Bulk Phonon Scattering by Perturbed Quasi-3D Multichannel Waveguides

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Scattering and localization phenomena in disordered mesoscopic systems are actually of renewed interest owing to advances in nanotechnologies, the basic motivation being the need to understand the limitations that structural disorder may have on the physical and mechanical properties of nanocrystalline materials. Our present knowledge of the related phenomena has been given by the work of Landauer who has related the conductance of the sample to its scattering matrix. His approach reveals the essential difference between elastic and inelastic scattering, the latter is responsible for the dissipation of energy, whereas the non-dissipative and phase conserving elastic process introduce quantum interference effects due to the coherent scattering between defects. This interpretation has stimulated many researchers to look for the effects of quantum coherence in dc transport. Recently, several authors have shown that multiple scattering and quantum interference become very important to describe transport phenomena, localization of electron states in disordered media, coherent magneto-transport and to investigate structural properties of low-dimensional samples.

In the present work, we concentrate on the influence of local defect on scattering properties of elastic waves in perturbed crystalline quasi-three-dimensional nanostructure in the harmonic approximation. The sample consists of three infinite atomic plans assimilated to a perfect waveguide in which a defect impurity is present in bulk. We are interested in the reflected and transmitted parts of the incidence wave, atom displacements in the perturbed region and their evolution relatively to the impurity mass and the bonding constants strength of the network. The mathematical treatment of the problem based on the Landauer approach resorts to the matching method initially employed for the study of surface localized phonons and resonances.

Numerical results show that the interference between the multiple scattered waves gives rise to a broad variety of structures in phonon transmission (or conductance) spectra, which can be regarded as identifying features of the specific defect structures and may therefore be used for their characterization. Some of these structures resulting from the interferences between incidental and reflected waves correspond to Fabry-Pérot oscillations and others, due to the coupling between transmitted modes and a defect induced states, are identified to Fano-like resonances. A third case of resonance may be interpreted as due to the coupling with the dispersionless modes.

In fact, defect induced mode coupling between propagating modes plays an important role in the theory of electromagnetic waveguides and has been the object of many investigations. Particularly, in the micro-wave regime, Fano-type interference resonances are commonly used to build filters.

Beyond the similarity with the quantum-mechanical case of electron scattering, the scattering behaviour of vibrational waves appears to be more complicated owing to the fact that the wave functions in the Schrödinger equation are complex scalars, whereas the vibrational amplitudes are complex vectors.

It should be noted that the interference phenomena discussed in this paper are derived from the dynamical equations, which can be applied to any length scale. In other words, the results obtained in the case of the vibrational waves are not limited to a nanometric scale, but can also interest the interference effects induced in the macroscopic systems.
Fig. 1: Functional behaviours $\Omega(Z)$ of the vibrational propagating and evanescent modes characterising the triple atomic plane in the case of a null incidence.

Fig. 2: Total transmission probability for the isolated defect in the case of null incidence. The indent-point histograms represent the total hypothetical phonon transmission capacity of the perfect waveguide. The broken and full lines are referred respectively to a light and a heavy defect.