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Phonons near interfaces

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Abstract. We discuss the nature of phonon spectra near interfaces and show by general thermodynamic arguments and by detailed analysis of linear chain models how it is that localised measurement of atomic motion on one side of an interface yields no information about the phonon structure of the material on the other.

1. Introduction

It is a curious fact that if measurements are made at a point in one material near to a boundary with another, then features of the phonon spectrum of the second material will not be observed. This is not an obvious result: one might expect phonons of one material to 'penetrate' another. It is the purpose of this paper to discuss this problem from various points of view in order to give some insight into localisation of phonon properties.

It is necessary to be clear what is meant by localisation in this context. When a measurement is made, the *mechanism* of measurement may be local but the *property* measured may be non-local. The distinction is illustrated in conventional electron tunnelling experiments with superconductors. Tunnelling currents depend on the amplitudes of electron wavefunctions at the surfaces of the potential barrier, so the mechanism of coupling is (fairly) localised and one may say that the *measurement* is local; but the wavefunctions themselves are non-local. In superconductivity, the coherence length of the superconducting state imposes a minimum spatial scale over which electronic properties may change, so that features in the electronic properties observed by tunnelling reflect interactions averaged over such distances even though the measurement is 'local'. In the present discussion, we are not concerned with mechanisms of measurement, which could also impose their own spatial scales on what is measured, but with local values of relevant parameters, such as atomic displacements, which are involved in interactions and depend on bulk structure.

In the literature, the term 'phonon density of states' is used loosely with several different meanings. The strict meanings of the term relate simply to counting of the phonon (eigen)states: number of states per frequency interval, for example. However, measurements are often said to show a (phonon) density of states when what they really show is the product of a density of states with the appropriate matrix element squared. The latter contains the details of the interaction of the phonons with the measuring field. The appearances of spectra measured by Raman, infra-red, neutron or inelastic tunnelling techniques may therefore be quite different (because of the different matrix

elements). These differing usages of the term 'density of states' lead to confusion. In this paper we restrict its use to its strict meaning as the number density of eigenstates.

From what has been said above, it is clear that the local quantity involved in *any* interaction with phonons is the product of the density of states $g(\omega)$ with the square of the local phonon displacement amplitude, $\xi^2(\omega)$. The former enters through summation over contributing transitions, and the latter through proportionality of the coupling potential to displacement. But this product is proportional to the local spectral energy density $u(\omega)$. The *local spectral energy density* is therefore the essential phonon quantity involved in any interaction. We shall discuss localisation of phonon properties from this point of view in sections 5 and 6.

It is, of course, obvious that when two materials are placed in contact, the density of phonon states changes. If the result of a local measurement near the interface is to remain unchanged, there must therefore be a compensating change in the intensities of the phonon modes. This is not simply a renormalisation to a larger volume if the materials are different since the proper boundary conditions have to be taken into consideration in calculating how amplitudes change in each material. It is the nature of the cancellation between densities of states and amplitudes which is explored in section 5.

In section 2 we give essential elements of the monatomic linear chain model for phonon structure in one dimension. In the following three sections we discuss localisation of phonon properties: in section 3 by using general arguments of classical thermodynamics, in section 4 by microscopic analysis of energy flow, and in section 5 by examining the eigenfunctions of a finite system. In section 6, we complete the analysis with discussion of evanescent modes.

2. The monatomic linear chain

Before discussing further the properties of phonons near to boundaries, it is appropriate to set out the relevant theory of the simple monatomic linear chain, which we shall use in later discussion.

We consider a linear chain of identical masses m , distance a apart and joined by springs of spring constant α . Elementary analysis of the equations of motion (Blakemore, 1985) shows that for frequencies ω below a cut-off value given by

$$\omega_c^2 = 4\alpha/m \quad (1)$$

there are propagating modes of the form

$$\xi_n = \xi_0 \exp[i(\omega t - kna)] \quad (2)$$

where ξ_n is the displacement of mass n , and k is the wavenumber given by

$$\omega/\omega_c \equiv \Omega = \sin(ka/2) \quad (\omega \leq \omega_c). \quad (3)$$

As $\omega \rightarrow \omega_c$, the wavenumber increases to π/a so that at ω_c neighbouring masses move in antiphase. Driven above ω_c , neighbouring masses continue to move in antiphase but the motion takes the evanescent form

$$\xi_n = \xi_0 (-1)^n \exp(i\omega t) \exp(-\gamma na) \quad (4)$$

with the tunnelling exponent given by

$$\Omega = \cosh(\gamma a/2) \quad (\omega \geq \omega_c). \quad (5)$$

We note that at low frequencies, the dispersion relation takes the form $\omega/\omega_c = ka/2$;

the wave motion is non-dispersive and the phase and group velocities are equal and given by

$$v_p = v_g = a\omega_c/2 = [a\alpha/(m/a)]^{1/2} = Y/\rho = v_s.$$

The penultimate expression is the classical continuum result for the speed of sound v_s with Y the Young modulus and ρ the density. As $\Omega \rightarrow 1^-$ and k approaches its limiting value π/a , $v_g \rightarrow 0$, as would be expected for the Bragg condition $k = \pi/a$.

To discuss the behaviour of the waves at boundaries between two linear chains, it is convenient to work in terms of the generalised wave impedance Z defined as

$$Z = F/\dot{\xi}$$

where F and $\dot{\xi}$ are the force and velocity at the point at which the wave is driven. In terms of wave impedances, the mean energy flux is given by

$$P = (F\dot{\xi}^* + F^*\dot{\xi})/4 = FF^*(Z + Z^*)/4ZZ^* = \dot{\xi}\dot{\xi}^*(Z + Z^*)/4 \quad (6)$$

which are generalisations for complex quantities of the standard expressions.

For continuous media, wave impedances are independent of position; but this is not the case for discrete systems such as those considered here. If the end element in a linear chain is a mass, then the wave impedance for driving the system at the mass is found to be

$$Z_m^\pm = \pm(\alpha m)^{1/2} \exp(\pm ika/2). \quad (7)$$

If the end element is a spring, then the impedance at the free end of the spring is

$$Z_s^\pm = \pm(\alpha m)^{1/2} \exp(\mp ika/2). \quad (8)$$

In these expressions, the upper signs correspond to waves propagating away from the end and the lower signs to waves arriving at the end.

When we later analyse in detail what happens when two chains are joined, it is convenient to preserve symmetry between the two by ending each in a half-spring, that is, in a different spring of spring constant 2α . The impedance at the free end becomes

$$Z_{s/2}^\pm = \pm(\alpha m)^{1/2}/\cos(ka/2). \quad (9)$$

(Two such identical chains joined together become a uniform chain with no discontinuity.) It must be pointed out, however, that this choice in no way affects the essential result of the analysis. Carrying the calculations through for other cases shows that localisation of phonon properties is unaffected by details of how the chains are coupled. This fact also allow us to take account of the possibility of structural relaxation (which can occur in real systems close to boundaries). That may likewise be incorporated as a modification to coupling, so the results are quite general.

It should be noted that reversal of the direction of propagation does not generally correspond to a simple change in sign of the impedance, as is always the case for continuous media. We see here that the general result for change of propagation direction is $Z \rightarrow -Z^*$. That is

$$Z^\pm = -Z^{\mp*}. \quad (10)$$

This is a general result which may be viewed as a direct consequence of time reversal symmetry. It allows us to express all results involving wave impedances in standard form using only the Z^+ s which are the conventional impedances defined for launching waves into a medium. In later parts of this paper we are therefore able to drop the \pm superscripts.

We see that Z_m and Z_s become pure imaginary as $\omega \rightarrow \omega_c$ as must be the case because, although force and velocity remain finite, there can be no net energy flow since $v_g \rightarrow 0$. At $\omega = \omega_c$, a chain behaves as a lossless simple harmonic oscillator driven at resonance, with the energy oscillating between kinetic and potential forms in the masses and springs respectively. In contrast to Z_m and Z_s , $Z_{s/2}$ becomes infinite at $\omega = \omega_c$ corresponding to a finite force at the centre of a spring but with zero displacement since at ω_c neighbouring masses move in antiphase.

For $\omega \geq \omega_c$, corresponding expressions for the wave impedances become

$$Z_m = -i(\alpha m)^{1/2} \exp(\gamma a/2) \quad (11)$$

$$Z_s = -i(\alpha m)^{1/2} \exp(-\gamma a/2) \quad (12)$$

$$Z_{s/2} = i(\alpha m)^{1/2} / \sinh(\gamma a/2). \quad (13)$$

Here there is no direction of propagation so the Z s carry no superscripts.

The expressions for the reflection and transmission coefficients at a junction between two chains are different from the standard expressions for continuous media because, as pointed out above, reversal of the direction of propagation does not generally correspond simply to a change of sign of the impedance. However, using (10), we may express the results in the equivalent of standard form:

$$r = -(Z_1^- + Z_2^+) / (Z_1^+ + Z_2^+) = (Z_1^* - Z_2) / (Z_1 + Z_2) \quad (14)$$

$$t = (Z_1^+ - Z_1^-) / (Z_1^+ + Z_2^+) = 2\text{Re}(Z_1) / (Z_1 + Z_2). \quad (15)$$

These coefficients are defined in terms of the ratios of the *extensive* variable, here the displacement or velocity.

For waves incident from one chain at a junction with a second for which $\omega \geq \omega_c$ we find $|r| = 1$ as expected. The transmission coefficient, giving the amplitude at the start of chain 2, is finite but there is no net energy flow since Z_2 is pure imaginary.

We now return to the problem of the behaviour of phonons near an interface.

3. A thermodynamic argument

We can show quite generally that in equilibrium the phonon spectral energy density near a boundary between two media is isotropic and characteristic of the medium in which it is measured.

Consider, two such adjoined media with the whole system in thermal equilibrium. Then, if the media are sufficiently extensive, the phonons arriving at the boundary from the left will certainly be characteristic of the left medium, and those arriving from the right characteristic of the medium to the right. But it follows from the Second Law of Thermodynamics that in thermal equilibrium the phonon spectrum at any point must be isotropic, for if it were not, it would be possible to intercept the disbalance by arranging similarly tuned directional collectors to receive different spectral intensities. Their temperatures would then diverge; but divergence of temperature within an isolated system initially in thermal equilibrium involves a decrease in entropy which would violate the Second Law. (This is the same argument as is conventionally applied to thermal radiation in an equal temperature enclosure; see Adkins 1983.) One therefore concludes that the spectral energy density in the phonon gas is isotropic, and, in particular, that near the boundary between the media, the phonon flux from the direction of the boundary must be identical to that approaching it.

Applied to semi-infinite media it follows that measurements made on phonons on one side of the boundary can yield no information about the medium on the other. The boundary therefore controls transmitted and reflected intensities in just the way required to maintain the quality of the radiation on either side. The restriction to semi-infinite media arises because it is only in that limit that we know that the phonon flux incident at the boundary is characteristic of the medium from which it comes. With finite systems, the phonon modes must be those of the whole system and individual intensities will fluctuate depending on the precise matching conditions. However, we shall show in section 5 by analysing a one-dimensional model, how the mean spectral intensity is still unchanged. Applied to finite systems, the thermodynamic argument always shows the phonon spectrum to be isotropic although its detailed nature must now involve the whole system.

While the thermodynamic argument given above is quite general, it gives no insight into the processes by which the quality of the phonon spectrum is maintained. For that, we must turn to detailed microscopic models for what happens at the interface between two media. For the most part, we shall explore the physics by considering the one-dimensional case.

4. Energy flux

We again consider semi-infinite media to avoid boundary effects and illustrate the physics by restricting discussion to the one-dimensional problem of two joined linear chains.

At frequencies below the cut offs of both chains, energy will be propagating throughout the system in the gas of phonons, although, in equilibrium, there will be no net transport. Using periodic boundary conditions, the density of states on a chain of length L is

$$g(\omega) = (L/2\pi) \partial k / \partial \omega$$

so the spectral energy density on the chain (including energy propagating in both directions) is

$$u(\omega) = (b(\omega)/\pi) \partial k / \partial \omega$$

where $b(\omega)$ is the Planck expression for the mean energy of an oscillator of frequency ω in thermal equilibrium. The spectral energy flux in each direction along the chain is therefore

$$P(\omega) = \nu_g(\omega)u(\omega)/2 = b(\omega)/2\pi$$

where we have used the general result for the group velocity, $\nu_g = \partial \omega / \partial k$. We note that this result is independent of the precise form of the dispersion relation and is therefore correct for any linear chain below cut-off. In particular, the power incident at the boundary between our two chains is the same on both sides of the junction.

We now look at the *power* reflection and transmission coefficients. These are

$$R = |(Z_1^* - Z_2)/(Z_1 + Z_2)|^2 \quad (16)$$

$$T = |t|^2 \operatorname{Re}(Z_2)/\operatorname{Re}(Z_1) = 4 \operatorname{Re}(Z_1) \operatorname{Re}(Z_2)/|(Z_1 + Z_2)|^2. \quad (17)$$

We note that these are symmetric as regards the direction of incidence. Since, in

equilibrium, the incident fluxes are also the same, we conclude that radiation leaving the boundary (consisting partly of reflected radiation and partly of radiation transmitted from the other side) is identical to that incident. We have thus shown, by considering the details of energy transport at the boundary in the one-dimensional model, that the spectral energy density in the phonons near the boundary is unaltered by the proximity of the second chain. This is a restricted case of the general result derived by thermodynamic arguments in the last section. Extension of the above arguments to higher dimensionality is far from trivial because of the mode mixing that generally occurs with oblique incidence at a boundary in two and three dimensions.

5. Finite systems

The arguments of the previous sections were based on energy flow near the boundary between semi-infinite chains. The condition that the chains should be semi-infinite ensured that phonons arriving at the boundary were of a character dependent solely on the medium from which they arrived. With finite chains (or more strictly, with chains that are shorter than the inelastic scattering length) we can no longer ignore the free ends. We are now forced to analyse the model in terms of the normal modes of the whole system. We shall show from the equations governing the normal modes that the spectral energy densities in the two chains are again identical to those that would be present if the second chain were not there.

This is a much more difficult problem but one which brings out clearly the distinction between the two usages of 'phonon density of states' discussed in the introduction. It is obvious that the density of phonon states (in the strict sense of number of states per energy interval) is a property of the whole system and that it must be the same at all points throughout the system. But experiments measure the spectral energy density which, as we shall show, does change discontinuously on passing from one medium to the other in just such a way as is required to give results characteristic of the medium in which the measurement is made.

5.1. Impedances of finite chains

We first required the generalised impedance presented by a chain of finite length at frequencies below ω_c . With a continuous medium, a free end defines an antinode of displacement but this is not the correct boundary condition for a discrete system. For the discrete system, the essential boundary condition is that there is no force applied to the last mass from the remote side. This is precisely equivalent to there being an antinode of displacement *half an atomic separation beyond the last mass*, for if one imagined the chain continued, this would ensure that the ultimate mass and the notional mass next beyond it have the same displacements at all times so that the intervening spring never changes length and there is never any force between them (figure 1). The same physics is obtained by using the amplitude reflection coefficient with $Z_2 = 0$. The displacements of the masses, numbered from the terminal mass are then of the form

$$\xi_n = \xi_0 \cos[ka(n - \frac{1}{2})] \exp(i\omega t) \quad (18)$$

and the generalised impedances taking account of the phasing of the two propagating components in the standing waves become

$$Z_m = i(\alpha m)^{1/2} \sin(kaN)/\cos[ka(N - \frac{1}{2})] \quad (19)$$

$$Z_s = i(\alpha m)^{1/2} \sin(kaN)/\cos[ka(N + \frac{1}{2})] \quad (20)$$

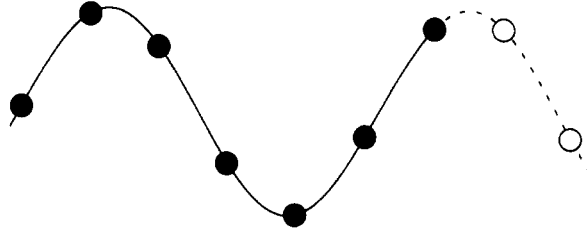


Figure 1. The boundary condition at a free end of a monatomic linear chain is that there is an antinode of displacement half an inter-mass spacing beyond the terminal mass.

$$Z_{s/2} = i(\alpha m)^{1/2} \tan(kaN)/\cos(ka/2). \quad (21)$$

In the following discussion, we shall only use the last of these.

5.2. The modes

When two finite chains are joined, the condition for the mode frequencies is that the sum of the impedances presented by the chains at the junction is zero. For the case of two chains ending in half springs this is

$$(\alpha_1 m_1)^{1/2} \tan(k_1 a_1 N_1)/\cos(k_1 a_1/2) + (\alpha_2 m_2)^{1/2} \tan(k_2 a_2 N_2)/\cos(k_2 a_2/2) = 0. \quad (22)$$

The relationships between the amplitudes in the two chains, ξ_1 and ξ_2 , for a given mode is obtained by applying an appropriate boundary condition at the junction. We equate the displacements. (With equation (22) this implies equality of forces.) Again, this boundary condition differs from the case for a continuous medium because the standing waves of equation (18) only have physical significance at the masses. The displacement of the free end of the half spring is therefore the mean of the displacements of the end mass (i.e. the n th mass) and of a notional $(n + 1)$ th mass if the chain were extended beyond the half spring. This then gives

$$\xi_1 \cos(k_1 a_1 N_1) \cos(k_1 a_1/2) = \xi_2 \cos(k_2 a_2 N_2) \cos(k_2 a_2/2). \quad (23)$$

5.3. The density of states

From equation (22) we see that mode frequencies are given by an equation of the form

$$c_1 \tan(k_1 a_1 N_1) = -c_2 \tan(k_2 a_2 N_2) = y \quad (24)$$

where c_1 and c_2 are positive and relatively slowly-varying quantities given by

$$c_i = (\alpha_i m_i)^{1/2}/\cos(k_i a_i/2). \quad (25)$$

We shall refer to y later. Both sides of this equation change between $-\infty$ and $+\infty$ once for each change in their arguments of π , but the first tan term has a positive gradient at all points and the second a negative. The number of intersections in a given frequency

interval is therefore $1/\pi$ times the sum of the changes in the arguments in the given frequency interval. This gives the density of states $g(\omega)$:

$$g(\omega) = (1/\pi)(\partial/\partial\omega)(k_1 a_1 N_1 + k_2 a_2 N_2) \quad (26)$$

which, with equations (1) and (3) gives

$$g(\omega) = (2/\pi)[(N_1/\omega_{c1})(1/\cos(k_1 a_1/2)) + (N_2/\omega_{c2})(1/\cos(k_2 a_2/2))]. \quad (27)$$

This is, as expected, just the sum of the densities of states for standing wave modes (fixed boundary conditions) of the individual chains.

5.4. The mean energy density on a chain

We first examine how the fact that the waves on the chains are standing waves affects the relationship between the mode amplitudes and the mean energy density on a chain.

The mean energy per atom on a chain of N atoms due to a mode of peak amplitude ξ_0 and frequency ω is, from equation (18),

$$\begin{aligned} U &= \frac{1}{2}m\omega^2 \xi_0^2 \sum_1^N \cos^2[ka(n - \frac{1}{2})/N] \\ &= \frac{1}{4}m\omega^2 \xi_0^2 (1 + \sin(2kaN)/2N \sin(ka)). \end{aligned} \quad (28)$$

The second term in the bracket is a correction resulting from the amount by which the mode does not have an integer number of half wavelengths on the chain. It has the form of a sinc function and becomes unimportant as kaN becomes large.

5.5. The spectral energy density

It is evident from the form of equation (20) that solutions will involve various values of the $kaNs$ and therefore, from (23), various ratios of amplitudes between the two chains. In thermal equilibrium, the *total* energy in a mode is simply given by the appropriate Planck expression for the mean energy of a simple harmonic oscillator, but the division of that energy between the two chains will vary from mode to mode according to the precise values of the $kaNs$. To compare the spectral intensities on the chains, we therefore need to perform an appropriate average over modes.

Now the ratio of the total energies on the two chains in a particular mode may, with the help of equations (23) and (24), be written

$$N_1 m_1 \xi_1^2 / N_2 m_2 \xi_2^2 = (g_1/g_2) c_1 \sec^2(k_1 a_1 N_1) / c_2 \sec^2(k_2 a_2 N_2) \quad (29)$$

where g_1 and g_2 are the densities of states on the individual chains. Since c_1 and c_2 are slowly-varying, to obtain the ratio of the spectral energy densities we require the statistical average of the \sec^2 ratio in (29). The neglect of the $1/N$ term in equation (28) will generally be a good approximation since, quite apart from the fact that N will usually be much greater than 1, we shall be averaging over modes and the correction term can be expected to average to zero.

Now the normal modes will generate a probability distribution $p(y)$ of the variable y defined in equation (24). But the arguments in the tangents will (normally) vary incommensurately from solution to solution. We may therefore take $p(y) dy$, the probability that a solution lies in the range y to $y + dy$, as proportional to the *product* of the

probabilities that each of the two $c \tan(kaN)$ terms lies in the given range. The probability that one such term lies in the given range is proportional to

$$\partial(kaN)/\partial y = \cos^2(kaN) = 1/[1 + (y/c)^2]. \quad (30)$$

Hence

$$p(y) = A\{1/[1 + (y/c_1)^2]\}\{1/[1 + (y/c_2)^2]\} = A \cos^2(k_1 a_1 N_1) \cos^2(k_2 a_2 N_2) \quad (31)$$

where A is a constant.

A further consequence of the incommensurability of the arguments in the tangent terms is that the secant terms in (29) may be taken as statistically independent of one another, so that in calculating the spectral energy density ratio we may replace the average of the \sec^2 ratio in (29) with the ratio of their averages. Then

$$\begin{aligned} \langle \sec^2(k_1 a_1 N_1) \rangle &= \int_{-\infty}^{\infty} \sec^2(k_1 a_1 N_1) p(y) dy \\ &= A \int_{-\infty}^{\infty} \frac{1}{1 + (y/c_2)^2} dy = A\pi c_2 \end{aligned}$$

and a corresponding expression is obtained for the other average. Substituting in (29), all terms on the right hand side cancel except the densities of states and we obtain for the ratio of the spectral energy densities on the chains:

$$u_1(\omega)/u_2(\omega) = g_1(\omega)/g_2(\omega). \quad (32)$$

Remembering that the density of states for the whole system is the sum of the densities of states of the individual chains (equation (27)) we see that the spectral energy density on each chain is identical to that which would be present if the other chain were not there:

$$u_1 + u_2 = (g_1 + g_2)b(\omega)$$

but from (32)

$$u_1 + u_2 = u_1(g_1 + g_2)/g_1$$

so that

$$u_1 = g_1 b(\omega).$$

5.6. Boundary effects

It must be pointed out in relation to the arguments given above that the proximity of an interface does modify local phonon structure because acoustic mismatch at the boundary produces standing wave components in the phonon field. This is similar to what happens near a free surface except that here the second medium imposes an end correction that varies with frequency. Measurements of changes in standing wave structure could therefore yield information about the changing impedance of the remote material and therefore, in principle, about its phonon properties also. Nevertheless, there is no reflection of the bulk phonon structure of the remote material in the local spectral intensities, so the essential conclusions of our discussion do not require qualification.

The presence of an interface or boundary also allows the possibility of surface modes. These do, of course, depend on the properties of both media so that measurement of

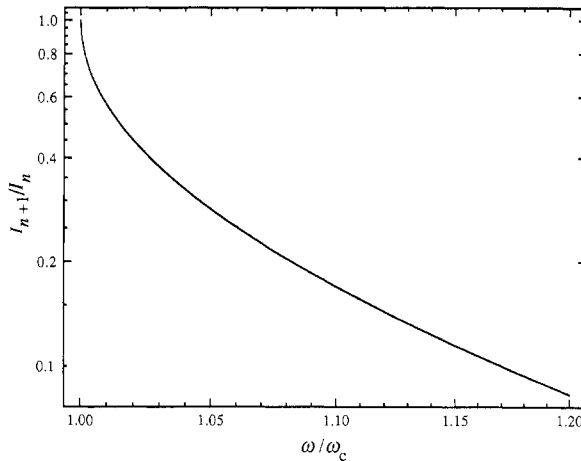


Figure 2. The reduction in intensity from one mass to the next in a monatomic linear chain at frequencies beyond cut-off.

their structure on one side of an interface would again yield information about the material on the other. These need not concern us here, however, because our interest is in whether the *bulk* phonon structure of one material can be observed by measurements in the other. Thus, we only need to consider modes that are delocalised in one or both of the media.

6. Evanescent modes

At frequencies such that $\omega_{c1} > \omega > \omega_{c2}$ modes are localised in chain 1 but penetrate as evanescent waves into chain 2. The density of states is essentially that of chain 1, differing only because of the end correction resulting from the loading of the first chain by the second. The modification is of order $1/N_1$. Measurements made in the second chain close to the interface will therefore show the density of states of chain 1 but coupling to these modes will fall off with distance into the second chain.

This situation is very different from that with propagating modes. There, measurements of spectral intensity at all points in chain 2 yield results characteristic of chain 2. Here, in chain 2, the spectral intensity varies with position and the density of states has the character of chain 1. The second chain now provides a means of coupling loosely to the modes of the first chain. This is a typical tunnelling phenomenon exemplified by quantum mechanical tunnelling of electrons into potential barriers, or by penetration of microwaves into waveguides beyond cut-off. The essential question is whether the extent of the penetration is sufficient to produce significantly measurable effects.

From (5) we obtain the tunnelling exponent γ in terms of the atomic spacing a and the reduced frequency Ω :

$$\pm \gamma a = 2 \ln(\Omega \pm \sqrt{\Omega^2 - 1}). \quad (33)$$

The attenuation of intensity from one mass to the next, $e^{-2\gamma a}$, is therefore

$$I_{n+1}/I_n = (\Omega - \sqrt{\Omega^2 - 1})^4. \quad (34)$$

This is shown in figure 2. We see that the attenuation increases rapidly as Ω becomes

greater than 1. For example, it only requires $\Omega = 1.015$ for the intensity to halve from one atom to the next. We conclude that evanescent modes will only be significant very close to the interface and very close to the cut-off frequency.

7. Summary

In this paper we have discussed the properties of phonons near interfaces. While placing two materials in contact obviously changes the density of allowed phonon states, localised measurements of phonon structure made on one side of the boundary show no features of the bulk phonon structure of the material on the other. We have shown how this must be so by applying general thermodynamic arguments to energy flow in thermal equilibrium. The transmission and reflection properties of interfaces must be such as to preserve the quality of the phonon radiation on either side. In order to gain insight into the mechanisms by which this comes about, we pursued detailed analysis of the model of two joined monatomic linear chains. Again, an energy transport argument could be applied, but a more illuminating approach was to examine the normal modes of a finite joined-chain system. We were able to show that the changed density of states resulting from joining the chains was precisely compensated by the averaged division of intensity between the chains so that the spectral energy densities in each material end up unchanged from their values with the chains isolated from one another. For modes delocalised between the chains, the only features of the phonon structure in one chain that relate to that of the other are the small phase changes in standing wave components that result from the changing boundary condition as the wave impedances of the media vary with frequency. At frequencies beyond the cut-off of one of the chains, modes are localised in one chain but penetrate the other as evanescent waves. In this case, measurements close to the boundary in the non-propagating medium can reveal the phonon structure of the other, but the rate of decay of the evanescent modes is such that only very close to the boundary and very close to the cut-off frequency would effects be significant. We therefore conclude that essentially any localised measurement of phonons made on one side of an interface will show only the phonon structure of the material in which the measurement is made.

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