Coherent Phonons Scattering by Interstitial Impurities in Quasi-Planar crystals

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Abstract—using the matching method formalism, this work presents the transmission and reflection coefficients of coherent phonons in a quasi 2D quantum waveguide perturbed by reticular defects as interstitial impurities. Our waveguide is modelled by two infinite atomic chains. The implied interactions refer only to the bonding strengths between nearest and next nearest close neighbours. .Numerical results show that the transmission spectra exhibit Fano-like resonance features which result from degeneracy of localized-impurity states and propagating continuum modes. In addition, the scattering by multiple impurities induces interferences between diffused and reflected waves in the defect region giving birth to Fabry-Pérot oscillations. This interference phenomenon could provide an interesting alternative to investigate structural properties of materials. The results could be also useful for the design of phonon devices.

Index Terms—Mesoscopic Disordered Systems; Reticular Dynamics; Phonons Scattering; Defect in Nanostructures, Matching Method; **N**umerical Simulation.

I INTRODUCTION

The survey of scattering and localization phenomena in the disordered mesoscopic systems interested the researchers at all times [1-3] because of the numerous applications found in classic metallurgy, in electrochemistry, in catalysis and in electronics.

Our present knowledge of the related phenomena has been given by the work of Landauer [4], in which the studied sample is represented by a set of scatterers (reticular defects) inserted in bulk or on surface of crystalline structure. He showed that the conductance of a quantum wire is bound directly to the scattering properties of such system, considered as a waveguide perturbed by defects. His approach has stimulated many researchers [5-10] to look for the effects of quantum coherence, most of the time by numerical methods, in dc transport particularly. Actually these phenomena are of renewed interest owing to advances in nanotechnologies, the basic motivation being to understand the limitations that reticular disorder may have on mechanical and vibrational properties of crystalline materials.

In the present work, we study the phonons scattering by an interstitial impurity localized in an infinite double atomic chain. We analyze the behaviour of a plan wave which propagates throughout this crystal which is assimilated to a quasi-planar crystallographic waveguide. We concentrate in calculating the reflected and transmitted parts of the incidental wave, the phononic conductance as well as the displacements of the irreducible atoms composing the perturbed region. We are also interested by the determination of the localized induced impurity states especially important for transmission spectra interpretation. Different defect configurations are considered. The mathematical treatment of the problem resorts to the matching method [7,11] in the harmonic approximation framework [12-14] while using scattering boundary conditions.

II STRUCTURAL MODEL

The considered model consists of two linear parallel periodic chains of masses, assimilated to a quasi-one-dimensional planar waveguide in which interstitial impurities are incorporated. The parallel chains are composed of specific masses aligned along the direction of propagation (x axis). The situation is depicted in Figure 1. Each mass is linked to its nearest and next nearest neighbours by harmonic springs of stiffness constants k_1 and k_2. The additional constants as K_{lv}, k_l and k_v, are represented on the figure. To simplify, the distances between adjacent masses are considered equal in the two Cartesian directions x and y of the plan. Also, to take account of the modification of the bonding strength field in the perturbed region (grey area M), we introduce a proportionality factor λ which indicates the ratio of the different force constants between the defect zone masses and those of the perfect lattice areas G (left) and D (right-hand side) located in sites separated by equivalent distances.

III 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

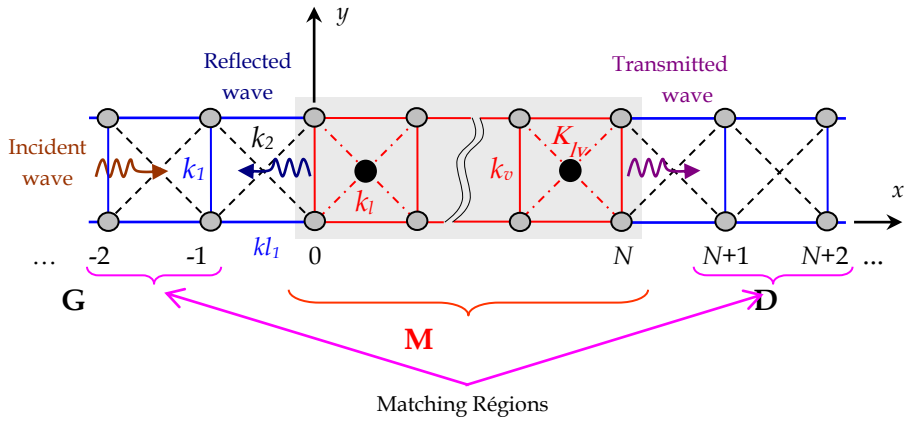

Figure 1: Schematic representation of a planar quasi-1D waveguide made up of two linear infinite chains perturbed by interstitial defects. The grey area M indicates defect region, G and D two semi infinite perfect waveguides.

general definition of the resonance concept and allows a more transparent analysis of the displacements behaviour in the vicinity of the Van Hove singularities [15]. 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.

A Perfect lattice dynamics

For an atom occupying the site (l) and vibrating at the frequency ω, the equations of motion can be written, using the harmonic approximation framework [14], in the following form:

$$\omega^2 m(l)\, u_\alpha\left(l,\omega^2\right) = -\sum_{l'\neq l}\sum_{\beta} k(l,l')\frac{r_\alpha r_\beta}{d^2}\left[u_\beta\left(l,\omega^2\right)-u_\beta\left(l',\omega^2\right)\right] \qquad (1)$$

where α and β represent the x, y directions of the plan; $m(l)=m$ indicates the atom mass located at site l; r_α is the component of the relative position vector between sites l and l', d the distance separating them and $k(l,l')$ the bonding strength constant between the two atomic sites.

Taking into account the problem symmetry and applying the scattering boundary conditions for which we get plan wave solutions, the perfect lattice atom equation of motion (1) rewrites itself in following matrix system:

$$\left[\Omega^2 I - D(Z,r_2)\right]|\vec{u}\rangle = |\vec{0}\rangle \qquad (2)$$

where $\Omega^2 = m\omega^2/k_1$ is the dimensionless frequency, I the identity matrix, $D(Z,r_2)$ the (3×3) dynamical matrix of the perfect lattice and $|u\rangle$ the vector displacement. The r_2 parameter denotes the force constants ratio between nearest and next-nearest neighbours.

The scattering problem in presence of defects imposes the knowledge of both propagating modes ($|Z|=1$) and evanescent ones ($|Z|<1$) of the perfect waveguide. In other words, for a given frequency, all solutions are necessary even those whose module is lower than unity. These solutions can be obtained by increasing the eigenvectors basis:

$$\vec{v}_\beta(l) = -\frac{1}{Z}\vec{u}_\alpha(l)\,; \quad \beta = 5,\cdots,8\,. \qquad (3)$$

We then rewrite equation (4) in the Z eigenvalue problem form,

$$A(\omega)\vec{W} = Z\,B\,\vec{W} \quad \text{with} \quad \vec{W} = \begin{pmatrix} u_\alpha(l) \\ v_\beta(l) \end{pmatrix}, \qquad (4)$$

where A and B are (4×4) matrices coming from the basis change. Let us note that the dimension of this generalized eigenvalue problem is twice as large as the original problem.

B Coherent phonons scattering at defects

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 incoming wave from the left of Figure 1 in the eigenmode $\bar{\nu}$, form must accompany your final submission. Authors are responsible for obtaining any security clearances.

$$\vec{V}_{in}^{\,i} = (Z_{\bar{\nu}})^i\,\vec{u}_{\bar{\nu}}\,; \quad i \le -1, \qquad (5)$$

where $Z_{\bar{\nu}}$ is the attenuation factor of the entering mode, $\vec{u}_{\bar{\nu}}$ its eigenvector; the superscript $i\,(\le -1)$ indicates the site occupied by the atom with respect to the direction of propagation.

The resulting scattered waves are composed of a reflected and transmitted parts, which can be expressed as a superposition of the eigenmodes of the perfect waveguide at the same frequency, i.e.,

$$\vec{u}_r^{\,i} = \sum_{\nu} r_{\nu\bar{\nu}} . \left[\frac{1}{Z_\nu}\right]^i . \vec{u}_\nu(\frac{1}{Z_\nu}); \quad i \le -1, \tag{6}$$

$$\vec{u}_t^{\,i} = \sum_{\nu} t_{\nu\bar{\nu}} . [Z_\nu]^i . \vec{u}_\nu(Z_\nu); \quad i \ge 2, \tag{7}$$

where $r_{\nu\bar{\nu}}$ and $t_{\nu\bar{\nu}}$ indicates the reflection and transmission coefficients normalized beforehand by group velocities (slopes of the dispersion curves) of the plan wave, set equal to zero for the evanescent modes. The evanescent modes are needed for a complete description of scattering in presence of defect, although they do not contribute at all to the energy transport.

With the definitions (6) and (7), we can rewrite the dynamical equations for the perturbed double chain. Since there are perfect waveguides in regions G and D, we only need to solve Eqs. (1) for the masses inside the perturbed zone M and in the boundary columns (-1) and (2), which are matched to the rest of the perfect waveguide by Eqs. (6) and (7). Isolating the inhomogeneous terms describing the incidental wave, we obtain an inhomogeneous system of linear equations

$$\left[D_f(\Omega, r_2, \lambda)\right][R]\vec{X} = -\left[D_f(\Omega, r_2, \lambda)\right]\vec{V}_{in} \tag{8}$$

where $D_f(\Omega, r_2, \lambda)$ indicates the dynamical defect matrix, $\vec{X}$ the vector gathering all the problem unknowns, $\vec{V}_{in}$ the incidental vector and R the matching matrix.

As example, for an isolated defect we obtain a dynamical matrix $D_f[18\times 26]$; from where a matching matrix $R[26\times 18]$ is deduced. Then the vector $\vec{X}$ will be composed of eighteen unknowns including the ten displacements $u_\alpha(l)$ of the irreducible atoms, the four transmission coefficients and four reflection ones.

IV IRREDUCIBLE ATOMS VIBRATION SPECTRA

In combining the matching procedure to the Green's functions and for a given wave vector parallel to the direction of propagation [16], the matrix phonon spectral density reads

$$\rho^{(l,l')}_{(\alpha,\beta)}(\Omega) = -2\Omega \sum_m P^l_{\alpha i} P^{l'}_{\beta i} \delta(\Omega^2 - \Omega_m^2), \tag{9}$$

where (l) ands (l') are two atomic sites, α and β designate two different Cartesian directions and $P^l_{\alpha i}$ is the component in direction α of the polarization vector of the atom (l) for the mode having a frequency Ω_m.

The vibration density of states (DOS) per atomic site $N_i(\Omega)$ in the perturbed defect region could be calculated by summing over the trace of the spectral density matrix (G $(\Omega^2+j\varepsilon) = ((\Omega^2+j\varepsilon)I-D_f(r_2,\lambda))^{-1}$ being the Green operator), i. e for (l)= (l'),

$$N_l(\Omega) = -\frac{2\Omega}{\pi} \lim_{\varepsilon\to 0^+} \left\{ \sum_\alpha \mathrm{Im}\left[G^{ll}_{\alpha\alpha}(\Omega^2 + j\varepsilon)\right] \right\} \tag{10}$$

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V RESULTS AND DISCUSSION

Phonons scattered by impurity are analyzed relatively to an incidental wave coming from the left of Figure 1, with unit amplitude and a zero phase on the border atom (-1) located just at the beginning of the defect region *M*.

A Single impurity scatterer

The numerical results for the transmission and reflection coefficients in terms of the incident phonon frequency are consigned in Figure 2 in the case of an impurity mass $m' = 1.5m$.

We notice that the presence of the interstitial defect leads to a general decrease of the probability amplitude. As expected, the influence of the impurity is relatively small in the acoustical regime because of the low implied frequencies. For $\Omega \to 0$, we get $T_\nu \to 1$; the subscript ν (=1 to 4) refers to the number of eigenmodes characterizing the double atomic chain [7-9]. Moreover, the transmission spectra are marked by pronounced typical Fano-like resonances (null transmission in Figures 2). These asymmetric resonances can be attributed to the presence of impurity-induced resonant states, whose frequency depends on the value of the bonding forces in the defect region *M*. Consequently, these resonances take place at low frequencies for heavy defects and inversely for the light ones. These findings are in good agreement with those of Tekman and Bagwell [2], who used a two mode-mode approximation.

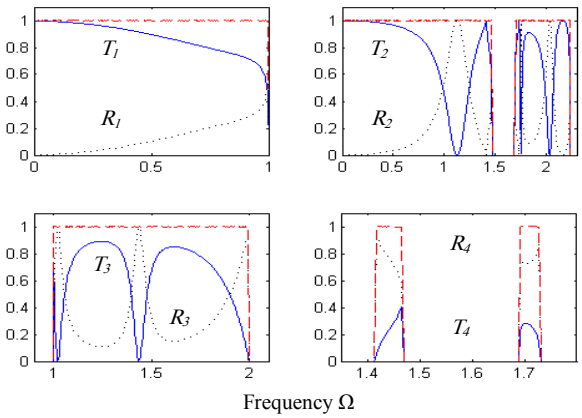

Figure 2: Transmission (full line) and reflection (doted line) coefficients vs. the phonon frequency for an isolated interstitial impurity mass *m'=1.5m*. The dashed curve shows the good complementarity between the two coefficients.

Lastly the well known theoretical relation translating the conservation of energy principle,

$$\left(\left|R_V\right|+\left|T_V\right|\right)=1 \qquad (11)$$

is fortunately satisfied and always checked for each frequency (dashed lines in Figures 2). Besides, this condition constitutes an effective control method of the results.

The results of the conductance $\Lambda(\Omega)$ are shown on Figure 3. In addition to the curves of conductance relating to each impurity mass considered, we also represented that of the perfect lattice (dash-dotted histogram). In this case, the entering wave is totally transmitted in each propagating mode. The conductance of the system becomes then more important where the modes overlap. For this reason, its value reaches more than unity in the concerned frequencies ranges. Otherwise the conductance spectrum is much more affected in the case of light impurity mass (dashed curve). In addition to resonances, this influence is translated by a less amplitude compared to for bigger masses at weak frequencies.

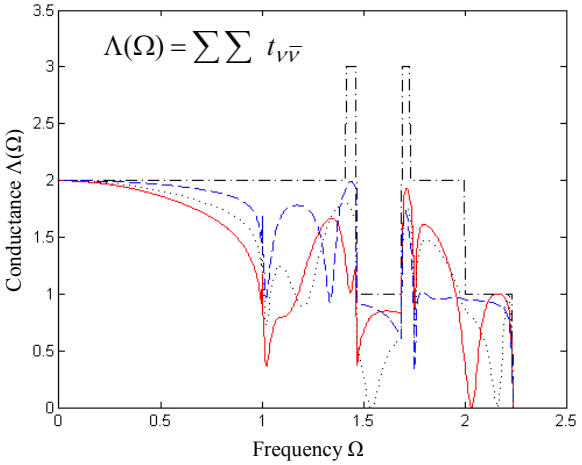

Figure 3: The total transmission probability vs phonon frequency for impurity masses $m'=0.5m$ (dashed line), $m'=m$ (dotted line) and $m'=1.5m$ (full line) in the case of a single impurity scatterer. The dashed-dotted histogram represents the total hypothetical phonon transmission capacity of the system.

B Extended defect

The increase of the defect region width doesn't bring anything of qualitatively new in relation to the case of the single impurity. The addition of impurities results solely in the increase of the size of the linear system (8), but the matrix $\tilde{D}$ keeps its structure. The supplementary blocks have the same shape as those characterizing a single defect. We have limited our study to only ten interstitial impurities which already generates a (72×80) defect matrix dimension. 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 scatterings of propagating states in the perturbed region.

The phonon scatterings, considered for an extended defect composed of several interstitial impurities, are presented in Figure 4 for heavy impurity mass ($m'=1.5m$) in the anti-symmetric mode 1 [8]. It can be seen that the transmission curves structure became richer of several peaks. We observe a drastic dependence of Fabry-Pérot oscillations with the number of impurities. However, the number of main dips remained the same corresponding to the total number of lattice parameter a contained in the width of the perturbed region.

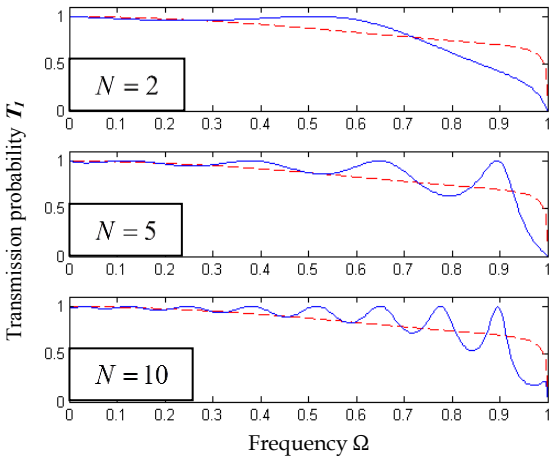

Figure 4: Transmission coefficient as a function of the phonon frequency for an extended defect composed of N defects of impurity mass $m'=1.5m$. The dashed curve refers to an isolated scatterer having the same mass.

The fact that their number seems to be lower on the figures is simply related to a resolution problem in the implied frequency range. Same results are observed by V. Pouthier and *al.* [17] on the transmittance spectrum of a nanowire containing a set of linear clusters separated by different spacing. 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 impurity (in dashed line on the figures).

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 transmission spectra. 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 of impurities. Similar results are obtained in the study of adatomic defects [8,9,17-20] and substitutional defect columns [8] in the perturbed double quantum chain. Defects are separated by

different spacing in both configurations.

C Phonons densities of states

In Figure 5 are shown the phonon densities of states (DOS) versus the non-dimensional frequency for defect irreducible atoms (see Fig. 1). The results were calculated, according to Eq. (10), for two inhomogeneity masses light (m'=0.5m) in dashed line and heavy (m'=2m) in full line in the case of stiffened force constants. Due to obvious symmetry effects, analogous behaviors are observed for both columns (0) and (1). Therefore, the density of states is shown only for atom (0,0). It can be seen that spectra for this kind of lattice atoms is quite similar and present five main features as in the overall transmission spectrum, mainly at resonant frequencies $\Omega \approx 1$, 1.4, 1.7, 2.0 and 2.3 for heavy impurity mass. For light mass, the resonant peaks happened at frequencies $\Omega \approx 1.0$, 1.4, 1.7 and 2.4. These resonances can be attributed to the presence of defect-induced resonant states.

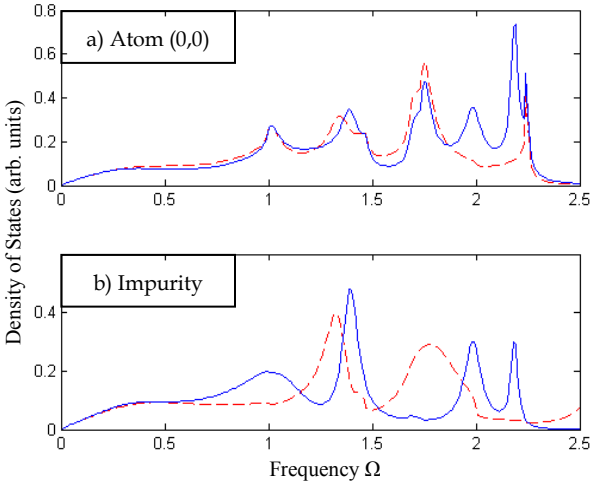

Figure 5: Density of states (DOS) of the irreducible atoms versus incident phonon frequency for a) light (*m'=0.5 m*, dotted line), and b) heavy (*m'=2 m*, full line) impurity masses.

The phonon modes of the impurity atom reveal four significant resonant peaks (two for light impurity mass) at high frequency. These strongly localized modes are due to interstitial defect induced states. These peaks correspond mainly to the longitudinal modes near the high Brillouin zone boundary. The low-frequency peaks are mainly contributed by the transverse modes. As previously, these resonant peaks shift to higher (lower) frequencies for smaller (larger) impurity mass as expected.

V CONCLUSION

In this work, we have analyzed the behaviour of elastic waves propagating through a quantum waveguide perturbed by interstitial impurities. Our calculation resorts to the matching procedure based on the Landauer-Büttiker approach. The scattering is considered for isolated and extended impurity defects. In both configurations, strong asymmetrical resonances are observed in the transmission spectra; these structures, identified to Fano resonances, describe usually the interference between a propagating transmitted mode and a local defect mode. The resonance frequency depends closely of the impurity mass (or of the bonding force constants) in accordance with the relation $\Omega^2=(k/m)$ defining the harmonic oscillator frequency.

For extended defects, resonance peaks and their number are determined by the perturbed region width given by the number of impurities. Moreover, the transmission spectrum is also characterized by other oscillations of Fabry-Pérot type due to the interferences between transmitted ant reflected waves in the perturbed region. Also their number depends closely of the defect region width.

The transmission spectra can thus be used for identifying defects of specific structures and then being used for their characterization. The interference effects are of interest for improvements in the design of transducers and noise control [21] whereas Fano-type resonances are commonly used to build filters [22]. The results could be also useful for the design of phonon devices.

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