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Lattice-dynamical calculation of phonon scattering at a disordered interface

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Abstract

For an FCC crystal with central force interactions and separately for a scalar model on a square lattice, we compute exactly the phonon transmission coefficient $T(\omega)$ through a disordered planar interface between two identical semi-infinite leads. At high frequencies $T(\omega)$ exhibits a strong frequency dependence which is determined by the correlation length of the disorder. © 1999 Elsevier Science B.V. All rights reserved.

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The problem of energy transfer between two solids occurs in a wide range of physical structures, including semiconductor quantum wells and superlattices. Early studies have assumed a perfect solid–solid interface and as a first approximation, an elastic continuum model accounting for acoustic mismatch has been employed to quantify heat flow through the interface [1]. Such a continuum theory describes generic low-frequency properties, but e.g. to account for experimental observations of the Kapitza thermal conductance between solids [2] at high temperatures, a lattice-dynamical approach [3] is required, which incorporates important parameters such as the phonon dispersion.

The theory of reference [3] provides a comprehensive lattice-dynamical description of perfect solid–solid interface. In this paper we discuss one extra mechanism which might play a significant

role in energy transfer, namely phonon scattering due to interfacial disorder. Breaking the translational invariance at the interface gives rise to the so-called scattering-mediated phonon transmission (reflection) [4], for which calculations based on perturbation theory predict a strong frequency dependence with a power-law crossover determined by the disorder characteristics [5]. We study these effects by analysing a lattice-dynamical model and calculate exactly the phonon transmission coefficient as a function of frequency. The disorder is introduced as a correlated or uncorrelated random variation of masses m_j along the lattice sites j of the interface layer.

We formulate the problem of phonon transmission across a disordered solid–solid interface by considering two identical semi-infinite leads attached to a ‘scattering region’. The two semi-infinite perfect crystals are envisaged as waveguides for incident and scattered phonons. The scattering region (disordered interface) consists of a single

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atomic plane where interactions with the impurities take place. A typical geometry is shown in Fig. 1.

As a model we take an FCC lattice of masses m_j coupled to each other by central force springs of stiffness κ . As a second example we also consider a square lattice described by a Born model with a single degree of freedom per site. In the latter, phonon polarization is neglected. In the harmonic approximation the lattice-dynamics in both cases is described by the linearized equations of motion of atomic displacements \mathbf{u}_j

$$m_j \ddot{u}_j^\alpha = - \sum_{\beta, i} K_{ij}^{\alpha\beta} u_i^\beta, \quad (1)$$

where $K_{ij}^{\alpha\beta} = \kappa(l_{ij}^{\alpha\beta} - 4\delta_{ij}\delta^{\alpha\beta})$, $l_{ij}^\alpha = (\mathbf{j} - \mathbf{i})^\alpha / |\mathbf{j} - \mathbf{i}|$, and $(\mathbf{j} - \mathbf{i})$ is taken from the first coordination sphere. The indices α, β run through x, y, z when phonons can be polarized and only through z when they are treated as scalars.

In the semi-infinite leads all atoms are of unit mass, whereas the masses at the interface have mean value $\langle m_j \rangle = 1$ and variance σ .¹ To generate an ensemble of N positive masses, we first introduce the following random numbers $\chi_j = \sum_k (a_k \cos(kj) + b_k \sin(kj))$ where a_k and b_k are Gaussian random numbers with zero mean value and $\langle a_k a_{k'} \rangle = \langle b_k b_{k'} \rangle = \delta_{kk'} e^{-k^2 \xi^2 / 4}$ and j labels a mass along the interface. Starting from these correlated quantities with correlation length ξ , which may assume positive and negative values, we define the non-negative quantities \tilde{m}_j and \hat{m}_j via the relations: $\tilde{m}_j = \chi_j - \chi_j^{\min}$, $\hat{m}_j = \sigma \tilde{m}_j / \sqrt{\langle \tilde{m}_j^2 \rangle - \langle \tilde{m}_j \rangle^2}$. Finally, the set of correlated mass $\{m_j\}$ used in the simulation is defined by $m_j = 1 - \hat{m}_j + \langle \hat{m}_j \rangle$. In what follows, to isolate the effect of correlations, we compare the transmission coefficient of such an interface, with that of an uncorrelated interface obtained by randomly ‘shuffling’ the above set.

To calculate the overall phonon transmittance we compute the unitary scattering matrix $S(\omega)$ at a fixed frequency using the Landauer–Büttiker formalism [6]. In addition to various tests on the numerical code, such as the calculation of the density of states or of isotropic scattering for a single

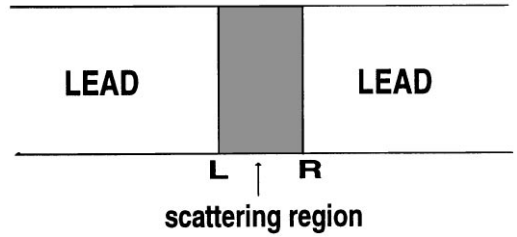


Fig. 1. A typical scattering geometry, where $L(R)$ refer to sites on the faces of left (right) lead.

mass defect, the unitarity of $S(\omega)$ is checked in all calculations. $SS^\dagger = 1$ reflects the conservation of flux. The S -matrix is extracted from the Green's function [7,8] (see Fig. 1 for definition of L, R)

$$G(\omega) = \begin{pmatrix} G(L, L; \omega) & G(L, R; \omega) \\ G(R, L; \omega) & G(R, R; \omega) \end{pmatrix}, \quad (2)$$

$$G(\omega) = (1 - g(\omega)D_s)^{-1}g(\omega), \quad (3)$$

where $g(\omega)$ is the Green's function for the leads calculated using an algorithm developed in Ref. [8]. D_s is the dynamical matrix $D = M^{-1/2}KM^{-1/2}$, $M_{ij}^{\alpha\beta} = m_i \delta^{\alpha\beta} \delta_{ij}$, which includes all the couplings between atoms on the interface and between the scattering region and the leads. Eq. (3) is Dyson's equation written in a convenient form.

In Fig. 2a and b the frequency dependence of the overall transmission coefficient $T(\omega)$ averaged over 10 disorder realizations of the interface masses for the FCC vectorial Eq. (1) and over 50 for the square lattice is shown. The lateral width of the interface is 29 and 100 in units of the nearest-neighbour spacing. The reason that we used the simplified scalar model is apparent. The computational time is quite large if we include phonon polarization because of the increase in the degrees of freedom. This prevents us from considering wider structures and eliminating finite-size effects evident in the structure of the plotted normalized to unity transmittance in Fig. 2a. It should also be noted that in this case periodic boundary conditions in the lateral direction were used, whereas in Fig. 2b fixed-end boundary conditions are adopted. The boundary conditions determine the precise frequencies at which propagating waveguide modes become

¹ To ensure that m_j are positive $\sigma < \frac{1}{3}$.

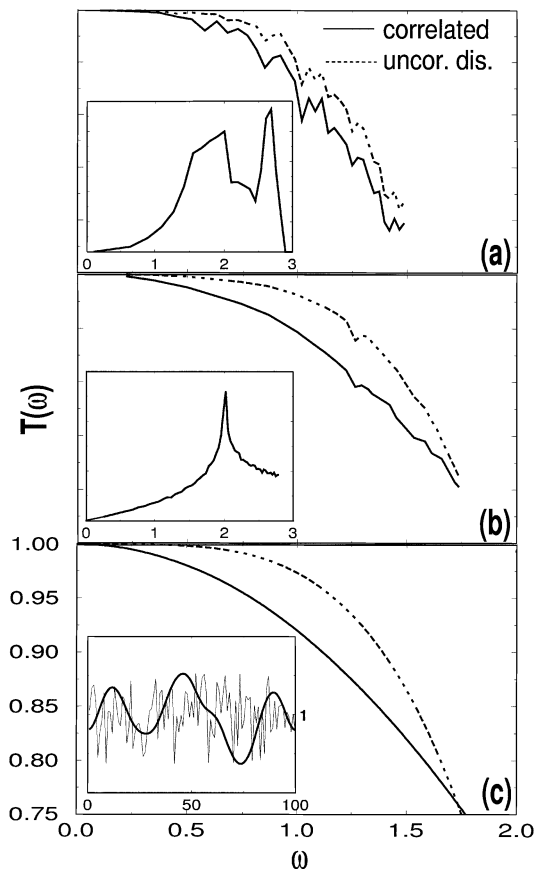


Fig. 2. Phonon transmission coefficient for the (a) FCC model ($\xi = 5.65$), (b) square scalar model ($\xi = 20$), and (c) estimates based on perturbation theory. In (a) and (b) insets the corresponding normalized DOS versus ω is plotted. Frequency is measured in units of $\sqrt{\kappa/m}$. Inset (c) shows a single realization of m_j versus j for a line of correlated and uncorrelated masses ($\sigma = 0.3$ in all plots).

available in the external leads, but apart from features which scale inversely with the number of such modes do not significantly affect the shape of the curves. In Fig. 2c the qualitative behaviour of $T(\omega)$

based on the results of perturbation theory [5] for both correlated and uncorrelated non-ideal interface layer is shown. These estimates are in good qualitative agreement with the results of the lattice-dynamical calculations.

Fig. 2 shows that a disordered interface of just a single atomic plane gives rise to strong scattering-controlled phonon transmission. The overall phonon transmission coefficient (reflection, $R(\omega) = 1 - T(\omega)$) exhibits strong frequency dependence with increasing incident phonon frequency. We also clearly demonstrate that the precise frequency dependence is determined by the characteristics of disorder. In particular, there exists a pronounced difference between the correlated and the uncorrelated disorder configuration. The exact $T(\omega)$ exhibits much slower frequency dependence for correlated distribution of masses m_j on the plane of the solid–solid interface than for uncorrelated configuration obtained by shuffling the same set $\{m_j\}$. Such an effect originates from the restrictions in the phase volume available for the scattered states due to the correlation-induced finite width of the disordered spectral distribution. For the future it would be interesting to simulate a finite thickness interface between dissimilar solids and to examine the role of anharmonicity of such an interface.

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