# Phonons transmittance behavior through a stepped nanowire

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Based on the matching method, this work presents the transmittance probability for acoustic phonons which propagate along a 1D waveguide perturbed by the presence a one-dimensional mono atomic step considered as a reticular defect. It is shown that the transmittance exhibits Fano-like resonance features whose origin results from degeneracy of step localized mode and propagating continuum mode. In addition, the scattering by multiple steps induce interferences between diffused and reflected waves in the step regions which generate Fabry-Pérot oscillations. The transmittance spectra can thus be regarded as identifying features and may therefore be used for their characterization. The results could also be useful for controlling thermal conductance artificially and the design of phonon devices.

## 1 Introduction

The presence of reticular defects in a structure affects substantially its dynamic, thermodynamic and kinetic properties. To study this influence, we must elucidate the phonons-defect interaction problem [1-5]. Interference effects generated in the elastic waves scattering by the lattice defects found a considerable interest since they can give rise to the resonant features of inter-crystalline interfaces which can be observed experimentally.

Based on the Landauer-Büttiker principle [2, 3], the matching method [6-8] to which we resort makes it possible to analyze the behaviour of the elastic waves through the defect perturbed region. We are interested, in particular, with the effects produced by this interaction on the phonons transmittance spectrum within the long-wave limit and low-frequency [1, 7, 8]. The results obtained for the 1D model [9] coincide with that obtained for 3D one [12] with the precision up to the numerical factor. In this work, however, we consider the propagation and the diffusion of the phonons by the structural defect in a 1D atomic chain. In spite of their simplicity, the one dimensional models give a qualitative description of many physical phenomena observed in the real three-dimensional systems.

## 2 Description of the model

The considered model depicted in Fig. 1, is made of an infinite atomic nanowire assimilated to a perfect quantum waveguide, so as to form an isolated step according to the z direction. The mono-atomic step (defect region indicated by the grey area *M*) is treated as the perturbed interface between two single semi infinite atomic nanowires *G* (left) and *D* (right) occupying the half spaces on either side of the step. The implied interactions refer only to the bonding strengths between nearest and next nearest close neighbours. The bonding force between two close atoms of the nanowire is symbolized by a spring constant $k_1$; the other additional constants as $k_{lv1}$ and $k_{lv2}$, are represented on the figure. There is experimental evidence that the frequencies of the localized vibrational states on the step can be either greater than the maximum frequency of the bulk phonon spectrum [13], or smaller than the frequency of the surface phonon mode [14] of the terraces. This has been modelled by attributing stiffened [15] or loosened [14] force constants in the neighbourhood of the step.

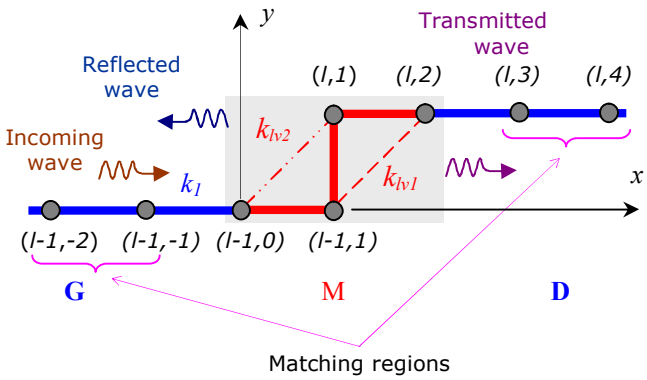


Figure 1: Schematic representation of a 1D waveguide. The mono-atomic step is treated as the perturbed interface (grey area M) between two single semi infinite atomic nanowires *G* and *D*.

## 3 Matching method principle

Initiated by Feuchtwang in the sixties then revisited by Szeftel and *al.* in the eighties, the matching method returns account in a satisfactory way for the phonons dispersion curves [7-9] and for surface resonances. It gives also a more general definition of the resonance concept and allows a more transparent analysis of the displacements behaviour in the vicinity of the Van Hove singularities [16]. However, its execution requires the crystal subdivision in three distinct regions having all the same periodicity along the surface. The procedure was described in details in references [8]. We will just present the necessary stages to the comprehension of the results analysis.

### 3.1 Dynamics of the perfect nanowire

For an atom occupying the site (*l*) confounded with the origin of the coordinates system and vibrating at the

frequency $\omega$, the equations of motion can be written, using the harmonic approximation framework [11], in the following form:

$$\omega^2 m(l) u_x(l) = -k_1(u_x(l) - u_{x+1}(l')) - k_1(u_x(l) - u_{x-1}(l')) \quad (1)$$

where $m$ indicates the atom mass; $u_x$ the atomic displacement and $k_1$ symbolises the bonding strength constant between the two adjacent atoms localized at sites *(l)* and *(l')*.

Taking into account the symmetry of the problem [17] and while applying the scattering boundary conditions for which we get plane wave solutions, the perfect lattice atom equation of motion (1) rewrites itself in following form:

$$\Omega^2 - 2 + (Z + 1/Z) = 0\,, \quad (2)$$

where $\Omega = \sqrt{m\omega^2/k_1}$ is the dimensionless frequency and $Z$ the phase factor of the plane wave.

For $Z = e^{iqa}$, the resolution of the equation (2) determines the eigenfrequencies $\Omega$ as well as the corresponding eigenvector $\vec{u}_x$. When the real wavevector $q$ is running over the first Brillouin zone, one obtains the dispersion curve $\Omega(q)$. Figure 2 shows the shape of this curve, symmetrical relatively to frequency axis in the case of a lattice parameter $a = 1$, $k_1 = 1$ and $m = 1$. Contrary to the electronic case where the curves are parallel sinusoids, we do not have here any hope to find a usable analytical expression. It will thus be necessary to resort to purely numerical methods to integrate this dispersion relation in the general problem in presence of defect.

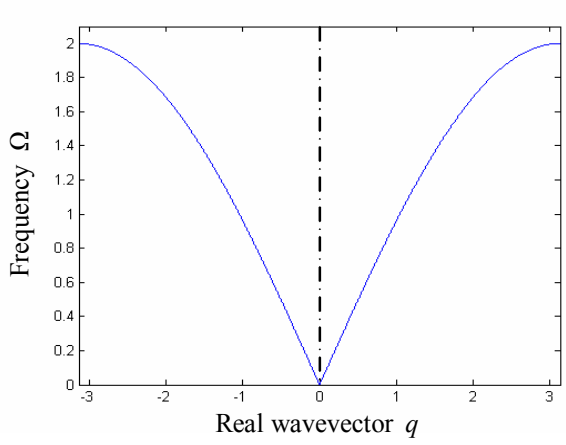


Figure 2: Dispersion of the propagating mode of the perfect atomic nanowire.

The result indicates that the only chain mode of vibration is acoustic ($\Omega \to 0$ as $q \to 0$).

The treatment of the scattering problem in presence of defects imposes the simultaneous knowledge of the propagating part ($|Z| = 1$) defined previously and the evanescent one ($|Z| < 1$) of the perfect 1D waveguide. In other words, for a given frequency, all solutions are necessary even those whose module is lower than unity. The solution which can be obtained by inversing the dispersion relation yields the functional behaviour of the vibrating eigenmode shown in Figure 3. The projection of the curves on the complex $Z$ plane shows that propagating mode solution follow the circle of unity radius equal to the module of the phase factor $Z$; this solution is identified to the dispersion curve of Figure 2. The evanescent solution ($|Z| < 1$) corresponds to the curve contained inside the unit circle.

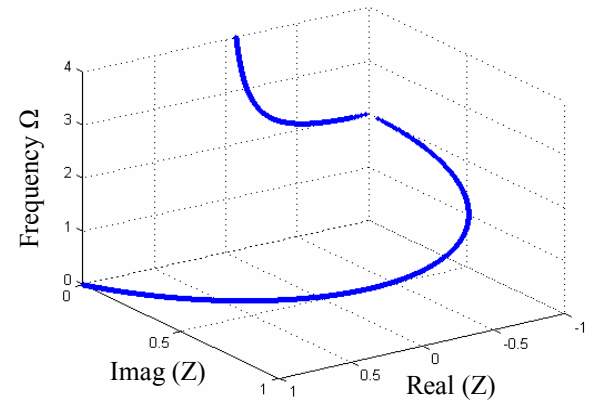


Figure 3: Functional behaviour $\Omega(Z)$ of the vibrating mode characterizing the perfect lattice atomic nanowire.

### 3.2 Coherent phonons scattering at the step edge

Since the perfect waveguides do not couple between different eigenmodes, we can treat the scattering problem for each vibratory eigenmode separately. Generalization to every combination of these modes does not pose a particular problem. For an incidental wave $V_{in}$ coming from the left of figure 1 in the eigenmode $\nu$,

$$\vec{V}_{in}^{\,i} = (Z)^{\,i}\,\vec{u} \quad (3)$$

where $Z$ is the phase factor of the entering mode, $\vec{u}$ its eigenvector. The superscript $i\,(\leq -1)$ indicates the site occupied by the atom relatively to the direction of propagation.

The resulting scattered waves, due to an elastic scattering by the defect, are composed of reflected and transmitted parts which generate vibrational fields in the two unperturbed half spaces G and D (Figure1). The Cartesian displacement components of an atom pertaining to these areas can be obtained by using the matching method [7]. For such a site, the displacement components are expressed as a superposition of the perfect waveguide eigenmodes at the same frequency, i.e.:

$$\vec{u}_r^{\,i} = \xi.\left[\frac{1}{Z}\right]^i.\,\vec{u}\left(\frac{1}{Z}\right), \quad i \leq (l-1,-1)\,, \quad (4)$$

$$\vec{u}_t^{\,i} = \eta.\left[Z\right]^i.\,\vec{u}\left(Z\right), \quad i \geq (l,3)\,, \quad (5)$$

where $\xi$ and $\eta$ indicate the reflection and transmission probabilities. The normalization of these coefficients with respect to the group velocity of the plane wave gives transmittance $\Lambda = \eta / Vg$ and reflectance $\chi = \xi / Vg$. In this case, we obtain unitarity of the scattering matrix.

By isolating the terms describing the incidental wave by using the relations (4) and (5), the inhomogeneous system of linear equations is finally put in the form:

$$\left[\tilde{D}(\Omega, k_{lv1}, k_{lv2})\right]\left[R\right]\vec{X} = -\left[\tilde{D}(\Omega, k_{lv1}, k_{lv2})\right]\vec{V}_{in}, \qquad (6)$$

where $\left[\tilde{D}(\Omega, k_{lv1}, k_{lv2})\right]$ represents the dynamical matrix of the defect, $\vec{V}_{in}$ the incidental vector and $\vec{X}$ the vector gathering all the problem unknowns: the atomic displacements $u_x$ of the defect atoms as well as the reflectance and the transmittance coefficients. These are necessary for the determination of atomic displacements in the boundaries as in the unperturbed areas *G* and *D* of the perfect waveguide.

As example, for the isolated step of Figure 1 we obtain a dynamical matrix $\tilde{D}\left[6\times 8\right]$; from where a matching matrix $R\left[8\times 6\right]$ is deduced. Then the vector $\vec{X}$ will be composed of six unknowns including the four vibrational displacements $u_x(l)$ of the step irreducible atoms and two transmittance and reflectance probabilities,

$$\vec{X} = \left\{u_x(l-1,0),\ u_x(l-1,1),\ u_x(l,1), u_x(l,2),\ \chi,\ \Lambda\right\}$$

# 4 Results and discussion

### 4.1 Scattering at the single surface step

Phonons scattered by the step are analyzed relatively to an incidental wave coming from the left in figure 1, with unit amplitude and a zero phase on the border atom (-1) located just at the site near the defect region *M*. Calculation is carried out for $k_1 = 1$, $k_{lv1} = 1.2$ and $k_{lv2} = 0.8$. The numerical results obtained for the transmittance and reflectance probabilities in terms of the dimensionless frequency are consigned in Figure 4.

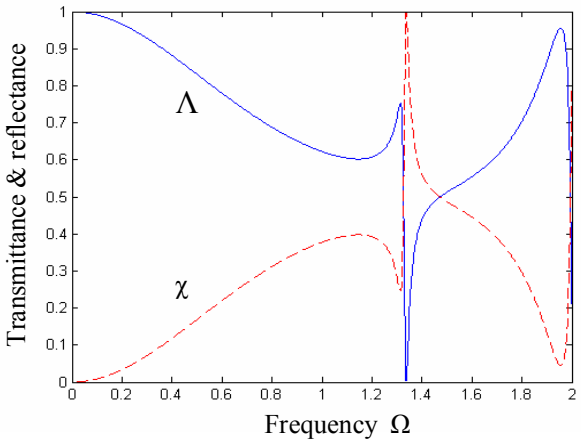


Figure 4: Phonon transmittance $\Lambda$ and reflectance $\chi$ as a function of scattering frequency for an isolated monatomic step in the case of stiffened force constants in the neighbourhood of the step.

We notice that the presence of the step leads to a general decrease of the probability. As expected, the influence of the defect is relatively small in the acoustical regime because of the low implied frequencies. For $\Omega \to 0$ we get $\Lambda \to 0$ in addition to the pronounced typical Fano-like resonance structure. This asymmetric resonance can be attributed to the presence of defect-induced resonant state, whose frequency depends on the value of the bonding forces in the step region.

This generalized behaviour is also observed when backscattering becomes more significant for wavevectors near the zone boundary where the transmittance probability tend towards zero. Lastly the well known theoretical relation translating the conservation of energy principle,

$$\left(\left|\Lambda\right| + \left|\chi\right|\right) = 1, \qquad (7)$$

is fortunately satisfied and always checked for each frequency. Besides, this condition constitutes an effective control method of the results.

Otherwise the spectrum is much more affected in the case of loosened force constants. In addition to resonance, this influence is translated by a less amplitude compared to the stiffened constants values.

### 4.3 Isolated double step

The surface-surface phonon scattering is now considered for a double step, schematized in top of Figure 5, where the two step edges are sufficiently far apart to justify decoupling the dynamics of the two edges. However, there exists a domain where the two edges are still sufficiently close ($\delta$ corresponds to a distance smaller than the surface phonon coherent length) where the two steps interact by exchanging coherent surface phonons.

Figure 5 gives the example of two identical steps separated by a plateau of variable length $\delta$ and the transmittance probabilities they produce.

The effects described previously in the case of isolated step appear, but they are even more difficult to isolate because of the biggest number of peak-dip structures near in frequencies. It is why we are not going to study in details these regions. On the other hand, we will limit ourselves to present a more global change of the transmission curves, provoked by the Fabry-Pérot oscillations issued from interferences between the multiple scattering of propagating states in the perturbed region.

The distance $\delta$ represents always a whole multiple of network parameters $a$. It can be seen in Figure 6 that the transmittance curves structure became richer of several peaks. We observe also a drastic $\delta$ dependence of Fabry-Pérot oscillations. However, the number of main dips remained the same corresponding to the number of steps ; but each of them divides in several secondary peaks that provide the total number of lattice parameter $a$ contained in horizontal distance $\delta$.

The fact that their number seems to be lower on the figure is simply related to a resolution problem in the implied frequency range. Same results are observed by V. Pouthier and *al.* [18] on the transmittance spectrum of a nanowire containing a set of linear clusters separated by different spacings. Some rapid oscillations in the boundary are due to the simultaneous presence of Fabry Pérot interferences which become more and more important with the increase of $\delta$. The transmission spectrum displays more complex oscillation behaviours especially for higher frequency. Otherwise, the upper level of the Fabry Pérot

oscillation can merge with the Fano-resonance peak. It should be noted that on average the global shape of the transmission curves is quite similar to that obtained in the case of an isolated step (in dotted line on the figure).

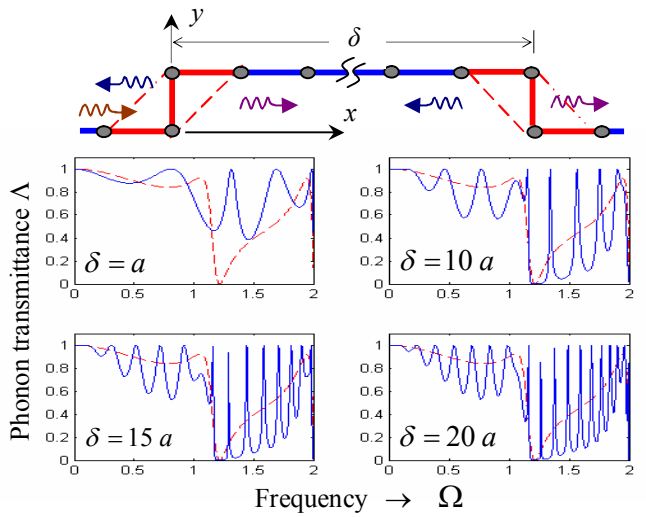


Figure 5**:** Magnitude of the phonon transmittance as function of the scattering frequency for two identical steps separated by a distance $\delta$ in the case of loosened force constants in the neighbourhood of the step. The dotted line refers to single step with the same parameters. The structure scheme is given above the figure.

### 4.3 Interaction of several steps

The increase of the sample defect region doesn't bring anything of qualitatively new in relation to the case of the isolated step. The addition of steps results solely in the increase of the size of the linear system (6), but the matrix $\widetilde{D}$ keeps its structure. The supplementary blocks have the same shape as those characterizing a lonely isolated step. Naturally, we can be interested by a disposition of consecutive steps forming a staircase. We have limited our study to only fifteen steps which already generates a $(34 \times 36)$ defect matrix dimension. In Figure 6, we investigate the dependence of the transmittance probabilities on the dimensionless frequency for different staircases. The dotted lines refer to a single isolated step. The transmission curves are turned into a number of peak-dip structures, the reason is that the modes will interfere with each other due to the multiple reflections of the phonon waves in the perturbed region. In general, the multiple interferences in the perturbed waveguide imply the more complex transmittance spectra, especially for higher frequencies. These interferences between multiply scattered waves result in Fabry–Pérot oscillations of increasing amplitudes with the frequency and whose number depends intimately of the number $N$ of steps that the staircase includes. Similar results are obtained in the study of adatomic defects [9, 12, 19-20] and substitutional defect columns [8] in the perturbed double quantum chain. Defects are separated by different spacings in both configurations.

An interesting feature is that the dips which correspond to positions of transmission zero, shown in the middle frequency interval broaden with the increase of the step number and develop gradually into a stop frequency gap at which all phonons are reflected by the defect quantum waveguide. Note that on average, the transmission curves follow a shape globally similar to that of the isolated step in both vibrating modes.

## 5 Conclusion

The undulatory behaviour of an elastic wave which propagates through a quantum waveguide containing geometric defects (steps) was analyzed while resorting to the matching procedure based on the Landauer-Büttiker approach. The scattering is considered for different defect configurations. In both cases, strong asymmetrical resonances are observed in the transmittance spectra; these structures are allotted to the coupling discrete continuum-states induced by the step region. The position and width of the resonance peaks are determined by the longitudinal length of the perturbed region M. Moreover, the transmittance spectrum is characterized by other oscillations of Fabry-Pérot type due to the interferences between transmitted ant reflected waves in the perturbed region. Their number depends closely of the plateau or staircase dimensions.

The transmittance spectra can thus be used for identifying defects of specific structures and then being used for their characterization. We hope that these findings can be verified in an easily realisable set of experiments. Such systems can find some useful applications in the designing of transducers and noise control devices (ultrasonic filters) [21] whereas resonances are commonly used to build frequency filters [22]. The results could also be useful for controlling thermal conductance artificially and the design of phonon devices.

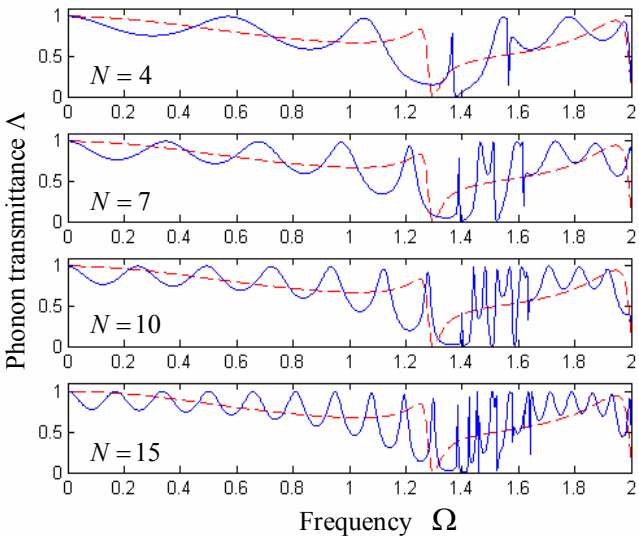


Figure 6: Phonon transmittance vs. scattering frequency for staircase having a variable number $N$ of steps in the case of stiffened force constants in the perturbed step region. The dotted line refers to single step for the same parameters.

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