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Phonon transmission across interfaces and the Kapitza resistance

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The transmission of phonons across an interface between a classical solid and liquid helium is calculated. Several simple models of the helium system are considered. Calculations for a solid with a clean and perfect surface give a transmission coefficient for low-energy phonons. ($\epsilon < 20$ K), which is very small (typically ≤ 0.1), and which decreases with decreasing energy. At energies above 30 K the transmission is predicted to have a larger value which is slowly varying with energy, and to be inversely proportional to the acoustical impedance of the solid. Possible mechanisms which increase the transmission for damaged or dirty surfaces are briefly discussed.

I. INTRODUCTION

When heat flows from a solid into superfluid helium, a temperature jump occurs across the interface. This effect was first observed by Kapitza[1] in 1941. Phenomenologically, the temperature jump can be considered to arise from a thermal boundary resistance (Kapitza resistance). It is now believed that a thermal boundary resistance occurs at all interfaces between dissimilar materials. The boundary resistance arises because not all thermal phonons incident on the interface are transmitted across into the other medium. Thus, to obtain a quantitative understanding of the Kapitza resistance, it is necessary to study the transmission and reflection of phonons at interfaces.

An important contribution to the theory of the Kapitza resistance was made by Khalatnikov.[2] He calculated the transmission coefficient of phonons across the boundary between a solid and liquid helium by applying the laws of classical acoustics. For a phonon at normal incidence to the interface the transmission coefficient is

$$\alpha_{S\text{-He}} = 4Z_S Z_{\text{He}}/(Z_S + Z_{\text{He}})^2 , \tag{1}$$

where Z_S and Z_{He} are the acoustical impedances defined by

$$Z_S = \rho_S c_S , \tag{2}$$

and

$$Z_{\text{He}} = \rho_{\text{He}} c_{\text{He}} , \tag{3}$$

where ρ_S and ρ_{He} are the densities in the solid and liquid, and c_S and c_{He} are the velocities of sound. For a typical solid ρ_S is 10 to 30 times larger than ρ_{He} and the velocity of sound c_S is also larger than c_{He} by a similar factor. Hence, the acoustical impedance of liquid helium is smaller by 100 to 1000 times than the impedance of most solids and so the transmission coefficient comes out to be of the order of 0.01.

At the present time the experimental situation regarding the transmission coefficients is not completely clear. *Most* experiments[3–16] have yielded transmission coefficients much larger than the values predicted by the acoustical-mismatch theory, except for phonons of very low energy. Typical results[4] are shown very qualitatively in Fig. 1. For phonons of energy less than 1 K the transmission coefficient is close to the acoustical-mismatch value.[5] In the energy range 1–5 K there is a rapid increase in transmission.[6] Above 10 K and up to the highest energy so far investigated[7] (around 40 K) the transmission is roughly constant, and is typically in the range 0.1–0.5. It is known that this anomalously large transmission of phonons also occurs across interfaces between a classical solid (e.g., silicon) and a quantum solid[17–19] (^{3}He, ^{4}He, H_2, or D_2) or liquid ^{3}He.[20] However, for interfaces between the two "classical" solids (e.g., indium and sapphire[21]) the acoustical-mismatch theory is in reasonable agreement with the experimental results. The difficulty thus appears to be present only when quantum effects are important.

Very recently Weber *et al.*[22] have studied the transmission of phonons of energy 14 K across interfaces between lithium fluoride or sodium fluoride and liquid helium. They found that when the alkali halide surface was cleaved at low temperature and surface contamination was avoided, the anomalous transmission was greatly reduced. For the same surfaces subsequent exposure to the atmosphere or "cleaning" with organic solvents increased the transmission to values comparable to those found in the earlier experiments. So far there is no information available about the energy dependence of the transmission coefficient for these very clean surfaces.

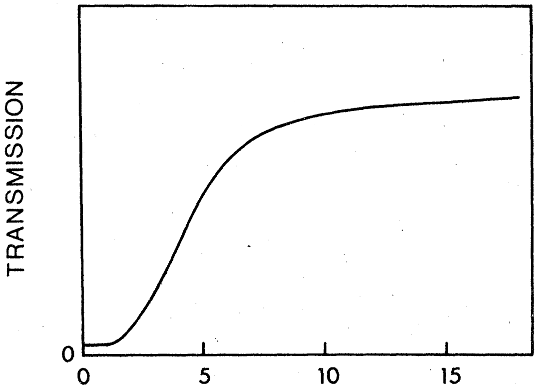

FIG. 1. Qualitative form of typical results for the phonon transmission coefficient as a function of energy. The vertical scale is linear and a typical value of the transmission coefficient at 10 K is in the range 0.1–0.5.

There have been many different calculations of the phonon transmission coefficient.[3,23] Generally, these calculations have been concerned with an explanation of the anomalously large transmission observed in most of the experiments mentioned above. Some of these ideas have been worked out in quantitative detail, while others have been supported by "hand-waving" arguments only. In this paper we investigate the transmission on the basis of calculations which, although crude, are nevertheless quantitative and based on first principles. Most of the analysis we present applies to transmission of phonons across an interface between a perfect solid with a clean surface and liquid helium. Thus, the theory is most applicable to experiments of the type performed by Weber *et al.*[22] In Sec. II we discuss the assumptions that the theory relies on. The actual calculations of the transmission for various models of the helium system are described in Sec. III. In Sec. IV we discuss the sum rules derived here that the transmission coefficient obeys. These have important implications for the transmission coefficient, particularly at low energy.

II. ASSUMPTIONS

Our basic approach in this paper is as follows: The incident phonon is assumed to have a wave vector normal to the interface and to come from the solid side. For a phonon of energy much less than $k\Theta_D$ (Θ_D is the Debye temperature of the solid) the phonon wavelength in the solid is much larger than the interatomic spacing. Thus, as a first approximation the helium sees the surface of the solid as oscillating almost rigidly. Hence, the displacement $\vec{D}$ of all points on the surface of the solid may be taken to be

$$\vec{D} = u_S \hat{e} \cos(\Omega t) , \tag{4}$$

where $\hat{e}$ is the unit polarization vector of the phonon, Ω is the phonon frequency, and the amplitude of oscillation u_S is independent of position on the surface. We will treat the oscillation of the surface as a time-dependent perturbation acting on the helium system. This perturbation is a potential whose value at a point $\vec{r}$ is

$$\delta H(\vec{r},t) = U_{S\text{-He}}(\vec{r}-\vec{D}) - U_{S\text{-He}}(\vec{r}) , \tag{5}$$

where $U_{S\text{-He}}(\vec{r})$ is the potential at $\vec{r}$ due to the Van der Waals forces between helium atoms and the solid surface when the surface is not displaced. To lowest order in u_S, Eq. (5) becomes

$$\delta H(\vec{r},t) = -u_S \hat{e} \cdot \nabla U_{S\text{-He}} \cos(\Omega t) . \tag{6}$$

We call this contribution to the coupling between the solid and the helium "displacement coupling", since it comes from the *rigid* displacement of the solid surface. In a higher approximation one should also take into account the fact that an incident phonon causes *relative* displacements of the atoms near the surface of the solid. We call this contribution "strain" coupling, because it arises from the oscillating strain in the solid surface. One expects that the strain perturbation will be smaller than the displacement perturbation by a factor which is roughly the ratio of the relative displacements of neighboring atoms to the absolute displacement.[24] This ratio is just

$$d_S/\lambda_S , \tag{7}$$

where d_S is the interatomic spacing in the solid and λ_S is the phonon wavelength in the solid. Although the distinction between displacement and strain coupling may appear rather academic, it turns out that it has important consequences (see Sec. IV).

The strain perturbation will not necessarily be small compared to the displacement perturbation if the surface of the solid is covered by adsorbed gas. For a gas which is physisorbed on the surface, the bonds between the gas atoms and the solid are much weaker than the bonds that hold a typical solid together. Thus, when the surface of the solid oscillates, the adsorbed gas atoms will not perfectly follow the motion of the solid surface. In this case the perturbation that acts on the helium can be written in the form

$$\delta H(\vec{r},t) = -u_S \hat{e} \cdot \nabla U_{S\text{-He}} \cos(\Omega t) - \sum_i u_i \hat{e}_i \cdot \nabla U_{i\text{-He}} \cos(\Omega t + \phi_i) , \tag{8}$$

where u_i and $\hat{e}_i$ are the amplitude and unit polarization vector of the ith absorbed atom, ϕ_i is a phase shift, and $U_{i\text{-He}}$ is the potential between the ith atom and the helium. Thus we can set

$$\delta H(\vec{r},t) = \delta H_{\text{disp}}(\vec{r},t) + \delta H_{\text{str}}(\vec{r},t) , \tag{9}$$

where

$$\delta H_{\rm disp}(\vec{r},t) = -u_S \hat{e}\cdot\nabla U'_{S-{\rm He}}\cos(\Omega t)\ , \tag{10}$$

$$\nabla U'_{S-{\rm He}} = \nabla U_{S-{\rm He}} + \sum_i \nabla U_{i-{\rm He}}\ , \tag{11}$$

and

$$\delta H_{\rm str}(\vec{r},t) = \sum_i [u_S\hat{e}\cos(\Omega t) - u_i\hat{e}_i\cos(\Omega t+\phi_i)]\cdot\nabla U_{i-{\rm He}}. \tag{12}$$

$\delta H_{\rm disp}$ is thus the perturbation due to a rigid oscillation of the solid plus the adsorbed atoms. This gives a displacement coupling with a new effective potential $U'_{S-{\rm He}}$. $\delta H_{\rm str}$ describes the extra effects that occur because the adsorbed atoms do not move with the same amplitude, direction, or phase as the solid. For the moment we consider just a clean surface and so neglect the strain coupling.

If we assume that the transmission coefficient of the phonon across the interface is much less than unity, and that the surface is clean, we will have

$$u_S \approx 2u_0\ , \tag{13}$$

where u_0 is the amplitude of the wave corresponding to the incident phonon. Now assume that the helium is initially in some state $|i\rangle$. The probability per unit time of a transition to the state $|j\rangle$ due to the influence of the perturbation is

$$P_{ij} = \frac{2\pi u_0^2}{\hbar}\,|\langle i|\hat{e}\cdot\nabla U_{S-{\rm He}}|j\rangle|^2 \times[\delta(E_i+\hbar\Omega-E_j)+\delta(E_i-\hbar\Omega-E_j)]\ . \tag{14}$$

Therefore, the rate at which energy is transmitted to the helium is

$$\dot{Q} = \sum_{ij}(E_j-E_i)P_{ij}e^{-E_i/kT}\Big/\sum_i e^{-E_i/kT}\ , \tag{15}$$

where T is the temperature. In what follows we will consider only $T=0$ K, and will come back to discuss the effect of a finite temperature later.

The energy flux incident on the surface is

$$\dot{Q}_{\rm inc} = \tfrac{1}{2}\rho_S u_0^2\,\Omega^2 c_S A\ , \tag{16}$$

where A is the area of the surface. Thus, the transmission coefficient for a phonon of energy ϵ $(\equiv\hbar\Omega)$ is

$$\alpha(\epsilon) \equiv \dot{Q}/\dot{Q}_{\rm inc} = \frac{4\pi\hbar}{\rho_S c_S \epsilon A}\sum_j |\langle 0|\hat{e}\cdot\nabla U_{S-{\rm He}}|j\rangle|^2\delta(E_0+\epsilon-E_j)\ , \tag{17}$$

where $|0\rangle$ denotes the ground state of the helium. Before considering models for the helium system, it is interesting to note some alternative forms of Eq. (17). Consider a situation in which the helium system is bounded only by the solid-helium interface and by a free surface (Fig. 2). This limits the discussion to helium in the absence of applied pressure. In such a case the only external potential acting on the helium is the interaction with the solid surface, i.e., the same potential whose gradient occurs in Eq. (17). Because of this special property one can derive the following equivalent forms for the matrix element in Eq. (17):

$$\langle 0|\hat{e}\cdot\nabla U_{S-{\rm He}}|j\rangle = (i/\hbar)(E_j-E_0)\,\langle 0|\hat{e}\cdot\vec{\rm P}|j\rangle \tag{18}$$

$$= (Nm/\hbar^2)(E_j-E_0)^2\langle 0|\hat{e}\cdot\vec{\rm R}|j\rangle\ , \tag{19}$$

where m is the mass of one helium atom, $\vec{\rm P}$ is the operator for the total momentum of the helium, $\vec{\rm R}$ is the center-of-mass of the helium system, and N is the number of helium atoms. Equations (18) and (19) hold regardless of the form of the interaction between the helium atoms, and can be derived in a straightforward way by considering commutators of the total helium Hamiltonian with the operators $\vec{\rm P}$ and $\vec{\rm R}$. Note that $\vec{\rm P}$ and $\vec{\rm R}$ commute with all parts of the helium Hamiltonian except the part that represents the potential due to the solid. We can now use Eqs. (18) and (19) to obtain the following equivalent forms for the transmission coefficient:

$$\alpha(\epsilon) = \frac{4\pi\epsilon}{\rho_S c_S A\hbar}\sum_j |\langle 0|\hat{e}\cdot\vec{\rm P}|j\rangle|^2\delta(E_0+\epsilon-E_j) \tag{20}$$

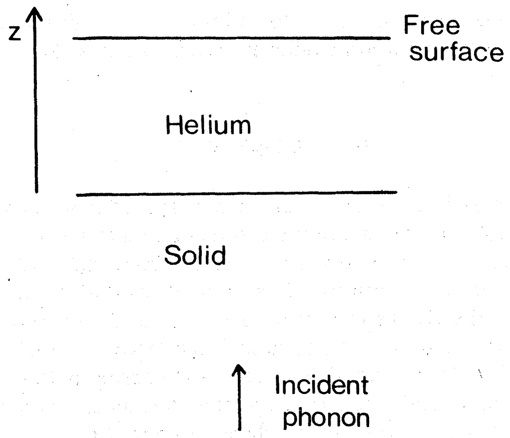

FIG. 2. Helium system bounded by the solid and by a free surface.

$$= \frac{4\pi i N m \epsilon^2}{\rho_S c_S A \hbar^2} \sum_j \langle 0|\hat{e}\cdot\vec{P}|j\rangle \langle j|\hat{e}\cdot\vec{R}|0\rangle \times \delta(E_0+\epsilon-E_j) \tag{21}$$

$$= \frac{4\pi N^2 m^2 \epsilon^3}{\rho_S c_S A \hbar^3} \sum_j{}' |\langle 0|\hat{e}\cdot\vec{R}|j\rangle|^2 \delta(E_0+\epsilon-E_j) \;. \tag{22}$$

These relations are interesting because the potential $\hat{e}\cdot\nabla U_{S\text{-He}}$ that couples the solid to the helium no longer appears explicitly in the matrix elements. However, the potential does appear implicitly on the right-hand side of Eqs. (20)–(22) because $U_{S\text{-He}}$ is involved in the determination of the helium eigenfunctions. These equations lead immediately to the following sum rules:

$$\int_0^\infty \alpha(\epsilon)\epsilon^{-1}\,d\epsilon = \frac{4\pi}{\rho_S c_S A \hbar} \langle 0|(\hat{e}\cdot\vec{P})^2|0\rangle \;, \tag{23}$$

$$\int_0^\infty \alpha(\epsilon)\epsilon^{-2}\,d\epsilon = \frac{2\pi N m}{\rho_S c_S A \hbar} \;, \tag{24}$$

and

$$\int_0^\infty \alpha(\epsilon)\epsilon^{-3}\,d\epsilon = \frac{4\pi N^2 m^2}{\rho_S c_S A \hbar^3} [\langle 0|(\hat{e}\cdot\vec{R})^2|0\rangle - \langle 0|\hat{e}\cdot\vec{R}|0\rangle^2] \;. \tag{25}$$

One can also derive positive-moment sum rules from Eq. (17). The lowest three are

$$\int_0^\infty \alpha(\epsilon)\,d\epsilon = \frac{2\pi\hbar}{\rho_S c_S A} \langle 0|\hat{e}\cdot\nabla\nabla U_{S\text{-He}}\cdot\hat{e}|0\rangle \;, \tag{26}$$

$$\int_0^\infty \alpha(\epsilon)\epsilon\,d\epsilon = \frac{4\pi\hbar}{\rho_S c_S A} \langle 0|(\hat{e}\cdot\nabla U_{S\text{-He}})^2|0\rangle \;, \tag{27}$$

and

$$\int_0^\infty \alpha(\epsilon)\epsilon^2\,d\epsilon = \frac{2\pi\hbar^3}{\rho_S c_S A m} \langle 0|\nabla(\hat{e}\cdot\nabla U_{S\text{-He}}) \cdot\nabla(\hat{e}\cdot\nabla U_{S\text{-He}})|0\rangle \;. \tag{28}$$

These formulas only apply if the coupling is of the displacement type.

At this stage the problem reduces to the calculation of the wave functions of the states of the helium system. Experiments[7–9] show that the transmission of phonons into a film is essentially the same as transmission into bulk helium, provided the film is at least three atomic layers thick. Thus, it is only necessary to calculate the wave functions for thin helium layers.[25] This assumption is also supported by experimental studies of transmission into bulk helium under pressure. It was found[18] that the transmission coefficient was independent of pressure for liquid helium up to the freezing pressure of 25 bars. In addition, when the pressure was further increased so that the helium solidified, no change in transmission occurred to within the experimental accuracy of ±5%. These results are consistent with the view that the helium atoms which are important in determining the energy transfer are those very close to the solid surface. Because of the Van der Waals attraction of the helium to the solid, these atoms are effectively in a region of very high pressure, even when the bulk helium above them is not under pressure. Thus, any additional pressure of a few tens of bars produces very little change in the states of the atoms near to the surface, and hence, negligible change in transmission.

III. CALCULATION OF THE TRANSMISSION

Let the interaction between one solid atom and one helium atom at distance r be approximated by the Lennard-Jones potential

$$\epsilon_{S\text{-He}}[(a/r)^{12} - 2(a/r)^6] \;. \tag{29}$$

The depth of the well is $\epsilon_{S\text{-He}}$, and the minimum of the potential occurs for r equal to a. If the solid atoms have a density n_s and fill the region $z<0$, the potential for large positive z is

$$U_{S\text{-He}}(\vec{r}) \approx -\pi\epsilon_{S\text{-He}} n_s a^6/3z^3 \;. \tag{30}$$

Sabisky and Anderson[26] write the long-range part of $U_{S\text{-He}}$ in the form

$$U_{S\text{-He}}(\vec{r}) \approx -\phi_{S\text{-He}} \frac{d_{\text{He}}^3}{z^3} \;, \tag{31}$$

where d_{He} is the mean spacing of atoms in liquid helium (3.58 Å) and $\phi_{S\text{-He}}$ is a constant. The relation between $\phi_{S\text{-He}}$ and $\epsilon_{S\text{-He}}$ is thus

$$\epsilon_{S\text{-He}} = \frac{3\phi_{S\text{-He}} d_{\text{He}}^3}{\pi n_S a^6} \;. \tag{32}$$

Measurements by Sabisky and Anderson, and calculations by them based on the theory of Lifshitz give values for $\phi_{S\text{-He}}$ which are typically in the range 15–40 K. If we take a to be the same as the range of the helium-helium interaction (2.869 Å) $\epsilon_{S\text{-He}}$ comes out to be between $\phi_{S\text{-He}}$ and $2\phi_{S\text{-He}}$ depending on the value of n_s.

A. Longitudinal phonons

The potential near to the surface of the solid is a very complicated function of position and will depend on the orientation of the surface and on the crystal structure. In addition, many Kapitza experiments probably have involved crystals which are rough on the atomic scale. Our simplest model of the potential ignores these subtleties and takes the solid atoms as distributed continuously with uniform density in the region $z<0$. For this "continuum model" the potential for $z>0$ is

$$U_{S\text{-He}}(\vec{r}) = \frac{3\phi_{S\text{-He}}\, d_{\text{He}}^3}{a^3}\left[\frac{1}{45}\left(\frac{a}{z}\right)^9 - \frac{1}{3}\left(\frac{a}{z}\right)^3\right] . \tag{33}$$

The minimum of this potential is at $z=5^{-1/6}a$ and the depth of the minimum is

$$-\tfrac{2}{3}(5)^{1/2}\phi_{S\text{-He}}\left(\frac{d_{\text{He}}}{a}\right)^3 = -2.889\phi_{S\text{-He}} . \tag{34}$$

This potential is shown in Fig. 3 for $\phi_{S\text{-He}}=30$ K. Since the potential is independent of x and y, this model is inadequate to consider the transmission of transverse phonons.

For a single helium atom moving in the potential (33) the eigenfunctions and eigenvalues are

$$\psi_{\vec{k}i} = e^{i\vec{k}\cdot\vec{r}}\chi_i(z) \tag{35}$$

and

$$E(\vec{k}i) = \frac{\hbar^2 k^2}{2m} + \epsilon_i , \tag{36}$$

where $\vec{k}$ is a vector parallel to the surface and χ_i and ϵ_i satisfy

$$-\frac{\hbar^2}{2m}\frac{\partial^2\chi_i}{\partial z^2} + U_{S\text{-He}}(z)\chi_i = \epsilon_i\chi_i . \tag{37}$$

Thus, χ_i is an eigenfunction for motion normal to the surface. For a rigid oscillation of the surface, transitions can only occur between states of the same $\vec{k}$. Hence, the spectrum of values of ϵ_i determines the energies of those phonons that can be absorbed by the helium atom. In Fig. 3 we show some of the χ_i functions corresponding to low energies. Table I shows how the energies of the low-lying states vary when the strength of the potential is changed. The simplest model (model 1) for the helium is obtained by completely neglecting interactions between helium atoms. The ground state of the helium is then the state in which all particles have zero momentum parallel to the surface and are in the lowest-energy z state χ_0. This model has the unphysical property that all atoms are in states next to the surface. For real helium, on the other hand, one expects that the number of atoms per unit area of the surface will have some definite value N_S. N_S will be determined by a balance between the Van der Waals attraction of the solid which pulls atoms into the surface, and the repulsive force between helium atoms at close distances. This effect of the repulsive force is augmented by the increase in the zero-point energy of helium at high density. Thus, in order for a model which completely neglects interactions between helium atoms to be reasonable, the total number of atoms in the helium system must be chosen to be equal to N_SA. In this case the model is a crude representation of a surface covered by a monolayer. The transmission coefficient for longitudinal phonons at normal incidence then becomes

$$\alpha(\epsilon) = \frac{4\pi N_S\hbar}{\rho_S c_S \epsilon}\sum_{i\neq 0}\left|\langle\chi_0|\frac{\partial U_{S\text{-He}}}{\partial z}|\chi_i\rangle\right|^2\delta(\epsilon_0+\epsilon-\epsilon_i) . \tag{38}$$

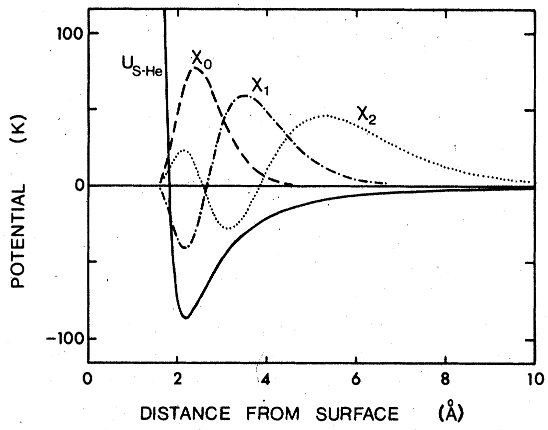

FIG. 3. "Continuum model" potential as a function of distance from the solid. The strength parameter $\phi_{S\text{-He}}$ equals 30 K. Also shown are the wave functions of the three lowest-energy eigenfunctions χ_i. The vertical scale for the χ_i is arbitrary.

We have evaluated this expression for several values of the strength of the Van der Waals force. For a given value of $\phi_{S\text{-He}}$, $\alpha(\epsilon)$ has a discrete spectrum at low frequencies (corresponding to transitions between bound states) and a continuous spectrum when $\epsilon+\epsilon_0$ is positive. Figure 4 shows α for $\phi_{S\text{-He}}$ equal to 20, 30, and 40 K. These results are plotted as a sequence of points at 5, 15, and 25 K, etc., which

TABLE I. Energy eigenvalues ϵ_i for motion normal to the surace as a function of the strength $\phi_{S\text{-He}}$ of the Van der Waals potential. These results are based on the potential (33).

Eigenvalue	Potential strength $\phi_{S\text{-He}}$ 20	30	40
ϵ_0	−31.4	−53.5	−76.6
ϵ_1	−8.0	−18.5	−31.3
ϵ_2	−1.4	−5.1	−10.9
ϵ_3	−0.1	−1.0	−3.1

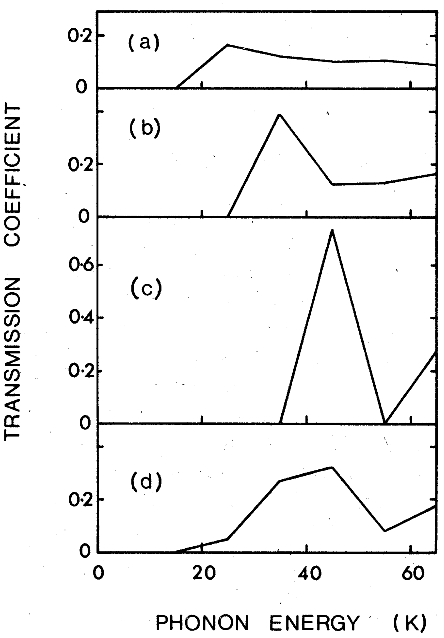

FIG. 4. Transmission coefficient as a function of energy. (a), (b), and (c) show results for the continuum potential (model 1) with $\phi_{S-\mathrm{He}}$ equal to 20, 30, and 40 K, respectively. The results for model 2, for which $\phi_{S-\mathrm{He}}$ has a range of values, is shown in (d).

represent the average value of α over a "box" 10 K wide around the point. The graphs are obtained by joining the points by straight lines. The eigenfunctions that correspond to the continuous spectrum were "quantized" by requiring that each χ_i be zero at 30 Å from the surface. The use of a truly continuous spectrum would have only a small effect on the results. As representative values we have taken $\rho_S = 3\,\mathrm{g\,cm^{-3}}$, $c_S = 4 \times 10^5\,\mathrm{cm\,sec^{-1}}$, and $N_S = a^{-2}$ in these calculations.

The structure in the results for α is somewhat unphysical, since, as mentioned above, the actual potential very near the solid surface will vary considerably with position along the surface. To simulate the effect of this variation we have also calculated α as the average transmission for a surface with a range of values of $\phi_{S-\mathrm{He}}$. Figure 4 includes the results obtained when it is assumed that the surface is equally divided into areas which have $\phi_{S-\mathrm{He}}$ values of 20, 30, and 40 K (model 2). The dip in transmission at 55 K would be removed if a continuous distribution of potential strengths were taken, and should be considered an artifact of the model.[27]

The calculated transmission for energy 30 K or greater is much larger than the acoustical-mismatch value. Between 30 and 60 K the average of α is about 0.2.

This model probably tends to underestimate the binding energy of the helium to the solid. For example, $\phi_{S-\mathrm{He}}$ is believed[26] to be 20.6 K for LiF. The use of the potential (33) with this value of $\phi_{S-\mathrm{He}}$ leads to a ground-state energy of −32 K. However, measurements by Houston and Frankl[28,29] give the value −65 K for a (100) surface. A model that leads to larger binding energies but has the same asymptotic value of the potential for large z is the following. Divide the solid up into planes parallel to the surface. Let the spacing between successive planes be d_S. Assume that in each plane the solid atoms are uniformly distributed. The last plane of atoms lies in the plane $z=0$. The potential for $z>0$ (i.e., outside the solid) is then

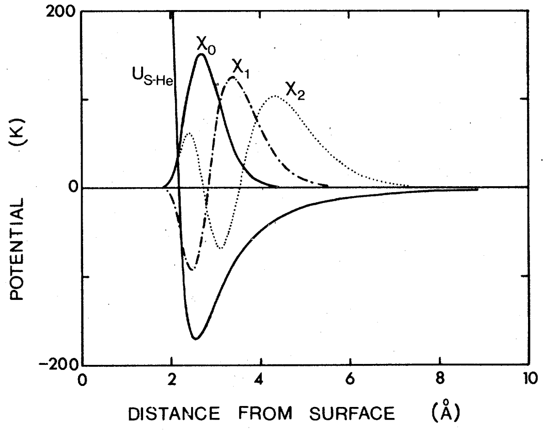

FIG. 5. "Planar model" potential as a function of distance from the solid. The strength parameter $\phi_{S-\mathrm{He}}$ equals 30 K. Also shown are the wave functions of the three lowest-energy eigenfunctions χ_i. The vertical scale for the χ_i is arbitrary.

$$U_{S-\mathrm{He}} = 3\phi_{S-\mathrm{He}} \frac{d_{\mathrm{He}}^3 d_S}{a^4} \sum_{p=0}^{\infty} \left[\frac{1}{5}\left(\frac{a}{z+p\,d_S}\right)^{10} - \left(\frac{a}{z+p\,d_S}\right)^{4} \right]. \tag{39}$$

For $\phi_{S-\mathrm{He}} = 30$ K and $d_S = 2.6$ Å this gives the potential and wave functions shown in Fig. 5. The energies of the lowest three states are −121, −56, and −22 K. For $\phi_{S-\mathrm{He}} = 20.6$ K the ground-state energy is −77 K which is reasonably close to the −65 K found for LiF by Houston and Frankl.[28] In Fig. 6 we show the results of the calculation of the phonon transmission $\alpha(\epsilon)$ when the potential (39) is used. This calculation assumes that equal areas of surface have $\phi_{S-\mathrm{He}}$ equal to 20, 25, 30, 35, and 40 K (model 3). Compared to model 2 there is a shift of the transmission to higher energies as expected from the above discussion of the depths of bound states.

These models have been presented as noninteracting models for the helium system. Another way to view them is as cell models. Consider a model in

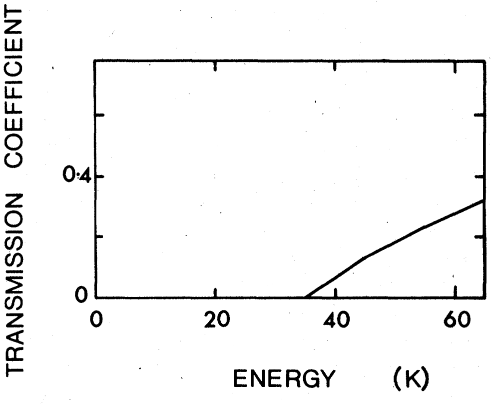

FIG. 6. Transmission coefficient as a function of energy for model 3.

which the surface of the solid is divided into square cells, each of side l such that

$$N_s l^2 = 1 . \tag{40}$$

Each cell contains one helium atom whose position in the x-y plane is constrained to be at the center of the cell. The wave function of the helium atom in the cell α with center at (x_α, y_α) is then

$$\psi_{\alpha i} = \delta(x - x_\alpha)\delta(y - y_\alpha)\chi_i(z) , \tag{41}$$

where χ_i satisfies Eq. (37). Calculation of the transmission for this model gives exactly the same transmission coefficient as for the model 2 or 3 when the appropriate potential for the motion in the z direction is used.

At low energy the transmission drops to zero because the phonons have insufficient energy to excite a helium atom to the first excited state. To consider the transmission in this range we must take account of the helium atoms in the second and subsequent layers. A crude model is based on the cell picture. Let each cell now contain n helium atoms, each of which can move only in the z direction. As mentioned before, it is necessary to put in some interaction between these atoms or the system will have the unphysical feature that all the atoms will be in the single-particle ground state. The simplest interaction (model 4) is to take an infinite-strength δ-function repulsion between helium atoms. Then the wave functions are obtained as follows. Choose n different single-particle eigenfunctions $\chi_i, \chi_j, \ldots$. For values of the coordinates $z_1, z_2, \ldots$ of the n particles such that

$$z_1 \leq z_2 \leq z_3 \leq \cdots \text{etc.} ,$$

the normalized wave function is the determinant

$$(n!)^{-1/2} \begin{vmatrix} \chi_i(z_1) & \chi_i(z_2) & \chi_i(z_3)\cdots \\ \chi_j(z_1) & \chi_j(z_2) & \cdots \\ \chi_k(z_1) & \cdots & \end{vmatrix} . \tag{42}$$

For other regions of space the wave function is either still given by Eq. (42), or differs from Eq. (42) just by an overall sign change. This sign change is made so that the wave function satisfies the requirements of Bose symmetry. The matrix elements for this wave function are also easy to calculate in terms of single-particle matrix elements. The transmission calculated for this model is shown in Fig. 7. The same form for the solid potential was used as in model 3. These results show several interesting features. The addition of the extra atoms per cell makes the transmission a more smoothly varying function of energy. The transmission at low energy is enhanced. Another very interesting feature is that for three atoms per cell the transmission is fairly insensitive to the strength $\phi_{S-\text{He}}$ of the substrate potential. This can be understood by the following argument, which is a highly simplified view of the problem but probably includes much of the essential physics. The atoms near the solid surface are in a strongly attractive potential and can only be excited to their first excited states by a very high-energy phonon. The atoms further away from the surface have lower excitation energies. When the surface of the solid oscillates at a frequency Ω, the atoms very near the surface will follow the motion of the surface adiabatically, because $\hbar\Omega$ is much less than the energy required to excite them. However, the disturbance will eventually reach a distance away from the surface such that the excitation energy is around $\hbar\Omega$. It is at this distance that the absorption takes place. When the strength of the solid potential is varied, the *distance* from the surface at which a phonon of a given energy can be absorbed will change. However, the actual magnitude of the absorption does not appear to be greatly affected.

B. Transverse phonons

To consider the absorption of a transverse phonon we must use a potential $U_{S-\text{He}}$ which has some dependence on the coordinates x and y that lie in the plane of the surface. However, it is tedious to solve the Schrödinger equation in three dimensions, even for only one helium atom. In addition, the approximation for the helium-helium interaction used in model 4 gives a simple solution only in one dimension. Accordingly, we consider the following highly simplified model. In general, the solid potential will be some complicated function $U_{S-\text{He}}(x,y,z)$ of x, y, and z. However, if the potential is strong, a helium atom will spend nearly all its time near where the potential is most negative. For each position on the surface there is a value of z, denoted by $z_{\min}(x,y)$, which minimizes the potential. We therefore make the approximation that the motion is two dimensional and governed by the effective potential

$$U_{\mathrm{eff}}(x,y) \equiv U_{S\text{-He}}(x,y,z_{\min}(x,y)) \ . \qquad (43)$$

Now we reduce the problem to one dimension, by dividing the surface into strips of width a, which run parallel to the direction $\hat{x}$ of the polarization vector of the transverse phonon. The atoms within a given strip are constrained to move in one dimension along the center of the strip.

A simple model for the x dependence of the potential in each strip is

$$U_{\mathrm{eff}}(x) = \phi_1 \cos(2\pi x/a) + \mathrm{const} \ . \qquad (44)$$

To estimate ϕ_1 note that the potential between a helium atom and a single solid atom has a depth of [see Eqs. (29) and (32)],

$$\epsilon_{S\text{-He}} = \frac{3\phi_{S\text{-He}} d_{\mathrm{He}}^3}{\pi n_S a^6} = 1.38\phi_{S\text{-He}} \ . \qquad (45)$$

This assumes $n_S = d_S^{-3}$. A helium atom just outside the solid surface will feel the attractive potential of a number of solid atoms, and the exact number will depend on the position on the surface. Thus, a rough guess at ϕ_1 is $2\phi_{S\text{-He}}$.

The single-particle states for the potential (44) are Bloch functions, and the band structures for ϕ equal to 20 and 80 K are shown in Fig. 8. We now assume the same sort of interaction between helium atoms as in model 4, and construct the many-particle wave function for each strip using Eq. (42). If the number of atoms per unit length of strip is a^{-1}, there will be one atom for each minimum of the potential (44). Thus, this corresponds to a crude model of a monolayer. In this model all of the single-particle states in the lowest energy band are used up to construct the many-particle ground state. We have calculated the transmission for this model (model 5). The surface was assumed to have the same distribution of values

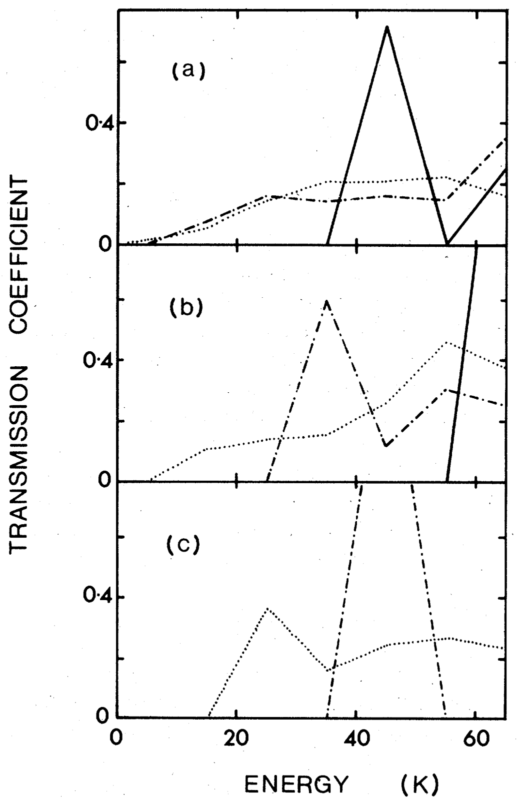

FIG. 7. Transmission coefficient as a function of energy for model 4. $\phi_{S\text{-He}}$ is equal to 20, 30, and 40 K in (a), (b), and (c), respectively. The solid line is the result for one particle per cell, and for two and three particles per cell the results are shown as dot-dash curves and dotted curves, respectively.

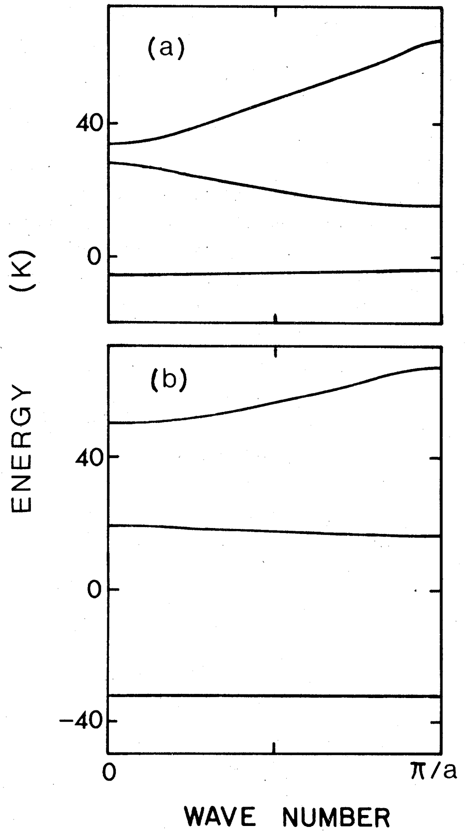

FIG. 8. Band structure for the potential (44) with ϕ, equal to (a) 20 K and (b) 80 K. The lowest three bands are shown.

of $\phi_{S\text{-He}}$ as in model 2. Thus, equal numbers of strips had $\phi_{S\text{-He}}$ equal to 20, 30, and 40 K, and therefore values of ϕ_1 of 40, 60, and 80 K, respectively. The transmission as a function of energy is shown as the solid line in Fig. 9. These calculations assume $\rho_S = 3\ \mathrm{g\,cm^{-3}}$ and $c_S = 3\times10^5\ \mathrm{cm\,sec^{-1}}$. The transmission has a large peak around 55 K, but this would be smeared out if a more smoothly varying distribution of potential strengths were taken, and hence, should be considered to be an artifact of the model.[27]

The transmission in this model is zero for phonons of energy below the band gap for the lowest value of ϕ_1 in the distribution. This band gap is 36 K. To get any transmission at lower energy one must consider more complicated models. It is clear that a second layer of helium atoms will be much more weakly bound to the solid surface, and will be able to absorb lower energy phonons. To treat this absorption, one can argue that for low-energy phonons the first layer of helium will oscillate rigidly with the solid surface (i.e., the whole layer will move with the same amplitude and phase as the solid surface). The potential $\tilde{U}_{\rm eff}(x,y,z)$ felt by the second helium layer will be the sum of the interactions with the solid and with the first helium layer, and since the first layer moves rigidly with the solid, the perturbation that acts on the second layer when the solid vibrates is just

$$u_S \hat{e}\cdot\nabla\tilde{U}_{\rm eff}\ .$$

Thus, to calculate the absorption of low-energy phonons by the second layer, one has to estimate the potential $\tilde{U}_{\rm eff}$ and then repeat the calculation that was done for the first layer, this time using this new potential. This calculation will only be correct below some cutoff energy ϵ_c at which the first layer of helium ceases to move rigidly. We have rather arbitrarily taken ϵ_c as 0.8 times the band gap. It is difficult to make a good estimate of $\tilde{U}_{\rm eff}$. The strength $\phi_{\rm He\text{-}He}$ of the Lennard-Jones potential of interaction between two helium atoms is 10 K. Thus, a repetition of the argument used for the first layer would give for the x dependence of $\tilde{U}_{\rm eff}$ the result

$$\tilde{U}_{\rm eff}(x) = \phi_2\cos(2\pi x/a) + \text{const}\ , \qquad (46)$$

with ϕ_2 about $2\phi_{\rm He\text{-}He}$. However, this argument ignores the potential due to the solid which tries to pull the second layer towards the first layer. This effect probably should increase ϕ_2. On the other hand, the effect of zero-point motion in the z direction of the second-layer atoms tends to move their mean position away from the solid. This should lead to a decrease in ϕ_2.

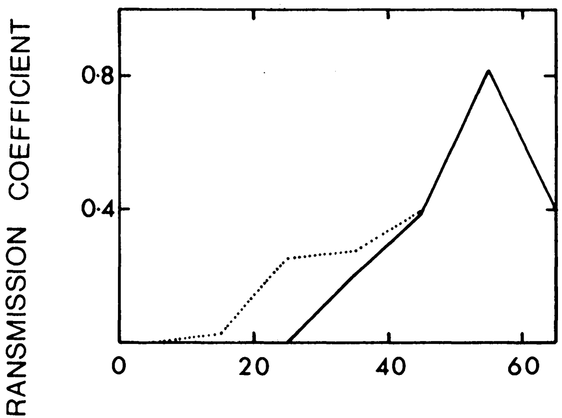

FIG. 9. Transmission coefficient as a function of energy for model 5 (solid line) and model 6 (dashed line). The large peak around 55 K would be smeared out if a more smoothly varying distribution of potential strengths were taken.

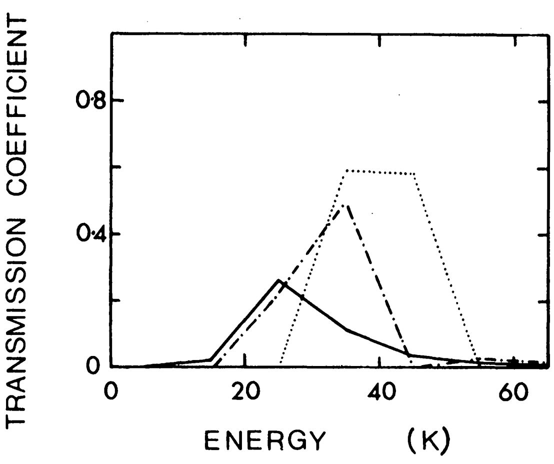

FIG. 10. Contribution to the transmission coefficient from a second layer. The solid, dashed, and dotted lines correspond to ϕ_2 equal to 10, 20, and 30 K, respectively.

The contribution to the transmission from the second-layer absorption is shown in Fig. 10 for ϕ_2 equal to 10, 20, and 30 K. These calculations do not include any cutoff energy ϵ_c at the high-energy end. The transmission for a two-layer helium model (model 6) is shown as the dashed line in Fig. 9. The first layer in this model has the same distribution of values of ϕ_1 as model 5. The second layer has ϕ_2 equal to 20 K. Below ϵ_c only the second layer contributes to the transmission, and above ϵ_c only the first layer contributes.

The addition of a second layer substantially increases the transmission in the energy range 20–30 K, and in this energy range the magnitude of the transmission is of the same order of magnitude as the typical experimental values. At lower energies, however, the transmission drops off very rapidly, and is zero below 19 K. This is therefore inconsistent with the majority of the experimental results which indicate a large transmission down to about a 5-K energy. One might try to get an increased transmission at low energy by adding further helium layers. It is hard to see how to calculate the effect of more helium by any simple extension of the present method. Another way in which one might hope to get an enhanced transmission at low energy is through the use of a nonperiodic potential instead of a cosine. This would then get rid of the band gap, and would make possible the adsorption of low-energy phonons even by a single layer of helium. There is certainly no reason to believe that the actual potential is periodic (except in the case of a very ideal perfect surface), and so this approach appears attractive. However, we have investigated the transmission for several nonperiodic potentials and have found that the transmission at low energy is not significantly enhanced. In fact, one can show fairly rigorously (see Sec. IV) that the experimentally observed anomalous transmission at low energy cannot be explained by the addition of another helium layer or by tinkering with the potential.

IV. APPLICATION OF SUM RULES

In this section we want to consider the following question: Can a more sophisticated model for the helium system give a transmission coefficient which agrees with the results found in most experiments? By "most experiments" we mean those experiments in which a large anomalous transmission is observed, i.e., all experiments except the recent measurements of Weber *et al.*[22] In most experiments a large transmission (e.g., 0.1–0.5) is observed at all energies above about 5 K. In our calculations as developed so far, however, the transmission is large only above about 25 K. Thus, we would like to know whether or not a more sophisticated model for the helium can extend the range of large transmission down to 5 K. There are several obvious deficiencies of our models that one could try to correct. Thus, for example, one could try to include the true helium-helium interaction instead of the δ-function repulsion. Another weakness of the models is that they are all one dimensional. Thus, two helium atoms are never able to pass each other and there can be no "backflow" effects that are known to be important in determining the properties of rotons. Yet another defect is the absence of more complicated motions of the helium atoms, such as tunneling between two positions of nearly equal energy.[30] Tunneling is a particularly attractive possibility because it leads naturally to low-energy states, and it appears that a phonon should couple well to these states.

However, we can show that although these physical effects may in fact occur within the helium system, they cannot lead to a large anomalous transmission at low energies. This result follows very directly from the sum rules that were derived in Sec. II. Consider the negative-moment sum rules (23)–(25). The interpretation of these sum rules is clearly more complex when there is bulk helium on the surface since the number N of helium atoms is effectively infinite. But for a helium film of finite thickness the application of the sum rules is straightforward. The Kinder and Dietsche experiments[7] have shown that the transmission coefficient $\alpha_{\mathrm{exp}}(\epsilon)$ is approximately 0.6 for slow transverse phonons in the energy range 6–42 K going from germanium into a three-layer helium film. A lower bound on the left-hand side of the sum rules can therefore be obtained if we make the approximation

$$\alpha_{\mathrm{exp}}(\epsilon)=\begin{cases}0, & \epsilon\leqslant 6\text{ K},\\ 0.6, & 6<\epsilon\leqslant 42\text{ K},\\ 0, & 42<\epsilon .\end{cases} \tag{47}$$

This gives

$$\int_0^\infty \alpha_{\mathrm{exp}}(\epsilon)\epsilon^{-1}\,d\epsilon \geqslant 1.17\text{ K}, \tag{48}$$

$$\int_0^\infty \alpha_{\mathrm{exp}}(\epsilon)^{-2}\,d\epsilon \geqslant 0.086\text{ K}^{-1}, \tag{49}$$

and

$$\int_0^\infty \alpha_{\mathrm{exp}}(\epsilon)\epsilon^{-3}\,d\epsilon \geqslant 0.0082\text{ K}^{-2}. \tag{50}$$

Since these are lower bounds on the left-hand sides, the right-hand sides of the sum rules must be larger than these values. The right-hand side is most easily estimated for the ϵ^{-2} sum rule, since this just involves the total number of helium atoms. For a three-layer film a reasonable estimate of the number of atoms per unit area is

$$\frac{N}{A}=\frac{3}{d_{\mathrm{He}}^2}=2.3\times10^{15}\,\mathrm{cm}^{-2}, \tag{51}$$

where d_{He} is the mean spacing of atoms in bulk helium. For germanium $\rho_S=5.34\,\mathrm{g\,cm^{-3}}$ and $c_S=2.77\times10^5\,\mathrm{cm\,sec^{-1}}$. Thus, the theoretical transmission coefficient $\alpha_{\mathrm{th}}(\epsilon)$ must satisfy

$$\int_0^\infty \alpha_{\mathrm{th}}(\epsilon)\epsilon^{-2}\,d\epsilon=\frac{2\pi Nm}{\rho_S c_S A\,\hbar}=0.0085\text{ K}^{-1}. \tag{52}$$

We have assumed in this calculation that the helium atoms in the gas can be ignored in the estimate of N/A. There are several pieces of evidence that support this view. For example, Guo and Maris[9] have measured the transmission from silicon into thin films of helium at temperatures of 1.85 and 3.35 K. For films of the same thickness the transmission at the two temperatures was the same. However, the gas densities at the two temperatures differed by several orders of magnitude. This strongly suggests that the transmission is determined by the properties of the film, and is unaffected by the amount of gas present. One can understand this by a rough estimate of the kinetics of the process. In Kinder and Dietsche' experiments[7] the temperature was 1.0 K, and a three-layer film was produced by a pressure of 49 m Torr. Thus the gas density was $n_G = 5 \times 10^{16}$ cm^{-3}. Now suppose that when a phonon is incident on the surface, the time that it takes for the absorption of energy to occur is τ. The number of gas atoms that make contact with unit area of the film during τ is of the order of $n_G \tau v_G$, where v_G is the mean speed of an atom in the gas. If we take $v_G = 10^4$ cm sec^{-1}, and $\tau = 10^{-11}$ sec (the period of oscillation of a 5-K phonon) we have

$$n_G \tau v_G \sim 5 \times 10^9 \text{ cm}^{-2} \ .$$

This is much less than the number of atoms per unit area in the film.

Different models for the helium system will lead to different results for $\alpha_{\text{th}}(\epsilon)$, but must always satisfy Eq. (52), provided that the number of helium atoms is always the same. Thus, since Eqs. (49) and (52) are in conflict, it is impossible to obtain agreement with experiment for $\alpha(\epsilon)$ for all energies, *regardless of the precise model assumed for the helium.* This result implies that to explain the transmission that is observed at low energies, it is necessary to reconsider the assumptions that led to the sum rule (24). This will be considered in more detail later in this section. The important point that comes out of the sum rule is that we cannot blame the lack of agreement of experiment and theory at low energies on the inadequacies of the models we have used for the helium.

This difficulty is revealed most clearly in the ϵ^{-2} sum rule we have considered in detail. This is because the right-hand side has a definite value, independent of any assumptions about the helium states. One can see signs of the same problem in the ϵ^{-3} sum rule, although now one has to make some assumptions about the helium. This rule is

$$\int_0^\infty \alpha_{\text{th}}(\epsilon)\,\epsilon^{-3}\,d\epsilon = \frac{4\pi N^2 m^2}{\rho_S c_S A\,\hbar^3} \times [\langle 0|(\hat{e}\cdot\vec{R})^2|0\rangle - \langle 0|\hat{e}\cdot\vec{R}\,|0\rangle^2] \ , \tag{53}$$

where $\vec{R}$ is the position of the center-of-mass. Let us try and construct a model of the helium that will lead to a large value of the right-hand side so that the experiments will not violate the sum rule. Assume that each of the helium atoms in one layer is fluctuating between two positions a distance ζ apart, and that there is no correlation between the fluctuations of the different atoms. We consider the direction of the vector between these positions to lie in the plane of the surface, but to be randomly oriented in the plane. Thus, this model corresponds to tunneling of helium atoms between some sites lying in a plane parallel to the surface. We consider a transverse phonon with $\hat{e}$ parallel to the x direction. Then the sum rule gives

$$\int_0^\infty \alpha_{\text{th}}(\epsilon)\,\epsilon^{-3}\,d\epsilon = \frac{\pi N_1 m^2 \zeta^2}{2\rho_S c_S A\,\hbar^3} \ , \tag{54}$$

where N_1 is the number of atoms in the layer. If we choose N_1 to be a^{-2}, i.e., 1.21×10^{15} cm^{-2}, the result is

$$\int_0^\infty \alpha_{\text{th}}(\epsilon)\,\epsilon^{-3}\,d\epsilon = 9.2 \times 10^{-5} \zeta^2 \text{ K}^{-2} \ , \tag{55}$$

where ζ is in Å. Thus, in order that the sum rule not be violated ζ must be greater than 9.5 Å. This is an unreasonably large distance for every helium atom in a plane to be tunneling.

We now reconsider the assumptions that led to the sum rules. It was assumed that the transmission coefficient was small, so that for a phonon at normal incidence on a clean surface the amplitude of oscillation of the surface was twice the amplitude of the incident phonon. Any reasonable correction to allow for the finite transmission coefficient of the phonon will reduce the amplitude of the surface oscillation, and hence, will give a lower transmission. This only makes the sum-rule violation worse. A second assumption was that we could calculate the phonon transmission into helium at zero temperature. To derive sum rules for nonzero temperatures one has to go back to Eq. (15) for the rate at which energy is transmitted into the helium and repeat the calculations. It turns out that the sum rule (52) should still hold in this case, and so a finite temperature should not eliminate the sum-rule violation.

Another important assumption is implicit in the way we have set up the problem. The phonon incident on the interface has been treated classically, and constitutes a classical driving force of frequency Ω which acts on the helium. Thus, when the helium is initially in its ground state the only sort of transition that is possible is one in which the helium absorbs energy $\hbar\Omega$. In a more general theory the solid should be treated quantum mechanically. If this is done, the resulting expression for the probability of absorption of energy $\hbar\Omega$ by the helium is the same as the one we have obtained by considering the solid classically. However, it is also possible for the helium to absorb only a certain part of the energy of the incident phonon, and for a phonon of lower energy $\hbar\Omega'$ to return into the solid. We have estimated the magnitude of this type of process and find that it is smaller than the simple absorption process considered here by at least one order of magnitude. Higher-order processes in which several low-energy phonons are produced in the solid are also possible. However, processes of this type tend to give a very small contribution to the energy transfer. For each extra phonon involved, extra powers of ρ_S and c_S enter into the denominator of the expression for the rate of energy transfer. ρ_S and c_S are large quantities on the scale of the corresponding parameters for the helium system.

As far as we can see the weakest points in the derivation of the sum rules are the assumptions that the surface of the solid is clean, and that the surface moves rigidly. We consider the effect of these assumptions in the following situations.

1. Clean and perfect surface

By a clean and perfect surface we mean a surface which is free of adsorbed gas or dirt, and on which the atoms have an ordered crystalline arrangement. When a long wavelength phonon is incident on such a surface the surface will certainly move rigidly as a first approximation. However, there will also be a small oscillatory strain at the surface. An oscillatory strain (or more generally any motion of different solid atoms relative to each other) has the possibility of being an important mechanism for energy transfer to the helium for the following reason. A *rigid* motion of the surface of the solid means that the helium is being "shaken." For a low-frequency oscillation, the helium follows the motion of the surface nearly adiabatically, and absorbs very little energy. It is for this reason that the matrix elements of the "displacement perturbation" are very small at low frequency [see Eqs. (18) and (19)]. However, *relative* motion of different surface atoms of the solid induces a more complicated oscillatory distortion of the helium which is more likely to lead to energy transfer.

The simplest sort of strain to consider is an oscillatory density change, i.e.,

$$\delta\rho/\rho = \eta_0 \cos(\Omega t + \phi) \ . \tag{56}$$

We assume that the magnitude η_0 and the phase ϕ of the strain are constant at all points within some distance ζ of the surface. Then, if ζ is considerably bigger than the range parameter a in the Van der Waals potential the perturbation that acts on the helium is just

$$\delta H_{\mathrm{str}}(\vec{r},t) = \eta_0 U_{S\text{-He}}(\vec{r}) \cos(\Omega t + \phi) \ , \tag{57}$$

where $U_{S\text{-He}}(\vec{r})$ is the potential exerted by the solid on a helium atom at point $\vec{r}$. This assumes that the Van der Waals forces are additive (this is not generally true), and therefore that the total potential is proportional to the density. Equation (57) only holds near the surface, i.e., roughly within a distance ζ of the surface. The contribution to the transmission coefficient from the perturbation (57) is

$$\alpha_{\mathrm{str}} = \frac{\pi \eta_0^2 \hbar}{\rho_S c_S u_0^2 \epsilon A} \sum_i |\langle i | U_{S\text{-He}}(\vec{r}) | 0\rangle|^2 \times \delta(E_0 + \epsilon - E_i) \ . \tag{58}$$

The magnitude of the strain at the surface is hard to estimate. The simplest assumption is to consider that the helium constitutes a very light loading of the surface, and so the normal component of the stress tensor must vanish at the surface. With this assumption the oscillating density change at the surface is zero for longitudinal and transverse waves at normal incidence on a surface of an elastically isotropic crystal. The density change is also zero at a surface of an anisotropic crystal provided the surface is a high symmetry plane. For phonons which are not at normal incidence, or which are incident on surfaces which are not symmetry planes, the density change will be given by Eq. (56) with

$$\eta_0 = b u_0 \Omega / c_S \ , \tag{59}$$

where b is a numerical constant of order unity. Then we have

$$\alpha_{\mathrm{str}} = \frac{\pi b^2 \epsilon}{\rho_S c_S^3 A \hbar} \sum_i |\langle i | U_{S\text{-He}}(\vec{r}) | 0\rangle|^2 \times \delta(E_0 + \epsilon - E_i) \ . \tag{60}$$

This leads to the sum rule

$$\int_0^\infty \alpha_{\mathrm{str}} \epsilon^{-1}\, d\epsilon = \frac{\pi b^2}{\rho_S c_S^3 \hbar A} \langle 0 | U_{S\text{-He}}^2(\vec{r}) | 0 \rangle \ . \tag{61}$$

The experiments of Kinder and Dietsche show that for transverse phonons in germanium the left-hand side has a value greater than 1.17 [see (48)]. Most of the phonons in this experiment were incident on a (110) surface at near normal incidence, so the largest value one can possibly expect for b is 1. We have estimated the expectation value of $U_{S\text{-He}}^2$ from the various models considered in Sec. III. The results vary from model to model, but the general conclusion is that the probable value of the right-hand side is around 0.02. It is most unlikely that it can be greater than 0.1. Thus, the sum rule is still violated by the experimental results. Note again that the use of the sum rule effectively preempts an explanation in terms of pecularities of the states of the helium atoms, since, for example, the expectation value of $U_{S\text{-He}}^2$ is not greatly affected if it is assumed that tunneling of the helium atoms takes place.[30]

2. Clean but damaged surface

For a damaged surface some new possibilities arise. The oscillating strain due to the incident phonon may cause some atoms *of the solid* to undergo relatively large displacements. These large displacements could lead to a much larger perturbation acting on the helium than the simple perturbation caused by the density change discussed above. It is very hard to give a serious estimate of this effect without detailed knowledge of the typical state of a damaged surface. The sort of displacement we are thinking of might arise from tunneling of a solid atom from one position to another. Another possibility is the motion of dislocations lying near the surface or intersecting the surface. We have not attempted to estimate the number of atoms moving in this way, and this number must in fact depend in a sensitive way on the details of the surface.

3. *Dirty surfaces*

The difficult question is—how dirty are the surfaces that have been used in most of the Kapitza resistance and phonon reflection experiments? Very little is known about the surface in most of the experiments. Generally, the surfaces have been polished in some way (chemically or mechanically) and have then been washed in a solvent (e.g., acetone, alcohol, or water). These surfaces will certainly not be clean in the atomic sense.

For a surface covered by a single layer of small molecules (oxygen, for example), one might anticipate a situation rather similar to a damaged surface, especially if the layer is chemisorbed. One expects that the majority of the adsorbed molecules would move almost rigidly with the solid, and so one can consider them as simply changing the effective potential seen by the helium system. However, there is the possibility that some of the molecules could undergo larger oscillations (e.g., of the tunneling type) and that these could couple energy to the helium.

Probably most of the surfaces[31] do have a significant coverage of larger molecules. These originate in the "cleaning" process or in subsequent handling. These molecules will seriously affect the sum rules and the results for the transmission coefficient in at least two ways. Let us first consider the dirt (Fig. 11) as a layer of elastic material of thickness L, density ρ_D and sound velocity c_D. When a phonon of frequency Ω is incident from the solid side of the dirt, the dirt will move rigidly in phase with the solid surface only if the phonon wavelength in the dirt is very long compared to the dirt thickness. Otherwise the oscillation is more complicated and the sum rules do not hold. The simplest way to treat this problem is to assume that the transmission into the helium is still fairly small, so that the stress at the surface of the dirt in contact with the helium is zero. Then it is straightforward to show that if the amplitude of the incoming phonon is u_0, the oscillation of the surface of the dirt has an amplitude

$$u_D = 2u_0[1-(1-Z_D^2/Z_S^2)\sin^2(\Omega L/c_D)]^{-1/2}\ , \qquad (62)$$

where $Z_D = \rho_D c_D$ and $Z_S = \rho_S c_S$ are the acoustical impedances of the dirt and of the solid. If the dirt consists of organic molecules, a reasonable value of ρ_D is a 1 $\mathrm{g\,cm^{-3}}$, and c_D might be 10^5 $\mathrm{cm/sec^{-1}}$ for transverse waves and 2×10^5 $\mathrm{cm/sec^{-1}}$ for longitudinal.

The dirt increases the oscillatory displacement seen by the helium for all phonon frequencies, since it is always true that

$$u_D \geqslant 2u_0\ . \qquad (63)$$

A large increase in amplitude occurs if the dirt is thick enough so that L is compareable to $\pi c_D/2\Omega$. For a 5-K energy phonon this requires $L = 24$ Å for transverse waves and 48 Å for longitudinal waves. These would be rather thick layers of dirt, but are not inconceivable. Since Z_D is considerably less than Z_S, u_D as given by Eq. (62) has large oscillations. However, one expects that for actual dirty surfaces the thickness varies considerably from place to place and so it makes sense to average (in the rms sense) u_D over a range of thicknesses (or equivalently a range of phonon frequency). The result of this averaging is

$$\langle u_D^2\rangle = (2u_0)^2 Z_S/Z_D\ . \qquad (64)$$

Thus, the mean-squared amplitude of the surface of the dirt is increased by a factor Z_S/Z_D relative to the mean-squared amplitude of the corresponding clean surface of the solid. This factor might typically be of the order of 10. This enhancement, of course, only holds for phonons for which $\pi c_D/2\Omega$ is comparable to, or larger than, the average dirt thickness. As a specific example consider the measurements of Kinder and Dietsche[7] on germanium which we discussed earlier in the contest of the sum rules. For transverse waves they found a transmission coefficient of 0.6 in the energy range 6–42 K. In order for the enhancement effect to work down to 6 K, the dirt layer must have a thickness of at least 20 Å. Germanium has $Z_S = 1.48\times10^6\ \mathrm{g\,cm^{-2}\,sec^{-1}}$,

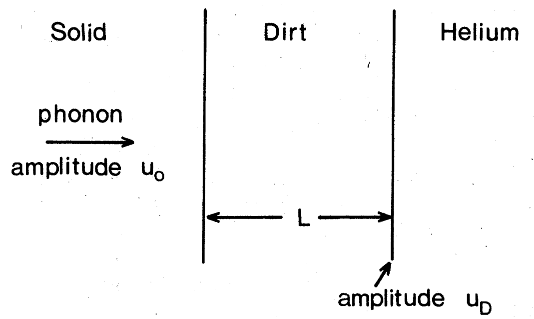

FIG. 11. Solid surface covered by a layer of dirt of thickness L.

whereas for transverse waves a reasonable value of Z_D is $10^5\ \mathrm{g\,cm^{-2}\,sec^{-1}}$. Thus, the ϵ^{-2}-sum rule Eq. (52) now becomes

$$\int_0^\infty \alpha(\epsilon)\epsilon^{-2}\,d\epsilon=\frac{2\pi Nm}{Z_D A\,\hbar}=0.126\ \mathrm{K}^{-1}\ . \tag{65}$$

Note that the value for the sum rule is independent of the acoustical impedance of the solid, and only depends on the acoustical impedance of the dirt. The experimental results of Kinder and Dietsche are not inconsistent with this sum rule. Their data in the range from 6–42 K gave a contribution of the left-hand-side integral of $0.086\ \mathrm{K}^{-1}$, which is less than the sum-rule prediction for the integral over the complete energy range. In fact, one can make the stronger argument that the data are in reasonable agreement with the sum-rule predictions. Below 6 K other data[6] (admittedly not measurements on germanium) indicate that $\alpha(\epsilon)$ begins to drop off rapidly, and so the sum-rule contribution in the energy range 0–6 K should not be large (certainly no larger than the contribution from 6–42 K). Even if α remains constant at 0.6 above 42 K the contribution to the integral above 42 K is very small because of the ϵ^{-2} factor. Thus a reasonable "experimental" estimate of the left-hand side of the sum rule is $0.1–0.2\ \mathrm{K}^{-1}$. This is in rough agreement with our estimate of the right-hand side.

A second way in which the sum rules may be modified is the following. If the surface is covered with large molecules, it may be wrong to think of the dirt and the helium systems as having a definite boundary. By this we mean that the dirt molecules may not be closely packed, and therefore the helium may penetrate between them. This would increase the number of helium atoms to which energy could be transferred, and raise the transmission coefficient. One expects that dirt with helium inside it would constitute a highly absorbing layer for phonons. Transmission of energy from the solid to the liquid helium could be considered as a two-step process. A phonon from the solid enters the dirt layer, and excites a helium atom inside the layer. This helium atom then returns to its ground state and produces another phonon (or phonons). This phonon may then either be transmitted into the liquid helium or may return to the solid. A similar phenomenological picture has been put forward by Cheeke and Ettinger.[32] An important difference is that their absorbing layer was the first layer of helium which they considered as a solid layer, whereas our layer is the surface dirt plus helium that it contains.

V. SUMMARY AND CONCLUSIONS

In this paper we have reported on the results obtained from a number of simple calculations of the transmission of phonon energy across interfaces between solids and liquid helium. For perfect clean surfaces the calculated phonon transmission coefficient at low energies ($\epsilon < 20$ K) is small (typically less than 0.1) and decreases with decreasing energy. At higher energies ($\epsilon > 30$ K) the transmission coefficient varies more slowly with energy. The transmission at high energy is found to be fairly insensitive to the strength of the Van der Waals potential binding the helium to the solid. The principal dependence of the transmission at high energy (30–60 K) on the properties of the solid can be described roughly by the law

$$\alpha \propto \mathrm{const}/\rho_S c_S\ . \tag{66}$$

The value of the constant is roughtly 3×10^5 or 4×10^5 cgs units.

The transmission coefficient satisfies several sum rules. These sum rules show that, given certain reasonable assumptions, the transmission at low energies for ideal surfaces must be small regardless of the physical nature of the states of the helium atoms near the surface.

The only measurements that have so far been made on very perfect surfaces are those of Weber *et al.*[22] Their data is just at the one energy 14 K. They find a very small transmission. It would be very interesting to have data over a wide range of energies, to see if our prediction that the transmission becomes larger above about 25 K is correct.

For dirty or damaged surfaces it is very hard to estimate the transmission because so little is known about the surfaces. We have argued that if there is a thick layer (e.g., 20 Å) of low-density low-velocity material on the surface the typical results that are found for dirty surfaces are understandable. Whether or not the surfaces that have been used really are this dirty should be capable of experimental verification. The dirt on the surface has at least two effects. It increases the amplitude of oscillation seen by the helium, and it may also be penetrated by the helium to form a highly attenuating system.

All of our calculations consider simply the excitation of single atoms or small groups of atoms at the surface. We have not attempted to calculate the type of excitations that should emerge in the bulk liquid helium (e.g., as rotons or as phonons), or the energy or momentum distribution of these excitations. Also, we have not calculated the transmission into hydrogen, or other materials. We hope to consider these problems in a future paper.

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[24] For a phonon (longitudinal or transverse) at normal incidence the strain vanishes at the surface if the loading effect of the helium is ignored. However, in the general case of a phonon at an arbitrary angle of incidence Eq. (7) is correct.

[25] Note, however, that the experiments of Refs. 7–9 presumably involve dirty surfaces, whereas we are attempting here to calculate the transmission for a clean surface. Thus, we are making an implicit assumption that both clean and dirty surfaces behave the same way as far as the dependence of transmission of film thickness is concerned.

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