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EXACT THEORY OF LONG-WAVELENGTH ONE-PHONON AMPLITUDES IN ATOM-SURFACE SCATTERING

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Exact Theory of Long-Wavelength One-Phonon Amplitudes in Atom-Surface Scattering

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ABSTRACT: We derive an expression for the probability of creating or annihilating one long-wavelength surface or bulk phonon during a scattering event, which depends on the bulk elastic constants but is independent of the details of the atom-target potential and of force constant changes near the surface. This expression is exact if the inelastic scattering is "weak" (the meaning of which is explained in the text). This theory should be experimentally verifiable, e.g. for 20 meV He atoms scattered from a W-surface.

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Introduction

Previous theoretical work on one-phonon processes has been based on (a) approximate force constants between both bulk and surface target atoms[1,2], (b) approximate atom-target interaction potentials[3,4,5,6,7] (usually a sum of pairwise potentials[3,4,5,6]) and (c) use of the distorted wave Born approximation[8,7,3,4,5,6].

This work shows that the creation (or annihilation) of *long-wavelength* phonons is independent of (1) changes of force constants in the surface region of the unperturbed target and (2) the functional form of the atom-surface interaction potential $V(\vec{r};\{\vec{u}_i\})$ where $\vec{r}$ is the position of the colliding atom and $\vec{u}_i$ the displacement of the ith target atom. The only requirements are that the target force constants reproduce correctly the bulk elastic constants and that the inelastic scattering is "weak"[9].

Therefore any disagreement between theory and experiment for long-wavelength phonons cannot be attributed to inadequacies of force constants or the interaction potential, nor can agreement be regarded as confirmation of approximations (a) or (b). *Short-wavelength* processes do provide tests of (a) and (b). Much of the published theoretical and experimental work gives only relative intensities of one-phonon processes as functions of momentum transfer[3,4,5]. Our work, which gives exact results for the intensity of long-wavelength processes, allows the determination of an absolute intensity scale. Our theory also shows that the use, in scattering calculations, of an effective incident energy which includes the well depth is not applicable to long-wavelength single-phonon processes. This correction, introduced by Beeby to estimate the Debye-Waller factor[10], has been used also for calculating the differential cross-section[11,12].

We now present a heuristic explanation of why the probability for the weak inelastic creation of a long-wavelength phonon is entirely determined by the bulk elastic constants of the target.

The displacements in the surface region associated with a (surface or bulk) phonon of small wave-vector $\vec{q}$ are locally rigid with a coherence length of q^{-1} both parallel and perpendicular to the surface. The restoring forces reside mainly in the interior (if $qa \ll 1$, where a is the lattice constant) and are determined by the static bulk elastic constants. Changes of the force constants in a few layers near the surface are irrelevant to the quasi-rigid displacements in the surface region.

To understand why the functional form of V is irrelevant we consider (for simplicity) a surface with negligible corrugation. The first-order-distorted-wave-Born approximation matrix element, adequate for weak scattering, is given to lowest order in qa by

$$M_{\vec{K}+\vec{Q},E\pm\hbar\omega;\vec{K},E} \approx \left(\Psi_{\vec{K},E}\,,\frac{\partial V(z)}{\partial z}\Psi_{\vec{K},E}\right) \tag{1}$$

provided that $qa \ll 1$. Here $V(z) = V(z;\{\vec{0}\})$, $\vec{Q}$ and ω are the parallel momentum and frequency of the phonon, and $\vec{K}$ and E are the parallel momentum and energy of the incident particle. If $\Psi_{\vec{K},E}$ is normalized to unit incident perpendicular flux, the right hand side represents the total force exerted by the rigid target per unit time and area. This is rigorously given by the change of perpendicular momentum per unit time and area, i.e.

$$\left(\Psi_{\vec{K},E}\,,\frac{\partial V(z)}{\partial z}\Psi_{\vec{K},E}\right) = -\Delta(\hbar k_z) = -2\hbar k_z \tag{2}$$

independent of the functional form of $V(z)$.

Our results are exact in the limit where the following conditions are satisfied (in addition to $qa \ll 1$):

$$\frac{\hbar}{M\bar{c}b} \ll 1 \quad (3a) \qquad \frac{m}{M}\left(\frac{V_o}{\hbar\omega_D}\right)^2 \ll 1 \quad (3b) \qquad E \lesssim \hbar\omega_D \quad (3c) \qquad k_BT \lesssim \hbar\omega_D \quad (3d)$$

Here $\bar{c}$ is a characteristic velocity of a phonon in the target, b is the range of the atom-target potential[13] and V_o is its depth. m is the mass of the colliding atom, M is the mass of a target atom, ω_D is the Debye frequency, and T is the temperature of the target.[14]

The condition (3a) allows one to stop the expansion of V after the first order term

$$V(\vec{r};\{u_i\}) = V(z) + \vec{u}_i \cdot \nabla_{\vec{u}_i} V(\vec{r};\{0\}) \tag{4}$$

Condition (3b) ensures that in calculating the inelastic scattering, the last term in (4) can be treated to lowest order (Fermi's golden rule). The equations (3a) and (3b) are derived in detail in the appendix.

Derivation of the Probability for Production of Long-Wavelength Phonons

To simplify the presentation, we will make the following assumptions in this section (see concluding remarks): (1) negligible diffraction scattering; (2) isotropy of the target; (3) interaction only with the uppermost layer of target atoms. The units are chosen so that the volume of the target and the area of the interacting surface of the target are 1.

To calculate the one-phonon amplitude we divide the Hamiltonian into an unperturbed Hamiltonian H_o, which ignores phonon coupling to the colliding atom, and H_1, which couples the atom linearly to the phonons[8].

$$H = H_{particle} + H_{target} + V(\vec{r};\{\vec{u}_i\}) = H_o + H_1 + \mathcal{O}(u^2) \tag{5}$$

where

$$H_o = \frac{p^2}{2m} + \sum_{\vec{q},\nu} \hbar\omega_{\vec{q},\nu}(a^\dagger_{\vec{q},\nu}a_{\vec{q},\nu} + \frac{1}{2}) + V(z), \qquad H_1 = \sum_{i,\alpha} \frac{\partial V}{\partial u_{i,\alpha}}(\vec{r})u_{i,\alpha} \tag{6}$$

Here α denotes a cartesian coordinate, $\vec{q}$ is the wavevector of a phonon and ν is its branch.

The colliding atom wavefunctions in the potential $V(z)$ have the form $\Psi_{\vec{K},E}(\vec{r}) = e^{i\vec{K}\cdot\vec{R}}\phi_{\vec{K},E}(z)$ for atom energy E. $\vec{K}$ is momentum parallel to the surface, and $\vec{R}$ is displacement parallel to the surface. $\phi_{\vec{K},E}(z)$ satisfies the equation

$$\left[-\frac{\hbar^2\partial_z^2}{2m} + V(z) - (E - \frac{\hbar^2K^2}{2m})\right]\phi_{\vec{K},E}(z) = 0. \tag{7}$$

$\phi_{\vec{K},E}(z)$ has the asymptotic form $(m/\hbar k_z)^{\frac{1}{2}}\left[e^{-ik_z z} + A_o e^{ik_z z}\right]$ as $z \to \infty$, where $k_z^2 + K^2 = 2mE/\hbar^2$.

Before calculation, we expand the $\vec{u}_i$ in normal modes,

$$H_1 = \sum_{i,\alpha,\vec{q},\nu} \frac{\partial V}{\partial u_{i,\alpha}}(\vec{r}) u_{\vec{q},\nu,\alpha} e^{-i\vec{q}\cdot\vec{R}_i} \quad + \text{h.c.} \tag{8}$$

which, for convenience, we rewrite as

$$H_1 = \sum_{\vec{q},\nu,\alpha} e^{-i\vec{q}\cdot\vec{R}}\, u_{\vec{q},\nu,\alpha} \sum_i \frac{\partial V}{\partial u_{i,\alpha}}(\vec{r})\, e^{-i\vec{q}\cdot(\vec{R}_i - \vec{R})} \quad + \text{h.c.} \tag{9}$$

If the wavelength of the phonon is much larger than the range of the coupling potential (similar to a and b), $\partial V/\partial u_i$ vanishes unless $q(R_i - R) \ll 1$ and the second exponential can be ignored. This yields

$$H_1 = \sum_{\vec{q},\nu,\alpha} e^{-i\vec{q}\cdot\vec{R}} u_{\vec{q},\nu,\alpha} \sum_i \frac{\partial V}{\partial u_{i,\alpha}}(\vec{r}) \quad + \text{h.c.} \tag{10}$$

Since $V(\vec{r}, \{\vec{u}_i\})$ depends only on $\vec{r} - \vec{u}_i$,

$$0 = \frac{\partial V(z)}{\partial r_\alpha} + \sum_i \frac{\partial V}{\partial u_{i,\alpha}}(\vec{r}). \tag{11}$$

Since $\partial V(z)/\partial x = \partial V(z)/\partial y = 0$, H_1 simplifies to

$$H_1 = -\sum_{\vec{q},\nu} e^{-i\vec{q}\cdot\vec{R}} \frac{\partial V}{\partial z}(z) u_{\vec{q},\nu,z} \quad + \text{h.c.} \tag{12}$$

The differential probability of scattering into final angle Ω with energy E', per unit incident perpendicular flux is given by the golden rule:

$$\frac{d^2P}{d\Omega dE'} = \frac{2\pi}{\hbar} |\langle \ldots n_{\vec{q},\nu} \pm 1 \ldots | \int_V \Psi^*_{\vec{K}',E'} H_1 \Psi_{\vec{K},E} d\tau | \ldots n_{\vec{q},\nu} \ldots \rangle|^2 \rho(E') \times \frac{\hbar k_z}{2m}, \tag{13}$$

where $n_{\vec{q},\nu}$ is the Bose occupation factor for the phonon $\vec{q},\nu$, and $\rho(E')$ is the density per unit solid angle of states $\Psi_{\vec{K}',E'}$. $\rho(E')$ is computed with continuum normalization in the

z-direction but box normalization in the $x-y$ plane. The matrix element for $E' < E$ (creation), appearing in equation (13), is

$$(n_{\vec{q},\nu}+1)^{\frac{1}{2}}\delta_{\vec{K}'+\vec{Q},\vec{K}}U_{\vec{q},\nu,z}\int_{\mathbf{Z}}\phi^{*}_{\vec{K}',E'}\frac{\partial V}{\partial z}\phi_{\vec{K},E}dz, \tag{14}$$

where $\vec{u}_{\vec{q},\nu}=\vec{U}_{\vec{q},\nu}(a^{\dagger}_{\vec{q},\nu}+a_{-\vec{q},\nu})$

The difference in energy and parallel momentum between the initial and final colliding atom states is very small. As a result, we may replace $\phi^{*}_{\vec{K}',E'}$ by $\phi^{*}_{\vec{K},E}$. The integral is now $\langle\partial V/\partial z\rangle$, the expectation value of the force. It is elementary to show, and it has been remarked in the context of other surface scattering problems,[15] that

$$\langle\frac{\partial V}{\partial z}\rangle=\frac{d\langle p\rangle}{dt}+-\frac{\hbar^2}{2m}\left[\partial_z\phi^{*}(z)\partial_z\phi(z)-(\partial_z^2\phi^{*}(z))\phi(z)\right]_{z=\infty}=-2\hbar k_z. \tag{15}$$

Using (14) and (15) in (13) results in

$$\frac{dP}{d\Omega dE'}(\Omega,E')=U^{2}_{\vec{q},\nu,z}\frac{k_z^3k}{\pi^2}g(E-E';\vec{Q})\{n_{\vec{q},\nu}+1\}. \tag{16}$$

$g(E-E';\vec{Q})$ is the density per unit energy of phonons with energy $\hbar\omega=E-E'$ and surface wavevector $\vec{Q}$.

The value of $U^{2}_{\vec{q},\nu,z}$ in the long-wavelength limit for an isotropic target, like tungsten, is well-known[7]. There are three types of phonons with displacement in the z-direction: (1) Rayleigh waves[16], with a dispersion relation $\omega=\xi c_tQ$ (c_t is the transverse speed of sound, Q is the momentum of the Rayleigh wave, and $0<\xi<1$); (2) mixed phonons[17,18], with dispersion relations $c_tQ\leq\omega<c_\ell Q$ (c_ℓ is the longitudinal speed of sound); (3) bulk waves[17,18] with dispersion relations $\omega\geq c_\ell Q$.

For Rayleigh waves[19], $U^{2}_{\vec{Q},z}=\hbar\tilde{F}(\sigma)/(\mu\rho)^{\frac{1}{2}}$, where ρ is the density of the target, $\tilde{F}$ is a dimensionless number depending only on the Poisson ratio σ, and λ,μ are the Lamé coefficients. For tungsten $\tilde{F}$ has the value 0.160. For a general isotropic target[20],

$$\tilde{F}^{-1}(\sigma)=8\xi^{-3}\left\{\frac{2-\xi^2}{2\sqrt{1-\xi^2}}-\frac{2-\xi^2}{\sqrt{1-(\xi\alpha)^2}}+\frac{(2-\xi^2)^2(2-(\xi\alpha)^2)}{8(1-(\xi\alpha)^2)^{\frac{3}{2}}}\right\} \tag{17}$$

where

$$\alpha = \sqrt{\frac{1-2\sigma}{2-2\sigma}} \tag{18}$$

and ξ, in the interval $0 < \xi < 1$, satisfies

$$\xi^6 - 8\xi^4 + 8\xi^2(3-2\alpha^2) - 16(1-\alpha^2) = 0. \tag{19}$$

There is only one Rayleigh wave for each value of the surface momentum, so $g(\hbar\omega;\vec{Q}) = \delta(\hbar(\omega - \xi c_t Q))$. When the integration over E' is performed, we find

$$\frac{dP}{d\Omega} = \frac{\hbar k_z^3 k \tilde{F}}{\pi^2(\mu\rho)^{\frac{1}{2}}}(n_{\vec{q},\nu}+1). \tag{20}$$

For mixed-mode phonons, $U^2_{\vec{q},z} = \hbar G(\sigma,\beta)/\rho\omega$ where $\beta = \omega/c_t Q$. G is a dimensionless number that depends on the Poisson ratio and the ratio, β, of the "surface velocity" ω/Q to c_t.

$$G = \frac{4\beta^2(\beta^2-1)(1-(\beta\alpha)^2)}{\left[16(\beta^2-1)(1-(\beta\alpha)^2)+(2-\beta^2)^4\right]}. \tag{21}$$

Since only the transverse part of a mixed-mode phonon extends through the bulk, the mixed mode density of states is identical to that of the transverse modes,

$$g(\hbar\omega;\vec{Q}) = \frac{\beta\sqrt{\rho}}{\pi\hbar\{\mu(\beta^2-1)\}^{\frac{1}{2}}}. \tag{22}$$

For bulk phonons, the only difference in $U^2_{\vec{q},z}$ from mixed modes is that

$$G = \left[\frac{\{(\beta\alpha)^2-1\}\beta^2}{4(\alpha^2-1)+\beta^4\alpha^2}\right]. \tag{23}$$

Finally, the density of states for bulk modes is

$$g(\hbar\omega;\vec{Q}) = \frac{\sqrt{\rho}}{\pi\hbar\sqrt{\mu}}\left\{\frac{\beta^5\alpha^2 - 4\beta(1-\alpha^2)}{\sqrt{(\beta\alpha)^2-1}\left[4\sqrt{\beta^2-1}\sqrt{(\beta\alpha)^2-1}+(2-\beta^2)^2\right]}\right\}. \tag{24}$$

Experimental Implications

We present below three graphs (Figures 1-3) of $dP/d\Omega dE'$ for 17 meV Helium atoms scattering off of a $70K$ tungsten surface[21] ($k_BT \sim \hbar\omega_D/4$) which happens to be weakly

corrugated. We chose tungsten because it is very isotropic[22] and the mass ratio $m/M \ll 1$. The results for Rayleigh phonons are presented on the same graphs by displaying $dP/d\Omega$.

Concluding Remarks

Our results were derived under three simplifying assumptions. The results remain unchanged if the third assumption (interaction with only the top layer) is dropped. For systems to which the first two assumptions (negligible diffraction, target isotropy) do not apply, exact model-independent results of the same general nature are still obtained but have a more complex form. The more general results will be presented in a separate publication[23].

Appendix

An estimate of higher-order contributions to the one-phonon amplitude provides reassurance that the first-order Born contribution dominates. The two types of new terms come from 1) higher order perturbation of the linear coupling term H_1 and 2) expansion of the potential $V(\vec{r};\{\vec{u}\})$ to higher order in the phonon coordinates $\{\vec{u}\}$. For both of these the next contributing term is third order. We find two parameters, λ and α, which characterise the higher order terms of type (1) and (2) respectively. These parameters are estimates of the ratio of the third-order processes to the first-order processes. The requirement $\alpha \ll 1$ is equation (3a) and $\lambda \ll 1$ is equation (3b).

Consider the third-order processes of type (1). These processes require a transition to an intermediate state with a second phonon and then the destruction of the same phonon. (Processes which interchange the creation and annihilation events are characterized by the same parameter λ). The transition to an intermediate state contributes a factor of

$\overline{\langle H_1 \rangle}\mathcal{N}/\overline{\Delta E}$; here $\overline{\langle H_1 \rangle}$ is a characteristic matrix element of the linear coupling term in the Hamiltonian, $\overline{\Delta E}$ is a characteristic energy denominator, and $\mathcal{N}$ is the number of intermediate states in the characteristic range of energies. If the intermediate particle state is unbound then $\mathcal{N} \sim \rho_{total}(\overline{E})\overline{\Delta E}$; here $\rho_{total}(\overline{E})$ is the density of states of the atom-target system at a characteristic energy. Since the destruction event allows no choice of the target's final state, the characteristic ratio of the third order processes to the first-order processes, λ, is $\overline{\langle H_1 \rangle}^2 \rho_{total}(\overline{E})\rho_{particle}(\overline{E}_{particle})$. The overline in equations and the adjective 'characteristic' in the text will henceforth be dropped.

The density of states $\rho_{total}(E)$ is

$$\int_0^E \rho_{particle}(E_p)\rho_{phonon}(E - E_p)dE_p = \frac{m^{\frac{1}{2}}\omega_D^2}{\hbar c^2\sqrt{E}} f(\frac{E}{\hbar\omega_D}). \qquad (A1)$$

$f(x)$ is bounded from above by $a_o x^2$ for $x \ll 1$ and by a_∞ otherwise; a_o and a_∞ are constants of order unity. The maximum value of $\rho_{total}(E)$ thus occurs for $E \sim \hbar\omega_D$. We will use $\rho_{total}(\hbar\omega_D)$ in our calculation of λ.

The matrix element $\langle H_1 \rangle$ is

$$\int d\tau \psi_1^* \frac{\partial V(\vec{r})}{\partial z} U \psi_2 \sim V_o U \sim V_o \sqrt{\frac{\hbar A_c}{M\omega_D}}. \qquad (A2)$$

U is a phonon amplitude and A_c is the area of the surface unit cell. Characteristic phonons will couple particle states that differ by a momentum of $1/a$. Intermediate particle energies will thus be of order $\hbar^2/2ma^2 \sim \hbar\omega_D$.

Combining these factors yields

$$\lambda \sim \langle H_1 \rangle^2 \rho_{total}(\hbar\omega_D)\rho_{particle}(\hbar\omega_D) \sim \frac{m}{M}\frac{V_o^2}{(\hbar\omega_D)^2}. \qquad (A3)$$

For helium on tungsten $\lambda \approx 7 \cdot 10^{-3}$.

The contribution from bulk phonons to λ is comparable to the contribution from surface phonons. For each surface momentum $\vec{Q}$ there is one surface phonon and there are N_z

bulk phonons. N_z is the number of layers of the solid in the $\hat{z}$ direction. However, the additional factor $1/N_z^{1/2}$ in $U_{\vec{Q}}$ cancels this N_z dependence.

The third-order processes whose intermediate particle states are bound are also characterized by λ. For this process $\langle H_1 \rangle \sim V_0 U a^{-1/2}$ and $\rho_{tot}(E) \sim m/\hbar^2$ so $\lambda \sim \frac{m}{M} \frac{V_0^2}{(\hbar\omega_D)^2} \sqrt{\frac{E_B}{\hbar\omega_D}}$. Here E_B is the energy of the bound state. There are no bound states with $E_B \gg \hbar\omega_D$. Other third-order processes not explicitly discussed here are quickly seen, by similar argumentation, to be characterized by λ.

The other parameter in the expansion is the ratio of the u^3 terms to the u terms in the expansion of $V(\vec{r}; \{\vec{u}\})$, both types of terms calculated in first-order perturbation theory. This ratio is $\langle \partial^3 V/\partial z^3 \rangle U^2 / \langle \partial V/\partial z \rangle$. If the potential $V(\vec{r})$ has range b then $\alpha \sim (U/l)^2$. For a surface phonon of the Debye frequency, $\alpha \sim (\hbar/2Mcb)$. The previous arguments concerning relative contributions of bulk and surface phonons apply. For helium on tungsten, $\alpha \approx 10^{-4}$.

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9. See below for a precise definition.

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13. We assume the potential does not have infinite range.

14. These conditions imply the Debye-Waller factor is approximately 1.

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19. In Reference 6 the notation $\hbar|e_z|^2/2\omega\rho$ is used to denote $U^2_{\vec{q},z}$. $\vec{e}$ is not a unit vector. The right side of Eq. 5.14 should be multiplied by 2.

20. For non-isotropic targets, $\tilde{F}$ depends in a more complicated way on the elastic constants, the Miller indices of the surface and the unit vector $\hat{Q}$.

21. The elastic constants for tungsten were obtained from F.H. Featherston, J.R. Neighbours, *Phys. Rev.* **130**, 1324, (1963). The density was obtained from G.D. Rieck, *Tungsten and its Compounds*, pp. 11,16 (Pergamon Press, New York, 1967).

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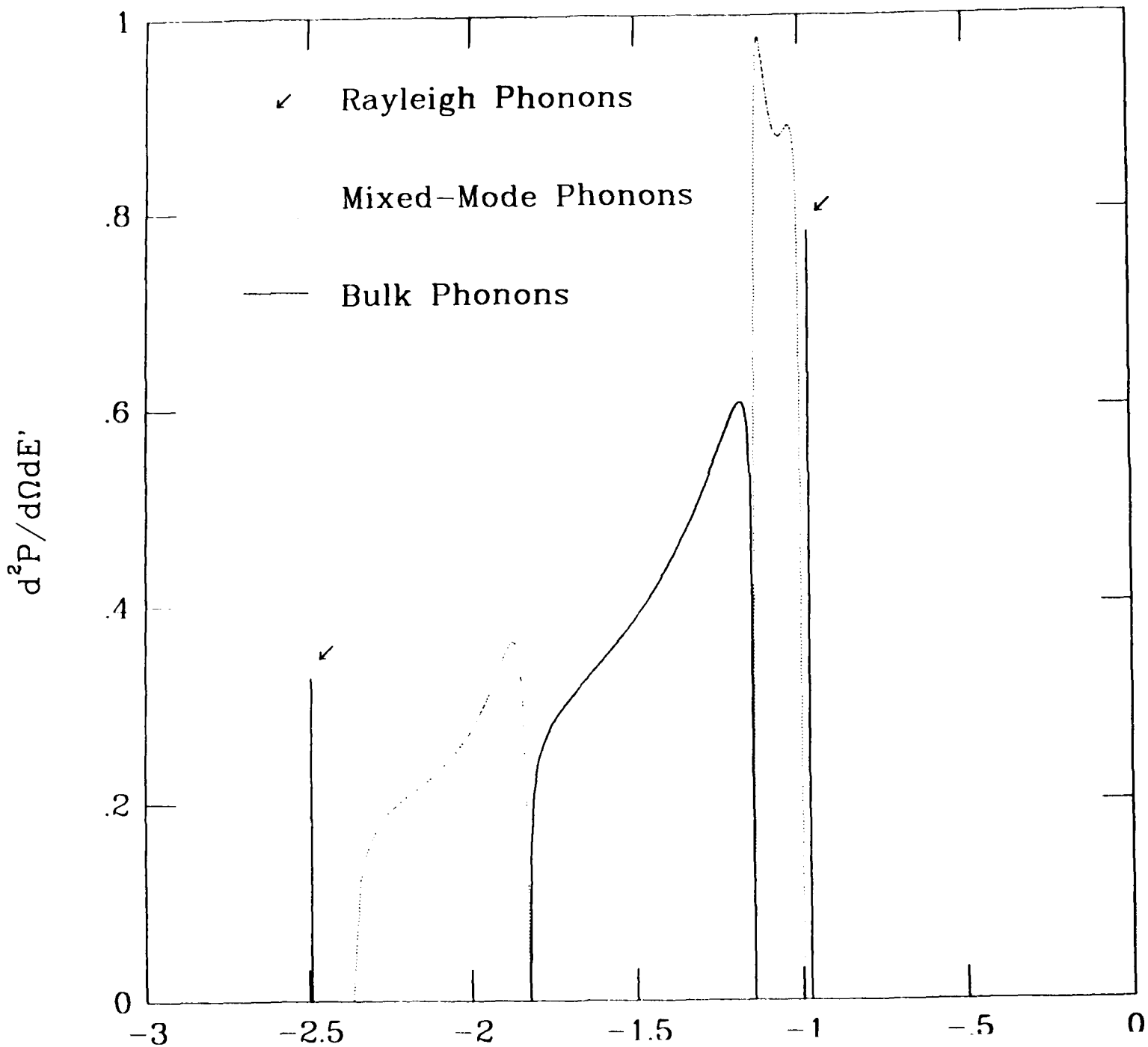
Figure Captions

1. Graph of $d^2P/d\Omega dE'$ ($dP/d\Omega$ for interaction with Rayleigh phonons) for 17 meV Helium atoms scattered by a $70K$ tungsten surface. The incident angle of the beam is 44^o from the perpendicular. The final angle is 46.5^o and is in the sagittal plane. The arrows point to the peaks which are caused by Rayleigh phonons.

2. The same parameters are used as in Fig. 1, except that the final angle is 47^o.

3. The same parameters are used as Fig. 2, except that the outgoing beam is displaced from the sagittal plane by 0.65^o.


Rayleigh Phonons
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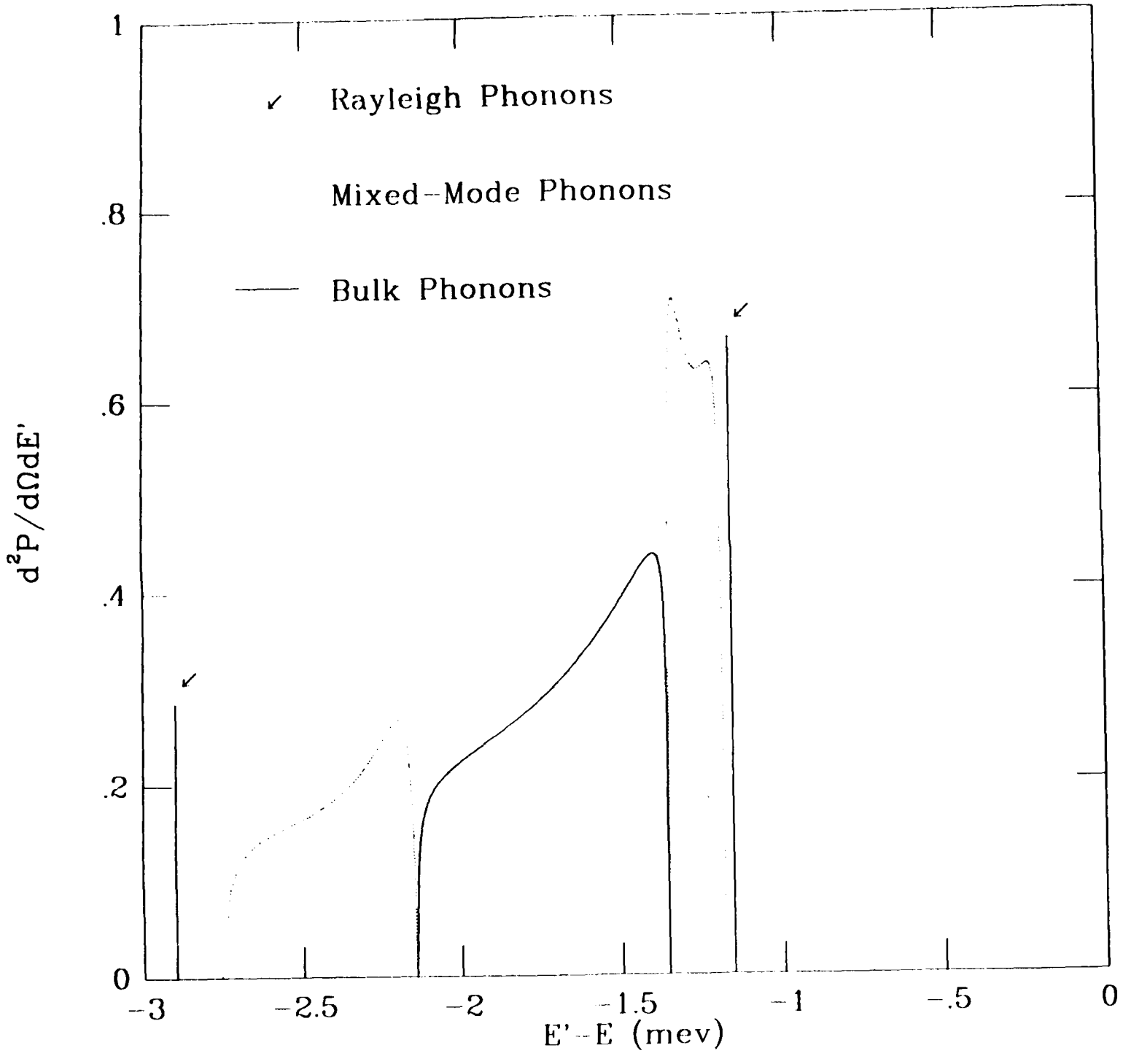
Rayleigh Phonons
Mixed-Mode Phonons
Bulk Phonons
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-1.5
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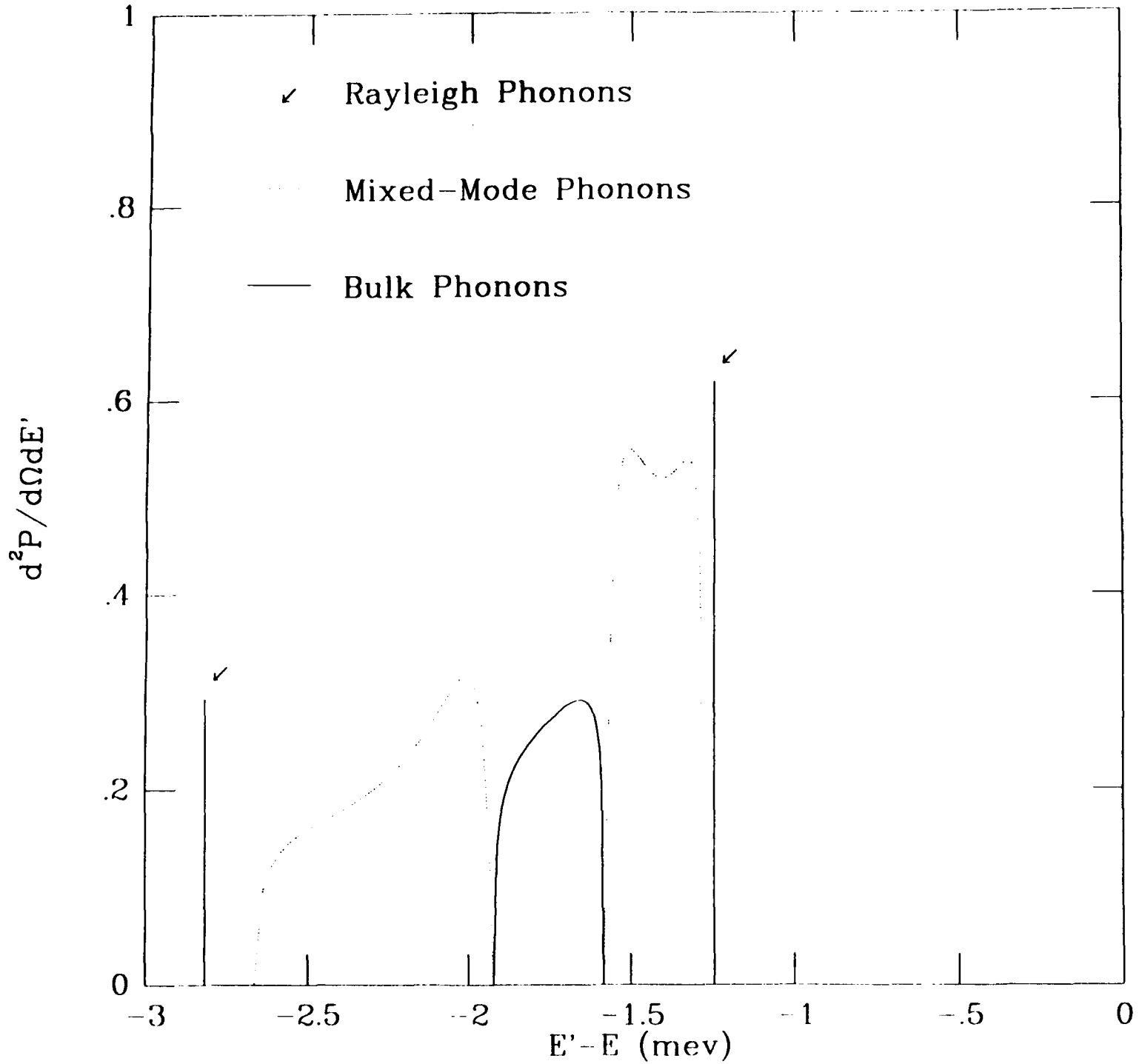
0
E'-E (mev)


Rayleigh Phonons
Mixed-Mode Phonons
Bulk Phonons
$d^2P/d\Omega dE'$
1
.8
.6
.4
.2
0
-3
-2.5
-2
-1.5
-1
-.5
0
E'-E (mev)