Microscopic Theory of the Kapitza Resistance at a Solid-Liquid ⁴He Interface

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We present the first completely quantum-mechanical calculation of the Kapitza resistance for the solid-liquid ⁴He interface. By using a realistic model of ⁴He, processes involving phonons and rotons in the liquid helium are treated in a unified manner. The coupling of the phonons in the solid to the excitations in the helium is derived in the form of a transfer Hamiltonian. In the long-wavelength limit the classical acoustic-mismatch theory is reproduced by transmission processes involving single phonons, but the coupling Hamiltonian also includes roton emission and higher-order processes involving two or more excitations in the helium. As in the theory of electron tunneling, the transfer-Hamiltonian formalism can serve as a basis for further studies taking account of many-body interactions in the solid or liquid, scattering by defects or surface structure, and the influence of attractive van der Waals forces at the interface.

I. MOTIVATION

The origin of the thermal contact resistance R_{κ} between a solid and liquid helium is thought to lie in the partial transmission of phonons across the interface between them. In the original Khalatnikov theory¹ the acoustic impedance which the liquid presents to the thermal vibrations of the solid surface, is calculated by treating the helium as a classical elastic fluid. An alternative and equivalent treatment by Little² uses the acoustic transmission coefficient which is again obtained from classical elasticity theory. However there are large discrepancies between experiment and theory and the observed resistances may often be one or two orders of magnitude smaller than these theoretical predictions. Discussion of experimental results with extensive bibliographies have been given in recent reviews by Pollack,³ Snyder,⁴ and Cheeke.⁵

Various modifications of the acoustic-mismatch theory have been proposed in attempts to account for the observed energy transfer. Challis, Dransfeld, and Wilks⁶ have considered the enhancement of the acoustic impedance due to a dense layer of helium near the interface. Adamenko and Fuks⁷ estimated the effect of surface roughness using a perturbation approach to the elastic wave equation. The effect of attenuation of the sound waves in the solid has also been shown to increase the transmission of acoustic energy but the description of the attenuation mechanism was purely classical. Khalatnikov and Adamenko⁸ described the damping by means of a viscosity tensor and the Rayleigh dissipation function, while Peterson and Anderson⁹ and Haug and Weiss¹⁰ employed complex wave vectors for the waves in the solid. The latter approach has recently been questioned

by Vuorio.¹¹ But all of these calculations have been based on classical acoustic theory and there is thus need for a microscopic description since ⁴He is a quantum liquid rather than a classical elastic fluid.

Microscopic quantum-mechanical calculations of the Kapitza resistance have so far been restricted to simplified models in which the liquid helium is viewed as a gas of independent atoms. The energy transfer then arises from inelastic collisions of the helium atoms with the vibrating solid surface. In this way the effect of the attractive van der Waals potential between helium atoms and the solid may be taken into account by computing the scattering matrix element from the atomic eigenfunctions of the van der Waals potential. For ⁴He Toombs and Challis¹² obtained an enhanced conductance and, in the low-temperature limit, their result was similar to that of Khalatnikov,¹ except that it contained the mean thermal atomic velocity rather than the sound velocity in liquid helium, which is nearly temperature independent. However they were forced to use Boltzmann statistics for the ⁴He atoms since Bose-Einstein statistics lead to unreasonably large occupancies at low temperatures. For ³He a Fermi-gas model has been used¹³⁻¹⁵ and the contribution of bound states of the van der Waals potential has also been considered.¹⁶

But in neglecting the interactions between helium atoms the independent-particle model ignores the existence of collective phonon-like excitations in the liquid helium, and as such can only have qualitative significance. Although in ³He there are quasiparticle excitations as well as collective zero-sound phonons, with corresponding contributions to the heat transfer,¹⁷ this is not the case in ⁴He where there are no stable single-particle

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excitations but only collective excitations (phonons and rotons). For a Bose liquid it is thus always necessary to include interparticle interactions in order to calculate a meaningful boundary resistance. A microscopic description, besides being of intrinsic interest, is thus necessary if earlier calculations of the effect of the attractive van der Waals potential are to be extended to a realistic model of liquid helium. Here we present a microscopic treatment of phonon transmission in which the coupling of the phonons in the solid to the complete excitation spectrum of liquid ⁴He is calculated in a unified manner.

In the formalism we shall develop, the coupling between the solid and the liquid ⁴He is derived in the form of a transfer Hamiltonian as in the theory of electron tunneling through a metal-insulatormetal junction. Just as the tunneling-Hamiltonian formalism has been successful in describing many-body effects¹⁸ due to electron interactions in the metal electrodes or interactions with impurities in the insulating barrier, the virtues of our formalism lie also in the possible generalizations. Thus, scattering processes which give rise to phonon damping in the solid may be incorporated into the theory of phonon transmission by including the appropriate scattering terms in the Hamiltonian for the solid-liquid system. A transfer-Hamiltonian analog of the acoustic-mismatch theory has been already proposed by Sheard and Toombs¹⁹ and applied to a simple model for scattering by surface defects in the solid.²⁰ However the solid-liquid interaction Hamiltonian was obtained by a heuristic argument. In the present paper the acoustic-mismatch results may also be reproduced, but the interaction Hamiltonian is derived rigorously from the interatomic potential between a helium atom and the solid. This paves the way for calculations of the influence of an attractive van der Waals force on the transfer matrix elements. A preliminary account of part of this work has already been published as a conference report.²¹

II. COLLECTIVE-VARIABLE THEORY OF LIQUID ⁴He

Our aim is to separate the total Hamiltonian of the composite solid-liquid system into unperturbed parts which describe the solid and the liquid ⁴He and a perturbation which represents the coupling between them. The central problem is to calculate the coupling Hamiltonian in terms of the phonon operators for the solid and operators describing the excitations in the liquid helium. For this purpose we must employ a realistic model of liquid ⁴He.

The original Bogoliubov theory²² depends on the assumption that a large fraction of the helium atoms are condensed into the zero-momentum state which does not appear to be justified²³ for liquid ⁴He and cannot adequately explain the observed excitation spectrum. These difficulties have been avoided in more recent theories²⁴⁻²⁶ in which the Bose liquid is described by collective hydrodynamic variables. As we shall see, these are particularly suited to our approach to the Kapitza-resistance problem and provide useful physical insight into the mechanism of the solidliquid coupling. We shall use the formalism given by Sunakawa, Yamasaki, and Kebukawa, which is lucidly presented²⁴ and has been developed through a series of papers. Here we briefly summarize the relevant points of the formalism which we shall need for future use.

The appropriate collective variables are the number density operator

$$\rho(\mathbf{\bar{r}}) = \psi^{\dagger}(\mathbf{\bar{r}})\psi(\mathbf{\bar{r}})$$

and the momentum density operator

$$\mathbf{\ddot{g}} = -\frac{1}{2}i\hbar \left[\psi^{\dagger}(\mathbf{\ddot{r}})\nabla\psi(\mathbf{\ddot{r}}) - \left\{\nabla\psi^{\dagger}(\mathbf{\ddot{r}})\right\}\psi(\mathbf{\ddot{r}})\right],$$

where $\psi(\mathbf{\dot{r}})$ and $\psi^{\dagger}(\mathbf{\dot{r}})$ are the usual boson field operators. Their Fourier components $\rho_{\mathbf{k}}$, $\mathbf{\dot{g}}_{\mathbf{k}}$ are defined by

$$\rho(\mathbf{\tilde{r}}) = \frac{N^{1/2}}{\Omega} \sum_{\mathbf{\tilde{k}}} \rho_{\mathbf{\tilde{k}}} e^{-i\mathbf{\tilde{k}}\cdot\mathbf{\tilde{r}}} = \frac{N}{\Omega} + \frac{N^{1/2}}{\Omega} \sum_{\mathbf{\tilde{k}}\neq 0} \rho_{\mathbf{\tilde{k}}} e^{-i\mathbf{\tilde{k}}\cdot\mathbf{\tilde{r}}},$$

$$\mathbf{\tilde{g}}(\mathbf{\tilde{r}}) = \frac{N^{1/2}}{\Omega} \sum_{\mathbf{\tilde{r}}} \mathbf{\tilde{g}}_{\mathbf{\tilde{k}}} e^{i\mathbf{\tilde{k}}\cdot\mathbf{\tilde{r}}},$$
(1)

where Ω is the volume of the helium system. We consider only states containing N particles so that in Eq. (1) ρ_0 , which commutes with the Hamiltonian, has been taken to be \sqrt{N} . An essential feature of the formalism is the introduction of a velocity operator $\overline{\mathbf{v}}(\mathbf{\hat{r}})$ by means of the implicit relation

$$\mathbf{\tilde{g}}(\mathbf{\tilde{r}}) = m\rho(\mathbf{\tilde{r}})\mathbf{\tilde{v}}(\mathbf{\tilde{r}}),$$

where *m* is the mass of a helium atom. If we Fourier expand $\vec{\nabla}(\vec{r})$ according to

$$\vec{\mathbf{v}}(\vec{\mathbf{r}}) = \frac{1}{mN^{1/2}} \sum_{\vec{k}} \vec{\mathbf{v}}_{\vec{k}} e^{i\vec{k}\cdot\vec{\mathbf{r}}},$$

then $\bar{v}_{\vec{k}}$ may be alternatively defined as the solution of the integral equation

$$\mathbf{\bar{v}}_{\mathbf{\bar{k}}} = \mathbf{\bar{g}}_{\mathbf{\bar{k}}} - N^{1/2} \sum_{\mathbf{\bar{p}} \neq \mathbf{\bar{k}}} \rho_{\mathbf{\bar{p}}-\mathbf{\bar{k}}} \mathbf{\bar{v}}_{\mathbf{\bar{p}}},$$

which may be obtained by iteration. This amounts to defining the inverse density operator by the series

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$$\rho^{-1}(\mathbf{\tilde{r}}) = \left(\frac{N}{\Omega}\right)^{-1} - \left(\frac{N}{\Omega}\right)^{-2} \rho'(\mathbf{\tilde{r}}) + \left(\frac{N}{\Omega}\right)^{-3} \rho'(\mathbf{\tilde{r}}) \rho'(\mathbf{\tilde{r}}) - \cdots,$$
(2)

where

$$\rho'(\mathbf{\bar{r}}) = \frac{N^{1/2}}{\Omega} \sum_{\mathbf{\bar{k}}\neq 0} \rho_{\mathbf{\bar{k}}} e^{-i\mathbf{\bar{k}}\cdot\mathbf{\bar{r}}}$$

represents only the fluctuations from the mean density N/Ω .

In terms of field operators the Hamiltonian for the liquid helium is

$$\begin{split} \Im C'_{L} &= \frac{\hbar^{2}}{2m} \int d\,\vec{\mathbf{r}}\,\nabla\psi^{\dagger}(\vec{\mathbf{r}})\cdot\nabla\psi(\vec{\mathbf{r}}) \\ &+ \frac{1}{2} \int d\,\vec{\mathbf{r}}\,d\,\vec{\mathbf{r}}\,'\,\psi^{\dagger}(\vec{\mathbf{r}})\psi^{\dagger}(\vec{\mathbf{r}}')\,V(\vec{\mathbf{r}}-\vec{\mathbf{r}}\,')\psi(\vec{\mathbf{r}}\,')\psi(\vec{\mathbf{r}}\,), \end{split}$$

where $V(\mathbf{\dot{r}} - \mathbf{\dot{r}}')$ is the potential energy between helium atoms. By showing that for any Bose system the operator

$$P = \psi(\mathbf{\tilde{r}})\rho^{-1}(\mathbf{\tilde{r}})\psi^{\dagger}(\mathbf{\tilde{r}})$$
(4)

must take the value unity, Sunakawa *et al.* express this Hamiltonian in the hydrodynamic form

$$\begin{aligned} \mathfrak{K}_{L}^{\prime} &= \int d\,\mathbf{\bar{r}} \left(\frac{1}{2}\,m\,\rho(\mathbf{\bar{r}})\mathbf{\bar{\nabla}}(\mathbf{\bar{r}})\cdot\mathbf{\bar{\nabla}}(\mathbf{\bar{r}}) + \frac{\hbar^{2}}{8m}\,\nabla\rho(\mathbf{\bar{r}})\cdot\rho^{-1}(\mathbf{\bar{r}})\nabla\rho(\mathbf{\bar{r}})\right) \\ &+ \frac{1}{2}\,\int d\,\mathbf{\bar{r}}\,d\,\mathbf{\bar{r}}^{\prime}\,\rho(\mathbf{\bar{r}})\rho(\mathbf{\bar{r}}^{\prime})V(\mathbf{\bar{r}}-\mathbf{\bar{r}}^{\prime}) \\ &- \sum_{\mathbf{\bar{r}}}\,\frac{\hbar^{2}k^{2}}{4m} - \frac{1}{2}\,NV(\mathbf{\bar{r}}=0). \end{aligned} \tag{5}$$

Using the expressions (1) and (2) for ρ and ρ^{-1} , \Im_L^{\prime} reduces to a bilinear form in the fluctuation operators with higher-order terms which give rise to interactions between the excitations. These terms renormalize the excitation energies and are important for an accurate description of the energy spectrum, particularly in the higher roton region. Since we shall mainly be interested in the phonon excitations we shall not include them here.

Provided the Hilbert space is restricted to states satisfying

 $\operatorname{curl} \overline{\mathbf{v}}(\mathbf{\bar{r}}) |\rangle = 0$

then ρ , \vec{v} have simple commutation relations which, in Fourier space, are

$$[\rho_{\vec{k}},\rho_{\vec{k}'}] = 0, [v_{\vec{k}}i,v_{\vec{k}'}] = 0, [\bar{v}_{\vec{k}},\rho_{\vec{k}'}] = \hbar \bar{k} \delta_{\vec{k}\vec{k}'},$$

where i, j denote Cartesian components. Boson excitation operators $B_k^{\ddagger}, B_k^{\ddagger}$ may thus be defined by²⁷

$$\rho_{\vec{k}} = -i\lambda_{k}^{1/2}(B_{-\vec{k}} - B_{\vec{k}}^{\dagger}), \quad \vec{\nabla}_{\vec{k}} = -i\frac{1}{2}\hbar\vec{k}\lambda_{k}^{-1/2}(B_{\vec{k}} + B_{-\vec{k}}^{\dagger}),$$
(6)

where

$$1/\lambda_k^2 = 1 + 4NmV(\vec{k})/\hbar^2 k^2 \Omega \tag{7}$$

and the Fourier transform of the interatomic potential is given by

$$V(\mathbf{\bar{k}}) = \int d\mathbf{\bar{r}} V(\mathbf{\bar{r}}) e^{-i\mathbf{\bar{k}}\cdot\mathbf{\bar{r}}}.$$

The Hamiltonian then becomes

$$\mathcal{H}'_{L} = E_{0} + \sum_{\vec{k}} \hbar \omega_{k} B_{k}^{\ddagger} B_{\vec{k}}^{\dagger} + \mathcal{H}_{I}$$

where E_0 is the ground-state energy and \Re_I corresponds to the anharmonic interactions between the excitations, whose energy spectrum is given by

$$\hbar\omega_{k} = \hbar^{2}k^{2}/2m\lambda_{k}. \tag{8}$$

For small wave vectors the excitations are phonons and

$$\omega_{k} = v_{L}k, \quad v_{L}^{2} = NV(0)/m\Omega, \quad \lambda_{k} = \hbar k/2mv_{L}, \quad (9)$$

where v_L is the velocity of sound in the helium.

III. SOLID-LIQUID INTERACTION HAMILTONIAN

In classical elasticity theory the transmission and reflection of sound waves at the interface between two media is determined by means of boundary conditions which require the equality of displacements and stresses on either side of the interface. But this procedure has no direct analog in a quantum-mechanical treatment since the dynamical variables for the solid and liquid helium are operators and equating them is a meaningless exercise. In quantum mechanics the only means of coupling two systems is through the mutual forces between them. We must therefore begin from the interatomic potential $V_a(\dot{\mathbf{R}}_n - \dot{\mathbf{r}})$, between an atom of the solid at lattice site $\ddot{\mathbf{R}}_n$ = (X_n, Y_n, Z_n) and a helium atom at $\dot{\mathbf{r}} = (x, y, z)$.

If the atomic displacement at site \vec{R}_n is \vec{u}_n then the total interaction energy between the vibrating solid and the liquid helium is

$$\int d\mathbf{\bar{r}} \psi^{\dagger}(\mathbf{\bar{r}}) \sum_{n} V_{a}(\mathbf{\bar{R}}_{n} + \mathbf{\bar{u}}_{n} - \mathbf{\bar{r}}) \psi(\mathbf{\bar{r}}).$$

At low temperatures it is sufficient to expand this to first order in the lattice displacements giving

$$\int d\mathbf{\bar{r}} \rho(\mathbf{\bar{r}}) \left(V_0(\mathbf{\bar{r}}) + \sum_n \mathbf{\bar{u}}_n \cdot \nabla_{\mathbf{\bar{R}}_n} V_a(\mathbf{\bar{R}}_n - \mathbf{\bar{r}}) \right)$$

where

$$V_0(\mathbf{\vec{r}}) = \sum_n V_a(\mathbf{\vec{R}}_n - \mathbf{\vec{r}})$$

is the total potential experienced by a helium atom

owing to interaction with the static solid. If a continuum model is assumed for the solid then V_0 only depends on the coordinate z which is perpendicular to the solid surface. Since the interatomic potential V_a is short ranged compared with the wavelength of the thermal phonons in the solid, we may take \bar{u}_n to be the displacement at the surface of the solid $z = Z_n = 0$. By the same argument we may replace the displacement at the point $(X_n, Y_n, 0)$ by that at the point (x, y, 0) since these points lie within the potential range; further,

$$\nabla_{\mathbf{\bar{R}}_n} V_a(\mathbf{\bar{R}}_n - \mathbf{\bar{r}}) = - \nabla_{\mathbf{r}} V_a(\mathbf{\bar{R}}_n - \mathbf{\bar{r}}),$$

so that the interaction energy becomes

$$\int d\mathbf{\bar{r}} \rho(\mathbf{\bar{r}}) \Big(V_0(\mathbf{\bar{r}}) - \mathbf{\bar{u}}(x, y, 0) \cdot \nabla_{\mathbf{\bar{r}}} \sum_n V_a(\mathbf{\bar{R}}_n - \mathbf{\bar{r}}) \Big)$$
$$= \int d\mathbf{\bar{r}} \rho(\mathbf{\bar{r}}) [V_0(\mathbf{\bar{r}}) - \mathbf{\bar{u}}(x, y, 0) \cdot \nabla_{\mathbf{\bar{r}}} V_0(\mathbf{\bar{r}})]$$
$$= \int d\mathbf{\bar{r}} \rho(\mathbf{\bar{r}}) V_0(z) - \int d\mathbf{\bar{r}} u_z(x, y, 0) \rho(\mathbf{\bar{r}}) \frac{dV_0}{dz} \cdot \mathbf{V}_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r}}) \nabla_{\mathbf{\bar{r}}} V_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r}}) \nabla_{\mathbf{\bar{r}}} V_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r}}) \nabla_{\mathbf{\bar{r}}} V_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r}}) \nabla_{\mathbf{\bar{r}}} V_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r})} - \mathbf{V}_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r}) - \mathbf{V}_0(\mathbf{\bar{r}}) - \mathbf{V}_0(\mathbf{\bar{r})} - \mathbf$$

The first term is the static interaction and should naturally be included in the unperturbed Hamiltonian \mathcal{H}_L for the liquid helium since it is the mechanism by which the helium atoms are prevented from penetrating the volume occupied by the solid. The latter term involving the dynamical coordinates of the solid is the means by which energy may be exchanged and is just the required solid-liquid interaction Hamiltonian \mathcal{H}_{SL} .

Thus the total Hamiltonian of the composite solid-liquid system is naturally separable into the form

$$\mathcal{H} = \mathcal{H}_{S} + \mathcal{H}_{L} + \mathcal{H}_{SL},$$
where
$$\mathcal{H}_{S} = \sum_{\bar{q}} \hbar \omega_{\bar{q}} a_{\bar{q}}^{\dagger} a_{\bar{q}}^{\dagger},$$
(10)

$$\mathscr{H}_{L} = \mathscr{H}_{L}' + \int d\mathbf{\bar{r}} \rho(\mathbf{\bar{r}}) V_{0}(z), \qquad (11)$$

$$\mathcal{H}_{\rm SL} = -\int d\,\vec{\mathbf{r}}\,u_z(x,\,y,\,0)\rho(\vec{\mathbf{r}})\,\frac{dV_0}{dz}\,,\qquad(12)$$

and \mathscr{K}'_L is given in Eq. (3) or (5). The unperturbed Hamiltonian \mathscr{K}_S for the solid contains the phonon annihilation and creation operators $a_{\overline{q}}^*, a_{\overline{q}}^+$ for the modes with wave vector \overline{q} and frequency ω_q , in terms of which u_g may be readily expressed.

The solid-liquid coupling (12) is essentially the form used by Toombs and Challis,¹² who took a Morse potential for $V_0(z)$ and computed the inelastic scattering of helium atoms using the single-particle eigenfunctions which are known for this particular model potential. Since our principal aim is to establish a quantum-mechanical formal-

ism for dealing with a Bose liquid rather than a gas of independent atoms, we shall consider a simplified model in which $V_0(z)$ is a repulsive potential step at the solid-liquid interface z = 0:

$$V_0(z) = V_0 \quad (z < 0)$$

= 0 (z > 0),

where $V_0 > 0$. The height of the step is not critical provided it is sufficiently great that the heliumatom wave functions do not penetrate significantly into the region z < 0 occupied by the solid. The presence of the potential step, which confines the helium to the half-space z > 0, implies the existence of phase coherence between incident and elastically reflected excitations. In the theory of tunneling such coherences are usually neglected²⁸ and in the same spirit we shall treat the helium excitations using a plane- (running-) wave representation even in the presence of the confining potential. We have already implied in Eq. (10) a similar treatment for the phonons in the solid but we shall return to this point later.

The interaction Hamiltonian (12) is in a rather inconvenient form since it involves the variation of $\rho(\mathbf{\dot{r}})$ in the region where the potential $V_0(z)$ is rapidly varying. Moreover for our simplified model of the potential we expect the interaction to be independent of the precise magnitude of the potential step. We now convert (12) to a more convenient form which demonstrates this property explicitly.

We first recognize that $-\rho(\mathbf{\tilde{r}})(dV_0/dz)$ is just the external force density exerted on the liquid helium by the solid. In classical hydrodynamics²⁹ the external force density $\mathbf{\tilde{F}}^{\text{ext}}$ enters the equation of motion for the momentum density $\mathbf{\tilde{g}}$ in the form

$$\dot{g}_i + \sum_j \frac{\partial \prod_{ij}}{\partial x_j} = F_i^{\text{ext}},$$

where Π_{ij} is the fluid stress tensor and i, j denote Cartesian components. For liquid helium we may derive a quantum-mechanical analog of this equation in the form

$$(i\hbar)^{-1}[g_{z},\mathcal{H}_{L}] = -\rho(\mathbf{\bar{r}}) \frac{dV_{0}}{dz} - \sum_{j} \frac{\partial \Pi_{zj}}{\partial x_{j}}, \qquad (13)$$

where the left-hand side is just g_z if the Heisenberg representation is chosen for the operators. Here, the static interaction potential $V_0(z)$ contained in \mathcal{K}_L has given rise to the external force term, and the kinetic energy and interparticle interactions of Eq. (3) contribute to the stress tensor term. Now integrate this equation from $z = -\epsilon$ to $z = +\epsilon$, where ϵ is of the order of the distance over which the average helium density decays from its bulk value to zero inside the potential step. We shall in fact consider the limit of an abrupt change of density when $\epsilon \rightarrow 0$. Since g_z remains finite the integral over the left-hand side of Eq. (13) gives zero by virtue of the infinitesimal range of integration. Thus

$$-\int_{-\epsilon}^{+\epsilon} \rho(\mathbf{\tilde{r}}) \frac{dV_0}{dz} dz = \int_{-\epsilon}^{+\epsilon} \left(\frac{\partial \prod_{zz}}{\partial z} + \frac{\partial \prod_{zx}}{\partial x} + \frac{\partial \prod_{zy}}{\partial y} \right) dz$$

The components π_{ij} of the stress tensor are also finite but decay rapidly from bulk values for $z > \epsilon$ to zero for $z < -\epsilon$. The derivates with respect to x or y behave similarly so we have³⁰

$$-\int_{-\epsilon}^{+\epsilon} \rho(\mathbf{\tilde{r}}) \frac{dV_0}{dz} dz = \left[\prod_{zz} (\mathbf{\tilde{r}}) \right]_{z=\epsilon} - \left[\prod_{zz} (\mathbf{\tilde{r}}) \right]_{z=-\epsilon}$$
$$= \prod_{zz} (x, y, 0),$$

where we have taken the limit $\epsilon \rightarrow 0$. Since in Eq. (12) we may similarly restrict the range of integration as $dV_0/dz = 0$ for $|z| > \epsilon$, we have

$$\mathcal{H}_{\mathrm{SL}} = \int u_{\mathbf{z}}(x, y, 0) \prod_{\mathbf{z}, \mathbf{z}}(x, y, 0) \, dx \, dy, \tag{14}$$

and the integration is now over the solid-liquid interface. Since Π_{zz} is the fluid pressure, \mathcal{K}_{SL} has the simple interpretation of the work done when the solid surface is displaced a distance u_z normal to the surface. This is exactly the form of interaction postulated by Sheard and Toombs, ¹⁹ who treated the helium simply as an elastic fluid and obtained a transfer Hamiltonian which gave results equivalent to the classical acoustic-mismatch theory. Our rigorous derivation here is preferable since it indicates the limitations of this expression for the interaction Hamiltonian. A more realistic model for the van der Waals potential $V_0(z)$ would contain, in addition to the strong repulsion which corresponds to our potential step, an attractive part which results in an increased helium density close to the solid surface. To deal with this situation we require a generalization of the theory of liquid helium to nonuniform states such as that recently given by Bowley.³¹ This problem is currently under study.

IV. DERIVATION OF STRESS TENSOR OPERATOR

The stress tensor operator is defined by Eq. (13). We obtain the equation of motion for g_z using the form of Hamiltonian given in Eqs. (11) and (3) and the usual Bose commutation relations obeyed by the field operators. There is hence a natural separation of the stress tensor into a part Π_{ij}^{KE} , which derives from the kinetic energy term in \mathcal{K}_L^{\prime} , and a part Π_{ij}^{FE} , which derives from the kinetic stress from the potential energy of the mutual interactions of the helium atoms.

We readily obtain the kinetic-energy part

$$\prod_{ij}^{KE} = \frac{\bar{\hbar}^2}{4m} \left(\frac{\partial \psi^{\dagger}}{\partial x_i} \frac{\partial \psi}{\partial x_j} + \frac{\partial \psi^{\dagger}}{\partial x_j} \frac{\partial \psi}{\partial x_i} - \frac{\partial^2 \psi^{\dagger}}{\partial x_j \partial x_i} \psi - \psi^{\dagger} \frac{\partial^2 \psi}{\partial x_j \partial x_i} \right)$$

the form of which is well known in the phenomenological theory of superfluidity³² when ψ is the superfluid wave function rather than a field operator. The diagonal component required in Eq. (14) may be written

$$\Pi _{xz}^{KE} = \frac{\hbar^2}{4m} \left(4 \frac{\partial \psi^{\dagger}}{\partial z} \frac{\partial \psi}{\partial z} - \frac{\partial^2 \rho}{\partial z^2} \right).$$
(15)

To express this in terms of collective variables ρ and $\vec{\mathbf{v}}$, we use the procedure of Sunakawa *et al.* in writing

$$\frac{\partial \psi^{\dagger}}{\partial z} \frac{\partial \psi}{\partial z} = \frac{\partial \psi^{\dagger}}{\partial z} \psi \rho^{-1} \psi^{\dagger} \frac{\partial \psi}{\partial z}$$

upon introduction of the unit operator P of Eq. (4). Using

$$\frac{\partial \psi^{\dagger}}{\partial z} \psi = (i\hbar)^{-1} \left(m\rho v_{z} + \frac{1}{2} i\hbar \frac{\partial \rho}{\partial z} \right)$$

with a similar expression for $\psi^{\dagger}(\partial \psi/\partial z)$, and the commutation relations for ρ and $\bar{\mathbf{v}}$, gives finally

$$\prod_{zz}^{KE} = m\rho v_z v_z + \frac{\hbar^2}{2m} \left(\frac{\partial \rho}{\partial z} \rho^{-1} \frac{\partial \rho}{\partial z} - \frac{\partial^2 \rho}{\partial z^2} \right) - \sum_{\vec{k}} \frac{\hbar^2 k_z^2}{2m \Omega}$$
(16)

The first term is familiar from classical hydrodynamics²⁹ and is just the pressure arising from the momentum flux $g_z v_z$, whilst the bracketed expression consists of quantum pressure terms peculiar to a quantum fluid and are analogous to a similar term in \mathcal{K}'_L of Eq. (5). The constant term, although infinite, gives a finite result when combined with the zero-point energy of the excitations. Again it is analogous to the corresponding term in Eq. (5). For later use we require Eq. (16) in terms of Fourier components, which is

$$\Pi_{zz}^{\text{KE}} = \sum_{\vec{k}\vec{k}\,'} \left(\frac{1}{m\Omega} v_{-\vec{k}z} v_{-\vec{k}\,'z} - \frac{\hbar^2 k_z k'_z}{4m\Omega} \rho_{\vec{k}} \rho_{\vec{k}\,'} \right) e^{-i(\vec{k}+\vec{k}\,')\cdot\vec{r}} + \frac{\hbar^2 N^{1/2}}{4m\Omega} \sum_{\vec{k}} k_z^2 \rho_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} - \sum_{\vec{k}} \frac{\hbar^2 k_z^2}{2m\Omega} \cdot$$
(17)

Here we have approximated ρ by the mean density N/Ω (and ρ^{-1} by Ω/N) in order to retain only linear and bilinear terms in the fluctuation operators. In Eq. (17) we must of course exclude those terms with $\vec{k} = 0$ or $\vec{k}' = 0$.

For the potential energy part of the stress tensor we start from the relation

$$\sum_{j} \frac{\partial \prod_{ij}^{\text{PE}}}{\partial x_{j}} = \psi^{\dagger}(\mathbf{\bar{r}}) \ \frac{\partial}{\partial x_{i}} \left(\int d\mathbf{\bar{r}}' \ \psi^{\dagger}(\mathbf{\bar{r}}') \psi(\mathbf{\bar{r}}') V(\mathbf{\bar{r}} - \mathbf{\bar{r}}') \right) \psi(\mathbf{\bar{r}}),$$

which follows directly from the equation of motion. Since we only have the derivative with respect to x_i on the right-hand side it follows that this part of the stress tensor is diagonal, $\prod_{ij}^{\text{PE}} = \prod_i^{\text{PE}} \delta_{ij}$. For physical and mathematical convenience we rearrange this equation in the form

$$\frac{\partial \Pi_{z}^{PE}(\mathbf{\dot{r}})}{\partial z} = -\rho(\mathbf{\dot{r}})F_{z}(\mathbf{\dot{r}}), \qquad (18)$$

where

$$F_{z}(\mathbf{\tilde{r}}) = -\frac{\partial}{\partial z} \left(\int d\mathbf{\tilde{r}}' \rho(\mathbf{\tilde{r}}') V(\mathbf{\tilde{r}} - \mathbf{\tilde{r}}') \right), \tag{19}$$

which can be interpreted as the average force on a particle at \vec{r} due to interaction with other particles at points \vec{r}' . To solve this equation for Π_s^{PE} we must Fourier transform each side. Defining

$$\prod_{z} PE(\mathbf{\bar{r}}) = \sum_{\mathbf{\bar{k}}} \prod_{z \in \mathbf{\bar{k}}} PE e^{-i\mathbf{\bar{k}}\cdot\mathbf{r}}$$

and a similar expression for $F_{z}(\mathbf{\tilde{r}})$ we get

$$ip_{\mathbf{z}}\prod_{\mathbf{z}} \frac{PE}{\mathbf{p}} = \frac{N^{1/2}}{\Omega} \sum_{\mathbf{\bar{k}}} \rho_{\mathbf{\bar{p}}-\mathbf{\bar{k}}} F_{\mathbf{z}\mathbf{\bar{k}}} \quad (\mathbf{\bar{p}}\neq 0).$$

The right-hand side is in the form of a convolution since the right-hand side of Eq. (18) is a product. Similarly from Eq. (19) we obtain

$$F_{z\bar{k}} = \frac{N^{1/2}}{\Omega} i k_z \rho_{\bar{k}} V(\bar{k}).$$

Combining these gives finally

$$\prod_{zz} PE(\vec{\mathbf{r}}) = \prod_{z} PE(\vec{\mathbf{r}}) = \frac{N}{\Omega^2} \sum_{\substack{\vec{\mathbf{k}} \ \vec{\mathbf{p}} \\ (\vec{\mathbf{p}} \neq 0)}} \rho_{\vec{\mathbf{p}}-\vec{\mathbf{k}}} \rho_{\vec{\mathbf{k}}} V(\vec{\mathbf{k}}) \frac{k_z}{p_z} e^{-i\vec{\mathbf{p}}\cdot\vec{\mathbf{r}}}.$$
(20)

By expanding ρ_k and $\bar{\mathbf{v}}_k$ in terms of the helium excitation operators B_k^{\star} and B_k^{\pm} we see we have terms in the stress tensor corresponding to single excitations (when $\vec{p} = \vec{k}$) and terms corresponding to two excitations. Upon insertion into the interaction Hamiltonian \Re_{SL} and using the standard phonon expansion for u_z , we have energy-transfer processes in which absorption of a phonon from the solid is accompanied by emission of one or two excitations into the helium and vice versa. There are also processes corresponding to inelastic scattering of helium excitations from the solid surface. Phonon and roton scattering were also considered by Khalatnikov¹ but the matrix elements were obtained in a more phenomenological fashion.

V. TRANSFER HAMILTONIAN

We now exhibit the solid-liquid coupling (14) explicitly in the form of a transfer Hamiltonian by expanding u_z and Π_{zz} in terms of the excitation operators for the solid and liquid, respectively. For the lattice displacement in the solid we have

$$\vec{u}(\vec{R}_n) = \sum_{\vec{q}} \left(\frac{\hbar}{2\rho_s \Omega_s \omega_q} \right)^{1/2} \left(a_{\vec{q}} e^{i\vec{q} \cdot \vec{R}_n} + a_{\vec{q}} e^{-i\vec{q} \cdot \vec{R}_n} \right) \vec{\epsilon}_{\vec{q}},$$

where $\tilde{\epsilon}_q = \tilde{q}/q$ is the unit polarization vector appropriate to longitudinal waves, and ρ_s and Ω_s are the mass density and volume of the solid, respectively. The inclusion of transverse waves as in the Khalatnikov theory¹ does not materially affect the formalism but for simplicity we retain only the longitudinal waves.

That part of the stress tensor associated with emission or absorption of single excitations in the helium is, from Eqs. (17) and (20),

$$\Pi_{zz}^{(1)} = \frac{N^{1/2}}{\Omega} \sum_{\vec{k}} \left(\frac{\hbar^2 k_z^2}{4m} + \frac{NV(\vec{k})}{\Omega} \right) \rho_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} .$$
(21)

The term with $\vec{k}=0$ is of course excluded from this sum as is the $\vec{q}=0$ term from the phonon expansion for the solid. Substituting these expansions into (14) gives the transfer Hamiltonian

$$\mathcal{H}_{\rm SL}^{(1)} = \sum_{\bar{q}} T_{\bar{q}\bar{k}}^{+} (a_{\bar{q}}^{+} - a_{-\bar{q}}^{-}) (B_{\bar{k}}^{+} - B_{-\bar{k}}^{+}), \qquad (22)$$

where the transfer matrix element is

$$T_{\bar{q}\bar{k}} = iA \,\delta_{\bar{q}_{\parallel},\bar{k}_{\parallel}} \,\epsilon_{\bar{q}z} \left(\frac{\hbar}{2\rho_{S}\Omega_{S}\omega_{q}}\right)^{1/2} \\ \times \frac{(N\lambda_{k})^{1/2}}{\Omega} \left(\frac{\hbar^{2}k_{z}^{2}}{4m} + \frac{NV(\bar{k})}{\Omega}\right) \,. \tag{23}$$

The integral over the interface of area A has given rise to the Kronecker delta which conserves the components of wave vector parallel to the surface, $\bar{q}_{\parallel} = \vec{k}_{\parallel}$. Clearly the transfer Hamiltonian gives rise to transmission of phonons from the solid into boson excitations in the liquid helium via terms of the form

$$T_{\overline{q}\overline{k}}a_{\overline{q}}^{\dagger}B_{\overline{k}} + T_{\overline{q}\overline{k}}a_{\overline{q}}B_{\overline{k}}'.$$

For long wavelengths the helium excitations are phonons. In this region the matrix element for phonon transmission simplifies considerably. Using the relations given in (9) we obtain the form

$$T_{qk}^{++} = iA\hbar \delta_{q_{\parallel}, k_{\parallel}}^{+} \in q_{\pi}^{+} \left(\frac{\rho_L v_L^3 k}{4\Omega\Omega_S \rho_S v_S q}\right)^{1/2} .$$
(24)

Here v_s is the velocity of sound in the solid and $\rho_L = Nm/\Omega$ is the mass density of the helium. We see at once the dependence on the ratio of the acoustic impedance of the two media, $\rho_L v_L/\rho_s v_s$. This matrix element was also obtained by Sheard and Toombs¹⁹ who treated the helium as a classical elastic fluid. It is clear why this is so since

in the long-wavelength limit the stress tensor (21) becomes

$$\Pi_{\mathbf{z}\mathbf{z}}^{(1)} = -\rho_L v_L^2 \Delta(\mathbf{\vec{r}}),$$

where

$$\Delta(\mathbf{\bar{r}}) = -\frac{\rho'(\mathbf{\bar{r}})}{(N/\Omega)}$$

is the fractional decrease in density owing to the fluctuations which is just the local dilatation. This form is identical to the stress tensor for a classical elastic fluid taken to first order in the fluid displacements,²⁹ since we may then neglect the momentum convection term $\rho_L v_z v_z$, which also appears in Eq. (16) but is second order.

It is interesting to compare the scattering of the helium atoms from the vibrating solid surface for the present case of a Bose liquid, with the scattering which would occur if the atoms were noninteracting as in a Bose gas. To do this we simply expand the field operators in terms of singleparticle plane wave states; thus

$$\psi(\mathbf{\ddot{r}}) = \Omega^{-1/2} \sum_{\mathbf{p}} c_{\mathbf{p}} e^{i \mathbf{p} \cdot \mathbf{r}},$$

where c_{p}^{+} annihilates a helium atom of momentum $\hbar \bar{p}$. The solid-liquid interaction Hamiltonian then takes the general form

$$\mathcal{H}_{\rm SL} = \sum_{\substack{\mathbf{q} \neq \mathbf{p} \\ \mathbf{k}}} A \,\delta_{\mathbf{q}_{\parallel}, \mathbf{k}_{\parallel}} \,\epsilon_{\mathbf{q} \mathbf{z}} \left(\frac{\hbar}{2\rho_{S} \boldsymbol{\Omega}_{S} \boldsymbol{\omega}_{q}} \right)^{1/2} M_{\mathbf{p}}^{\mathbf{p} + \mathbf{k}} \\ \times c_{\overline{\mathbf{b}} + \mathbf{k}}^{\dagger} c_{\overline{\mathbf{p}}} (a_{\overline{\mathbf{q}}}^{\dagger} - a_{-\overline{\mathbf{q}}}^{\dagger})$$
(25)

for processes involving only two helium atoms. Equation (25) defines a matrix element for the inelastic scattering of a helium atom from state \vec{p} to $\vec{p} + \vec{k}$. We use the form of stress tensor given in Eq. (21) which for small momentum transfer $\hbar \vec{k}$ describes phonon transmission into the helium. In this limit the scattering matrix element is dominated by interparticle interactions and we find

$$M \vec{p}^{+\vec{k}} = NV(0) / \Omega^2 = \rho_L v_L^2 / N.$$

Thus for an interacting Bose liquid the scattering of the helium atoms from the solid surface during phonon transmission is completely isotropic being independent of both initial and final momenta. To compare with the behavior of a gas of independent atoms, we must use the stress tensor given in Eq. (15), which gives

$$M_{\underline{p}}^{\overline{p}+\overline{k}} = (\hbar^2/m\Omega)(p_z + \frac{1}{2}k_z)^2 . \qquad (26)$$

Thus, by contrast, for noninteracting atoms the scattering is angular dependent and for small momentum transfers is strongly weighted towards normal incidence. For an independent-particle model of ³He Rice¹³ has also considered the scattering of free atoms from a surface and obtained the diagonal matrix element by an argument involving the pressure in a Fermi gas which is similar to our use of the stress tensor.

VI. ENERGY TRANSFER BY ONE-PHONON PROCESSES

The energy-transfer processes may be categorized by specifying the number of excitations involved in the helium. Thus the transfer Hamiltonian (22) describes one-excitation processes and the excitation may be a phonon or a roton (or even in between), but the approximate form of matrix element (24) is restricted to one-phonon processes. It is now readily verified that a perturbation calculation of the heat current J_{SL}^{ph} due to one-phonon transmission processes, leads to essentially the same results as the classical acoustic-mismatch treatment. Taking the temperature of the solid to be $T + \Delta T$ and that of the liquid to be T, the net heat flow is

$$J_{\rm SL}^{\rm ph} = \Delta T \sum_{\substack{q,k \\ q,k}} \left(\frac{2\pi}{\hbar^2} \right) \left| T_{\overline{q},\overline{k}} \right|^2 \hbar \omega_q \delta(\omega_q - \omega_k) \left(\frac{\partial n_q^0}{\partial T} \right), \qquad (27)$$

where n_q^0 is the Bose-Einstein distribution function for temperature *T*. Note that we reserve the label $\bar{\mathbf{q}}$ for phonons in the solid. Conservation of energy, $\omega_q = \omega_k$, together with the wave-vectorconservation condition, $\bar{\mathbf{q}}_{\parallel} = \bar{\mathbf{k}}_{\parallel}$, contained in $T_{\bar{\mathbf{q}}\bar{\mathbf{k}}}$, are equivalent to the law of refraction of sound waves at the solid-liquid boundary. Thus the transfer Hamiltonian formalism preserves this basic feature of phonon transmission. In particular owing to the disparity in the sound velocities in the solid and in the liquid, the emission of phonons into the helium is confined to a narrow critical cone of semiangle $\theta_c \cong v_L/v_s$.

The Kapitza resistance evaluated from Eqs. (27) and (24) is given by

$$R_{K}^{-1} = \frac{J_{SL}^{pn}}{A\Delta T} = k_{B} \frac{\pi^{2}}{45} \left(\frac{\rho_{L} v_{L}}{\rho_{S} v_{S}^{3}} \right) \left(\frac{k_{B} T}{\hbar} \right)^{3}$$
(28)

We may compare this directly with the acousticmismatch theory since Little² has given results for a model involving only longitudinal phonons. Classical elastic theory gives a transmission coefficient

$$\alpha_{\rm SL} = \frac{4\rho_L \rho_S / k_z q_z}{(\rho_L / k_z + \rho_S / q_z)^2} \cdot$$

From energy conservation $v_S q = v_L k$ and since $v_L \ll v_S$ we have $k \gg q$. Moreover $\rho_L \ll \rho_S$, so that, neglecting the term ρ_L/k_z in the denominator, an adequate approximation for the solid-liquid ⁴He interface is

$\alpha_{\rm SL} = 4\rho_L q_s / \rho_S k,$

where we have also put $k_s \cong k$ by virtue of the restriction imposed by the critical cone. This gives an acoustic-mismatch value for the Kapitza conductance which is greater than that of Eq. (28) by a factor of 4 but otherwise identical. The origin of this discrepancy lies in our use of a planerunning-wave representation for the phonons in the solid and the excitations in the helium, which neglects the phase coherences between incident and reflected waves. In the theory of tunneling such coherences in the electronic states are usually ignored since one is not concerned with the absolute magnitude of the tunneling current. However in the Kapitza-resistance problem one of the major sources of discrepancy between theory and experiment lies in the magnitude of the heat flow, so it is important to be able to account for the missing factor of 4.

In the unperturbed Hamiltonian \mathcal{K}_{S} for the solid the interaction with the helium is completely absent and the solid thus has a free surface at z = 0. We should therefore use standing waves for the zdependence of the lattice displacements with the phase chosen such that the surface is a vibrational antinode. Since a standing wave is a coherent superposition of two progressive waves, the surface vibrational amplitude is twice that for a single plane progressive wave. On the other hand if the two plane waves are phase incoherent the surface amplitude is $\sqrt{2}$ times that for a single plane wave. It follows that a decomposition of the lattice vibrations into standing-wave modes will give rise to an additional factor $\sqrt{2}$ in the transfer matrix element. A similar decomposition is necessary for the wavelike fluctuations in the helium. But the unperturbed Hamiltonian \mathcal{K}_{L} of Eq. (11) contains the static potential step $V_0(z)$ which is equivalent to an impenetrable wall. The unperturbed modes are again standing waves but the vibrational amplitude must vanish at the wall z = 0. This means that the plane z = 0 is a node for velocity fluctuations but an antinode for density fluctuations as at the closed end of an organ pipe. Again an additional factor $\sqrt{2}$ will appear in the matrix element (24) so that the transition probability and energy flow are increased by the required factor of 4. We may of course put this on a more formal basis by writing down the appropriate expansions in standing-wave modes. For the present paper we have preferred to retain the more familiar running-wave expansions since we may then use in unchanged form the theory of Sunakawa et al., and the physics of the problem is basically unaltered. However to deal with the case of a general van der Waals potential requires a more detailed

investigation of the excitations close to the solid surface. It is then necessary to use modified standing waves which are determined self-consistently from the van der Waals potential in a theory of nonuniform states of liquid helium such as proposed by Fetter³³ and Bowley.³¹ For the case of an impenetrable wall the appropriate standing-wave expansions of the density- and velocity-fluctuation operators have also been given by Bowley.³¹

VII. ENERGY TRANSFER BY ONE-ROTON PROCESSES

Our transfer Hamiltonian (22) and (23) couples the solid to the complete excitation spectrum of helium. In the region of the minimum in the dispersion curve for the excitations a phonon in the solid is transmitted into a roton in the helium. These processes have not been previously calculated although Khalatnikov¹ did consider inelastic roton scattering at the solid surface. Such tworoton processes are also included in our treatment via the bilinear terms in the stress tensor. At low temperatures only the high-frequency tail of the Bose-Einstein distribution gives rise to thermally excited rotons but owing to the large density of states they may nevertheless influence the transport properties.

In the vicinity of the roton minimum the dispersion relation (8) approximates to^{34}

$$\hbar \omega_{k} = \Delta + \hbar^{2} (k - k_{0})^{2} / 2m_{r}$$
⁽²⁹⁾

where Δ and k_0 are the energy and wave number at the minimum and m_r is the roton effective mass. Since $k_0 \cong 1.9 \times 10^8$ cm⁻¹ is very much greater than the thermal phonon wave vectors in the solid at the temperatures of interest ($T \le 2$ K); $k_{\parallel} = q_{\parallel}$ can be neglected in comparison with k. Rotons are therefore emitted strictly normal to the surface and we may take $k_z = k$ in the matrix element (23). Recalling the definition (7) of λ_k and the relation (8), it follows that the transfer matrix element for one-roton emission-absorption processes is

$$T_{\bar{q}k} = iA\delta_{\bar{q}\|,\bar{k}\|} \epsilon_{\bar{q}} \left(\frac{\hbar}{2\rho_S \Omega_S \omega_q}\right)^{1/2} \\ \times \frac{N^{1/2}}{\Omega} \frac{\omega_k (2m \hbar \omega_k)^{1/2}}{2k} \cdot$$

After computing the roton density of states from (29), evaluation of the corresponding heat current J_{SL}^{rot} gives

$$J_{\rm SL}^{\rm rot} = A \Delta T \frac{k_B \rho_L (2\Delta/m_r)^{1/2}}{12\pi^2 \rho_S v_S^3} \frac{2m_r \Delta}{\hbar^2 k_0^2} \\ \times \left(\frac{\Delta}{\hbar}\right)^3 (\beta \Delta)^{3/2} e^{-\beta \Delta} I ,$$

where

$$I = \int_0^\infty \left(1 + \frac{z^2}{\beta \Delta}\right)^6 \left(1 + \frac{z}{(\beta \hbar^2 k_0^2 / 2m_r)^{1/2}}\right)^{-1} e^{-z^2} dz$$

and $\beta = 1/k_B T$. Here we have taken the thermalroton distribution to be adequately described by a Maxwell-Boltzmann function since in experimental situations $\beta \Delta \gg 1$. Under these conditions the integral $I \cong \frac{1}{2} \pi^{1/2}$. We see that this contribution to the Kapitza conductance then has the temperature dependence $T^{-3/2} e^{-\Delta/k_B T}$.

The ratio of the one-roton contribution to the one-phonon contribution (28) can now be expressed conveniently in terms of dimensionless ratios:

$$\frac{J_{SL}^{\text{for}}}{J_{SL}^{\text{ph}}} = \frac{15}{4\pi^4} \left(\frac{\pi\Delta}{2m_r v_L^2}\right)^{1/2} \frac{2m_r \Delta}{\hbar^2 k_0^2} (\beta \Delta)^{9/2} e^{-\beta \Delta}$$

Taking numerical values of the parameters of liquid ⁴He at s.v.p. from Wilks³⁴ we find this ratio is 0.042 at 2 K. Roton emission cannot therefore affect the numerical discrepancies between experimental and theoretical values of the Kapitza resistance principally because of the freezing out of the roton population at low temperatures.

VIII. SECOND-ORDER PROCESSES

As we have mentioned the bilinear terms in the stress tensor link the phonons in the solid to two excitations in the helium. Thus we have a multitude of higher-order processes such as emission of two phonons, two rotons or a roton and a phonon and inelastic scattering of phonons, rotons or phonon-to-roton scattering. In general we expect processes involving rotons to be small for $k_B T$ $\ll \Delta$ on account of the low thermal occupancy. We also expect emission of two phonons to be unimportant since energy conservation restricts the available density of states. Khalatnikov¹ has also considered phonon scattering and roton scattering and concluded that although they are comparable with, but smaller than, the acoustic-mismatch value at 2 K they rapidly become completely negligible at lower temperatures. However the appropriate transition probabilities were obtained by Khalatnikov from semiclassical arguments and his treatment is sufficiently different from ours that we feel it worthwhile to discuss one of these processes in more detail.

The relevant parts of the stress tensor are obtained from Eqs. (17) and (20). With a slight change of notation in Eq. (20) these are

$$\Pi_{zz}^{(2)} = \sum_{\vec{k},\vec{k},'} \left(\frac{1}{m\Omega} v_{-\vec{k}z} v_{-\vec{k}\,'z} - \frac{\hbar^2 k_z k_z'}{4m\Omega} \rho_{\vec{k}} \rho_{\vec{k}\,'} + \frac{N}{\Omega^2} \frac{V(\vec{k}) k_z}{k_z + k_z'} \rho_{\vec{k}\,'} \rho_{\vec{k}} \right) e^{-i(\vec{k} + \vec{k}\,') \cdot \vec{r}},$$

where the terms with $\vec{k} = \vec{k}' = \vec{k} + \vec{k}' = 0$ are excluded. We shall discuss phonon scattering and therefore substitute

$$\begin{split} \rho_{\vec{k}}^{\star} &= -i \left(\frac{\hbar k}{2m v_L} \right)^{1/2} \left(B_{-\vec{k}} - B_{\vec{k}}^{\dagger} \right), \\ v_{\vec{k}z}^{\star} &= -i \hbar k_z \left(\frac{m v_L}{2\hbar k} \right)^{1/2} \left(B_{\vec{k}}^{\star} + B_{-\vec{k}}^{\dagger} \right). \end{split}$$

In the long-wavelength limit the second term in the above stress tensor can be neglected since it contains higher powers of k than the remaining terms. Retaining only the two-phonon scattering terms gives

$$\Pi_{gg}^{\text{ph scat}} \iota = \sum_{\vec{k},\vec{k}'} \frac{\hbar v_L (kk')^{1/2}}{2\Omega} \left(-\frac{k_z k'_z}{kk'} + \frac{k_z}{k_z + k'_z} \right) \times (B_{-\vec{k}} B_{\vec{t}'}^{\dagger} + B_{\vec{t}}^{\dagger} B_{-\vec{k}'}^{-1}) e^{-i(\vec{k} + \vec{k}') \cdot \vec{r}}$$

Upon manipulation involving reversing the signs of \vec{k} and \vec{k}' and interchange of \vec{k} and \vec{k}' at various stages, we find the more convenient form

$$\prod_{zz}^{\text{ph scat}} = \sum_{\vec{k},\vec{k}'} M_{\vec{k},\vec{k}'} B_{\vec{k}} B_{\vec{k}}^{\dagger}, e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}}, \qquad (30)$$

where

$$M_{\vec{k}\vec{k}'} = \frac{\bar{\hbar} v_L (kk')^{1/2}}{2\Omega} \left(\frac{2k_z k'_z}{kk'} + 1 \right).$$
(31)

The diagonal matrix element $M_{\bar{k}\bar{k}} \sim \hbar k v_L / \Omega$ corresponds roughly to the flux of momentum carried by a phonon with momentum $\hbar k$ moving with velocity v_L . This is similar to the form (26) for free particles since a particle of momentum $\hbar p$ has velocity $\hbar p/m$. The matrix element is weighted towards wave vectors normal to the solid surface. To estimate this contribution to the Kapitza conductance we approximate the matrix element by the value at normal incidence³⁵

$$M_{\vec{k}} = 3\hbar v_L (kk')^{1/2} / 2\Omega .$$
 (32)

The solid-liquid interaction describing two-phonon scattering events is then

$$\mathscr{K}_{SL}^{ph \ scat} = \sum_{\substack{\mathbf{a},\mathbf{b},\mathbf{k}'\\\mathbf{q},\mathbf{k}}} T_{\mathbf{q},\mathbf{k}}^{\mathbf{k}'} B_{\mathbf{k}}^{\dagger} B_{\mathbf{k}'}^{\dagger} (a_{\mathbf{q}}^{\star} - a_{-\mathbf{q}}^{\dagger}), \qquad (33)$$

where

$$T_{\bar{q}\bar{k}}^{\bar{k}'} = A \delta_{\bar{q}_{\parallel}+\bar{k}_{\parallel},\bar{k}_{\parallel}}^{+} \epsilon_{\bar{q}z} \left(\frac{\hbar}{2\rho_s \Omega_s \omega_q}\right)^{1/2} M_{\bar{k}\bar{k}}^{+},$$

is the transfer matrix element for the process $\bar{q} + \bar{k} \rightarrow \bar{k}'$. There is some formal similarity here with the theory of acoustic attenuation in which an ultrasonic wave \bar{q} is attenuated by anharmonic interactions with thermal phonons \bar{k} and \bar{k}' . However in phonon-phonon interactions in bulk media

all three components of wave vector are conserved which leads to the requirement that the thermal phonons have a greater phase velocity than the ultrasonic wave.³⁶ This is not the case here since $v_L < v_S$ and the above processes are only allowed because of the nonconservation of the *z* component of wave vector.

Computing the transition probability from the golden rule gives the net heat flow for a temperature difference ΔT

$$J_{SL}^{\text{ph scat}} = \Delta T \sum_{\overrightarrow{q \ k \ k}} \frac{2\pi}{\hbar^2} |T_{\overrightarrow{q \ k}}^{\overrightarrow{k'}}|^2 \ \hbar \omega_q$$
$$\times \delta(\omega_q + \omega_k - \omega_{k'}) \ \frac{\partial n_{\overrightarrow{q}}^0}{\partial T} (n_{\overrightarrow{k}}^0 - n_{\overrightarrow{k'}}^0).$$

Conservation of wave vector removes the sum over k'_x and k'_y , and the sum over k'_z is performed using the energy conservation condition. Again making the approximation $|k'_z| \sim k'$, which avoids complicated angular integrations, we find the integral over k reduces to

$$\int \omega_k^3 \omega_{k'} (n_{k}^{\underline{0}} - n_{k'}^{\underline{0}}) d\omega_k,$$

where now $\omega_{k'} = \omega_k + \omega_q$. By expanding the integral in powers of ω_q and taking only the first term we obtain the leading term in the temperature dependence. The above integral is then approximately

$$\frac{\hbar \,\omega_a}{k_B T} \left(\frac{k_B T}{\hbar}\right)^3 \frac{4 \pi^4}{15}$$

The sum over \bar{q} reduces essentially to the heat capacity C_s of the solid giving finally the simple expression

$$J_{SL}^{ph \ scat} = A \Delta T \, \frac{\pi^2}{10} \, \hbar \, k_T^4 \frac{C_s}{\rho_s \Omega_s} \,, \tag{34}$$

where $k_T = k_B T / \hbar v_L$ is the wave number of thermal phonons of energy $k_B T$ in the helium. This form is in fact very similar to the expression for the Kapitza conductance for the Fermi-gas model^{13,14} of ³He if k_T is replaced by the Fermi wave number k_F . The inelastic scattering of phonons in ⁴He is therefore analogous to the inelastic scattering of the quasiparticles in ³He, but because of the different statistics the average momentum $\hbar k_T$ of the phonons in ⁴He is temperature dependent whereas $\hbar k_F$ is not. This accounts for the rapid T^7 temperature dependence of this contribution to the conductance.

In a Fermi liquid, interactions between quasiparticles give rise to collective zero-sound modes which couple to the vibrations of the solid via the same mechanism which scatters the quasiparticles.¹⁷ In a similar way, momentum conserving phonon collisions (N processes) give rise to second-sound modes in a phonon gas and correspond to fluctuations in phonon density rather than particle density.³⁴ Our interaction Hamiltonian (33) for two-phonon scattering includes coupling to fluctuations in the local number density of phonons, which is represented by the operator

$$p(\mathbf{\tilde{r}}) = \mathbf{\Omega}^{-1} \sum_{\mathbf{\tilde{k}},\mathbf{\tilde{k}}'} B_{\mathbf{\tilde{k}}}^{\dagger}, B_{\mathbf{\tilde{k}}} e^{i(\mathbf{\tilde{k}}-\mathbf{\tilde{k}}')\cdot\mathbf{\tilde{r}}'}$$

whose form closely resembles the stress tensor (30). By including phonon-phonon interactions our theory may therefore be generalized to describe emission and absorption of second-sound modes but it is doubtful if this could greatly enhance the energy transfer via two-phonon scattering.

The acoustic-mismatch heat flow can be put into a similar form to (34) by rewriting Eq. (28),

$$J_{\rm SL}^{\rm pn} = A \Delta T \rho_L v_L C_{\rm S} / 6 \rho_S \Omega_S , \qquad (35)$$

remembering that for our model C_s only includes longitudinal modes. The acoustic impedance $\rho_L v_L$ for direct phonon emission corresponds to the value $\sim \hbar k_T^4$ for phonon scattering (or $\sim \hbar k_F^4$ for scattering of free fermions¹⁴). Comparing Eqs. (34) and (35) we find the ratio

$$\frac{J_{\rm SL}^{\rm ph \ scat}}{J_{\rm SL}^{\rm ph}} = \frac{3\pi^2}{5} \frac{\hbar k_T^4}{\rho_L v_L} ,$$

which is only 0.033 at 2 K. Owing to the rapid temperature dependence the two-phonon contribution soon becomes negligible at lower temperatures. The general form of our result agrees with Khalatnikov's calculation and the ratio also agrees to within an order of magnitude despite the approximations we have made. Our approach to the Kapitza resistance confirms Khalatnikov's general conclusion¹ that higher-order processes do not contribute significantly to the energy transfer at temperatures below 2 K.

IX. OUTLOOK

Our calculation is the first completely quantummechanical theory of the Kapitza resistance for the solid-liquid ⁴He interface. By using a realistic model of a Bose liquid we have treated processes involving phonons and rotons in the helium in a unified and conceptually more satisfying manner than in previous treatments. The acousticmismatch theory is recovered in the appropriate limit and we have calculated the contribution of direct roton emission-absorption processes which apparently have been previously overlooked.

Although we have not shed any dramatic light on discrepancies between theory and experiment our approach has the advantage that it is capable of generalization in a relatively straightforward way. Phonon interactions in the solid or in the helium may be incorporated into the theory by including appropriate terms in the total Hamiltonian. The effects of these on the transition rate appear in second and higher orders of time-dependent perturbation theory.²⁰ In this way the influence of damping of the waves in the solid or of scattering by defects or surface structure may be calculated in a systematic way and some of the difficulties of the classical theory¹¹ avoided. We have also indicated the way to modify the transfer matrix elements to include attractive van der Waals forces at the interface.

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The transfer-Hamiltonian formalism allows the

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