$$\int d^3r\, \psi^{\dagger}(\vec{r}) \sum_n U_a(\vec{R}_n + \vec{u}_n - \vec{r})\, \psi(\vec{r})$$

At low temperatures one can expand this to first order in $\vec{u}_n$ to obtain

$$\int d^3r\, \rho(\vec{r}) \left\{ U_0(\vec{r}) + \sum_n \vec{u}_n \cdot \nabla_{R_n} U_a(\vec{R}_n - \vec{r}) \right\}$$

(33)

where $U_0(r) = \sum_n U_a(R_n - r)$ is the total potential energy experienced by the helium atom owing to the interaction with the static solid. The interaction energy is rewritten by making the following assumptions.

(i) A continuum model of the solid is assumed. There U_0 depends only on the z coordinate. The surface of the solid is taken to be the $x-y$ plane.

(ii) The inter atomic potential is short ranged compared with the wavelength of the thermal phonons in the solid. Thus the displacement $\vec{u}_n$ is taken to be along the surface of the solid.

(iii) The displacement at the point $(X_n, Y_n, 0)$ is replaced by the displacement at $(x, y, 0)$.

(iv)

$$\nabla_{R_n} U_a(\vec{R}_n - \vec{r}) = -\nabla_{\vec{r}} U_a(\vec{R}_n - \vec{r})$$

Thus

$$\int d^3r\, \rho(\vec{r}) \left\{ U_0(\vec{r}) - u(x,y,0) \cdot \nabla_r \sum_n U_a(r - R_n) \right\}$$
$$= \int d^3r\, \rho(\vec{r})\, U_0(z) - \int d^3r\, u_z(x,y,0)\, \rho(r) \frac{\partial V_0}{\partial z} \qquad (34)$$

The second term facilitates the exchange of energy between theliquid and the solid and is the solid-liquid interaction hamiltonian H_{sl}.

$$H_{Total} = H_{liq} + H_{Solid} + H_{sl} \qquad (35)$$

$$H_{solid} = \sum \omega_q a_q^{\dagger} a_q$$
$$H_{liq} = H_{liq}^{d} + \int d^3r\, \rho(\vec{r})\, V_0(z)$$
$$H_{sl} = -\int d^3r\, u_z(x, y, 0)\, \rho(\vec{r})\, \frac{dV_0}{dz} \qquad (36)$$

$a_q^{\dagger}$, a_q are the phonon operators for the solid for the q^{th} mode. The term $-\rho(r)\frac{dV_0}{dz}$ is the external force density exerted on the liquid by the solid and it can be written in a convenient form by using the equation of motion for the momentum density

$$\dot{\vec{j}}_i + \sum_j \frac{\partial \Pi_{ij}}{\partial x_j} = F_i^{ext} \quad = \text{external force density}$$

(37)

Quantum mechanically

$$-i\left[j_z, H_{liq}\right] = -\rho(\vec{r})\frac{dV_0}{dz} - \sum_j \frac{\partial \Pi_{zj}}{\partial x_j} \qquad (38)$$

Integrating this equation from $z=-\varepsilon$ to $z=+\varepsilon$, ε being the order of the distance over which the average helium density decays from its bulk value to zero

$$-\int_{-\varepsilon}^{+\varepsilon} \rho(r)\frac{dV_0}{dz}\,dz = \int_{-\varepsilon}^{+\varepsilon} \left\{ \frac{\partial \Pi_{zz}}{\partial z} + \frac{\partial \Pi_{zx}}{\partial x} + \frac{\partial \Pi_{zy}}{\partial y} \right\} dz$$

(39)

The components of the stress tensor are finite and decay rapidly from bulk values to zero. The derivatives also behave similarly. Hence

$$-\int_{-\varepsilon}^{+\varepsilon} \rho(r)\, \frac{dV_0}{dz}\, dz = \pi_{zz}(x, y, 0) \quad \text{as } \varepsilon \to 0$$

so that

$$H_{sl} = \int u_z(x, y, 0)\, \pi_{zz}(x, y, 0)\, dx\, dy \tag{40}$$

the integration is over the solid-liquid interface.

The next step is the calculation of the stress tensor operator. There is a natural separation of the stress tensor into a part π_{ij}^{KE} which results from the Kinetic energy and another part π_{ij}^{PE} which results from the potential energy.

The diagonal component π_{zz}^{KE} can be written as (Khalatnikov, 1965)

$$\pi_{zz}^{KE} = \frac{1}{4m}\left\{ 4\, \frac{\partial \psi^{+}}{\partial z}\, \frac{\partial \psi}{\partial z} - \frac{\partial^2 \rho}{\partial z^2} \right\} \tag{41}$$

which can be expressed in terms of the collective variables as

$$\pi_{zz}^{KE} = m \rho\, v_z v_z - \sum_k k_z^2 / 2m\Omega + \frac{1}{2m}\left[\frac{\partial \rho}{\partial z}\, \rho^{-1}\, \frac{\partial \rho}{\partial z} - \frac{\partial^2 \rho}{\partial z^2} \right]. \tag{42}$$

On approximating ρ^{-1} by means of the mean value Ω/N, π_{zz}^{KE} can be expressed in terms of the Fourier components

$$\pi_{zz}^{KE} = \sum_{k,k'} \left\{ \frac{1}{m\Omega}(v_{-k})_z (v_{-k'})_z - \frac{k_z k_z'}{4m\Omega} \rho_{kk'} \right\} e^{-i(\vec{k}+\vec{k}')\cdot\vec{r}}$$
$$+ \frac{\sqrt{N}}{4m\Omega} \sum_k k_z^2 \rho_k e^{-i\vec{k}\cdot\vec{r}} - \sum_k \frac{k_z^2}{2m\Omega} \quad (43)$$

To derive the potential part of the stress tensor, first observe that

$$\sum_j \frac{\partial \pi_{ij}^{PE}}{\partial x_j} = \psi^\dagger(\vec{r}) \frac{\partial}{\partial x_i} \left\{ \int d\vec{r}' \, \psi^\dagger(\vec{r}') \psi(\vec{r}') V(r-r') \right\} \psi(\vec{r}) \quad (44)$$

The right side of this equation involves only the derivative with respect to x_i only. Consequently this part of the stress tensor is diagonal

$$\pi_{ij}^{P.E} = \pi_i^{PE} \, \delta_{ij}$$

We can rearrange the equation as

$$\frac{\partial \pi_z^{PE}(\vec{r})}{\partial z} = -\rho(\vec{r}) \, F_z(\vec{r}) \quad \text{where } F_z(\vec{r}) = -\frac{\partial}{\partial z} \int d\vec{r}' \rho(\vec{r}') V(r-r') \quad (45)$$

So that $F_z(r)$ can be interpretted as the average force on a particle at $\vec{r}$ due to interactions with other particles at points $\vec{r}'$. Let

$$\pi_z^{PE}(\vec{r}) = \sum_k \pi_{z\vec{k}}^{PE} \, e^{-i\vec{k}\cdot\vec{r}}$$
$$F_z(\vec{r}) = \sum_k F_{zk} \, e^{-i\vec{k}\cdot\vec{r}} \quad (46)$$

so that $F_{z\vec{k}} = \frac{\sqrt{N}}{\Omega}\, i\, k_z\, \rho_k\, V(k)$

$$i p_z \pi_{zp}^{PE} = \frac{\sqrt{N}}{\Omega} \sum_k \rho_{p-k} F_{zk} \quad (p \neq 0) \tag{47}$$

Thus

$$\pi_{zz}^{P.E}(\vec{r}) = \pi_z^{PE}(\vec{r})$$

$$= \frac{N}{\Omega^2} \sum_{\substack{k,p \\ (p\neq 0)}} \rho_{p-k}\, \rho_k\, V(k)\, \frac{k_z}{p_z}\, e^{-i\vec{p}\cdot\vec{r}} \tag{48}$$

One can now use the expansions (31) for ρ_k and v_k. Then stress tensor will have terms corresponding to single excitations and corresponding to two excitations. Or using this in (40) and expanding u_z in terms of phonon operators, one obtains an energy transfer process in which absorption of a phonon from the solid is accompanied by emission of one or two excitations into the helium and 'vice versa'.

Note that

$$\bar{u}(\vec{R}_n) = \sum_q \sqrt{\frac{1}{2\rho_s \Omega_s \omega_q}}\; \vec{\varepsilon}_q \left\{ a_{\vec{q}}\, e^{i\vec{q}\cdot\vec{R}_n} + a_q^{\dagger}\, e^{-i\vec{q}\cdot\vec{R}_n} \right\} \tag{49}$$

where $\vec{\varepsilon}_q = \vec{q}/|\vec{q}|$ is the unit polarization Vector.

Then stress tensor associated with emission or absorption of single excitations in the liquid is

$$\Pi^{(1)}_{zz} = \frac{\sqrt{N}}{\Omega} \sum_{k \neq 0} \left\{ \frac{k_z^2}{4m} + \frac{NU(k)}{\Omega} \right\} \rho_k e^{-i\vec{k}\cdot\vec{r}} \tag{50}$$

Use these in ( )

$$H^{(1)}_{sl} = \sum_{\vec{q},\vec{k}} T_{\vec{q},\vec{k}} (a_q^{\dagger} - a_{-q})(B_k - B_{-k}^{\dagger}) \tag{51}$$

where the transfer matrix element is

$$T_{q,k} = i A \delta_{q_{\parallel}, k_{\parallel}} (\epsilon_{\vec{q}})_z \sqrt{\frac{1}{2\rho_s \Omega_s \omega_q}} \frac{(N\lambda_k)^{\frac{1}{2}}}{\Omega} \left(\frac{k_z^2}{4m} + \frac{NU(k)}{\Omega} \right) \tag{52}$$

The Kroniker delta yields momentum conservation parallel to the surface and arises due to the integral over the interface area A

In the long wave length limit (phonon transmissions)

$$T_{q,k} = i A \delta_{q_{\parallel}, k_{\parallel}} (\epsilon_{\vec{q}})_z \left\{ \frac{\rho_L v_L^3 k}{4\Omega \Omega_s \rho_s v_s q} \right\}^{1/2} \tag{53}$$

v_s being the velocity of sound in the solid.

$\rho_L = \frac{Nm}{\Omega}$ = Mass density of the liquid. Note that this depends on the acoustic impedence $\rho_L v_L / \rho_s v_s$ of the two media.

Also in the long wave length limit

$$\pi^{(1)}_{zz} = -\rho_L v_L^2 \, \Delta(r)$$

$$\Delta(r) = -\rho'(r) \Big/ \left(\frac{N}{\Omega}\right) \tag{54}$$

$\Delta(r)$ is the fractional decrease in the density owing to the fluctuations which are just the local latation. Then heat current $J^{(1)}_{SL}$ is given by

$$J^{(1)}_{SL} = \Delta T \sum_{q,k} 2\pi \, |T_{qk}|^2 \delta(\omega_q - \omega_k) \left(\frac{\partial n_q^0}{\partial T}\right) \tag{55}$$

n_q^0 being the Bose-Einstein distribution function at temperature T.

Kapitza resistance is given by

$$R_K^{-1} = \frac{J_{SL}^{PA}}{A \, \Delta T} = k_B \frac{\pi^2}{45} \left(\frac{\rho_L v_L}{\rho_S v_S^3}\right) (k_B T)^3 \tag{56}$$

The results here are essentially the same as the one obtained from classical acoustic mismatch treatment. Thus there is the usual discrepancy between the experiment and the theory by a factor of ~ 4. One can think of improving the situation by including roton transfer processes. This also does not help in reducing the numerical discrepancy. This is essentially due to the freezing out of the roton population at low temperatures. Inclusion of higher order processes also does not improve the situation. In conclusion this seems to be a very interesting theoretical investigation.

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