

Research Article

Phonon Conductance of Potassium- and Sodium-Doped Transpolyacetylene Chain

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A theoretical approach for the study of phonon dynamics and scattering properties of doped transpolyacetylene chain is presented. The coherent reflection and transmission scattering cross-sections for phonons incident on the doped unit cell boundary are calculated in accordance with the Landauer-Buttiker electron scattering description, using the matching procedure with the nearest and next nearest neighbor elastic force constants. This is done for two different dopants, namely, the potassium and sodium atoms. Our numerical results yield an understanding of the transpolyacetylene chain dynamical properties and the effects on phonon conductance due to phonon incident on the doped unit cell boundary. The coherent reflection and transmission coefficients show characteristic spectral features, depending on the cutoff frequencies for the propagating phonons and on the nature of the dopants. They illustrate the occurrence of Fano resonances in the scattering spectra that result from the interactions of propagating elastic waves of the undoped transpolyacetylene chain with the localized modes due to the breakdown of the translation symmetry in the x direction.

1. Introduction

Conjugated polymers have been studied intensively because of their fascinating properties. These materials are of great fundamental interest in that they are exotic, low-dimensional semiconductors [1–3]. More recently, the use of such conjugated polymers has been explored in a variety of technological applications such as field effect transistors [4, 5], light emitting diodes [6, 7], and solar cells [8–10]. They are especially interesting in their doped state, when exhibiting the conductivity ranging from the conductivity typical for insulators to the conductivity typical for metals [11, 12]. For instance, as pointed out by Heeger [13], the nature of the elementary excitations, mobile charge carriers, or bound neutral excitants remains controversial.

Among these conjugated polymers, transpolyacetylene a quasi-one dimensional conductor, has been the subject of many investigations [14, 15]. Most of the theoretical works on elementary excitations in these materials have focused on a single-polyacetylene chain. In its doped state, polyacetylene

chain forms a new class of conducting polymers, in which the electrical conductivity can be varied over a range of eleven orders of magnitude [16, 17]. It is well known that the existence of dopants in conjugated polymers can greatly modify the transport properties of the system. Previous studies have reported the doping dependence of the conductivity of conjugated polymers [18–20], and showed that the effects are crucial for the improvements of device performance. Understanding phonon scattering properties due to dopants in such systems will be essential to extend elementary excitations physics into the mesoscopic regime, where a variety of size and geometry effects are important for scattering and transport properties. Phonon conductance plays a fundamental role in controlling the performance of molecular devices.

Transport properties of low-dimensional systems have been subjects of interest for a long time. Most of the recent research in this area has been oriented toward the study of electronic scattering. The understanding of coherent electronic transport in the mesoscopic regime has been

provided by the formalism of Landauer [21] and Büttiker [22] for electron transport in mesoscopic systems, who related the conductance of the system to its scattering matrix. Multiple scattering and quantum interference phenomena are not limited, however, to the electronic transport, but in a variety of problems they can become important for the coherent transport of other types of excitations such as phonons [23, 24] and magnons [25, 26] in low-dimensional systems.

The purpose of this work is to perform theoretical investigations on phonon dynamics and phonon conductance of potassium- and sodium-doped transpolyacetylene chain, by the use of the matching procedure, [27, 28] with nearest and next nearest neighbours elastic force constants. The scattering properties are calculated in full accordance with Landauer-Buttiker formalism for electron transport in mesoscopic systems. The defect is treated as the doped unit cell by substituting two hydrogen atoms by two potassium or two sodium atoms.

The paper is organized as follows. In Section 2, we present a brief description of the model used and the theoretical approach employed for studying the dynamic properties of undoped transpolyacetylene chain. In Section 3, we present the mathematical framework for determining the scattering properties due to given incorporated atoms or dopants in the unit cell of the undoped transpolyacetylene chain. Some numerical results and discussions are given in Section 4 for each case along with the conclusion of the paper.

2. Model and Its Dynamical Properties

The prototype of the conjugated polymers is polyacetylene $(\text{CH})_x$. In its simplest form, a single-polymer chain consists of a zigzag backbone of carbon atoms. One hydrogen atom is bonded to each carbon atom, so that every carbon atom is threefold coordinated. In Figure 1(a), we show, within the box defined by the dotted lines, the unit cell for transpolyacetylene chain. This unit cell of an infinite one-dimensional chain contains two inequivalent carbon atoms A and B. The simplest system model used in this study is depicted in Figure 1(b).

The atoms in the transpolyacetylene chain are held together by the chemical bonds between the atoms. These bonds are not rigid, but act like rings, which connect the atoms, creating a spring mass system with defined stiffness constants. Consider k , k_1 , and k_2 and k' , k'_1 , and k'_2 to denote the elastic force constants between nearest and next nearest neighbor sites as shown in Figure 1(b). We define for convenience the ratio: $\gamma_1 = k_1/k$, $\gamma_2 = k_2/k$, $\gamma_3 = k'/k$, $\gamma_4 = k'_1/k$, and $\gamma_5 = k'_2/k$. The approximation that we make is to neglect the motion of side groups relative to the backbone by compressing the atoms in the groups into masses m or M . Each mass m or M corresponding to the mass of a (C–H) or (C–K or C–Na) group, respectively, is linked to its neighbors by harmonic springs.

When an atom is displaced in the chain, this displacement can travel as a wave through the medium. These waves

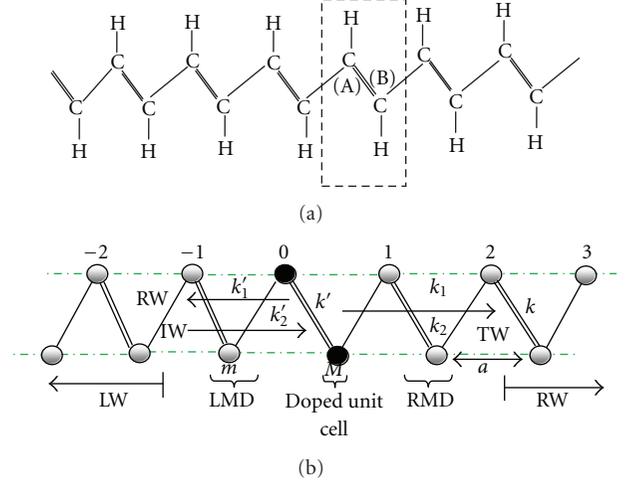


FIGURE 1: (a) A transpolyacetylene chain structure, showing the unit cell bounded by a box defined by the dotted lines with two inequivalent Carbon atoms A and B in the unit cell. (b) A schematic representation of doped transpolyacetylene chain. The doped unit cell may contain different masses and force constants. The elastic constants in the boundary may also be different from the rest of the undoped transpolyacetylene chain. The doped unit cell, the incident waves (IW), the reflected waves (RW) and the transmitted waves (TW) are shown. The two perfect wave guides (LW) and (RW) and the two matching domains (LMD) and (RMD) are also indicated.

can either be longitudinal, where the displacement of the atom is in the same direction as the propagation of the wave, or can be transverse, where the atomic displacement is perpendicular to the direction of propagation. The equation of motion for an atom located at site l in the two semiinfinite transpolyacetylene chains is given by:

$$\omega^2 m(l) u_\alpha(l, \omega) = - \sum_{l' \neq l} \sum_{\beta} k(l, l') d_\alpha \cdot \frac{d_\beta}{d^2} [u_\beta(l, \omega) - u_\beta(l', \omega)], \quad (1)$$

where the indices $(\alpha, \beta) \in \{x, y\}$ denote Cartesian coordinates. Identical mass m is considered for all the sites in the semiinfinite undoped polyacetylene chain. $m \equiv m(l)$ is the mass of the (CH) group and $u_\alpha(l, \omega)$ is the corresponding displacement vector of the atom along the Cartesian direction. The radius vector \mathbf{d} between l and l' , has Cartesian components d_α , and $d = |\mathbf{d}|$. Equation (1) is applied systematically for the transpolyacetylene chains, at the doped unit-cell boundary and in the domains to the left (LW) and the right (RW) of the doped unit cell. The same interatomic distance a is taken between nearest neighbour sites throughout the system.

The solutions to (1) for the two sites in the unit cell of the semiinfinite undoped transpolyacetylene chain far from the doped unit cell of the structure illustrated in Figure 1(b) may hence be expressed as

$$[\Omega^2 I - D(Z, \gamma_1, \gamma_2)] |U\rangle = 0, \quad (2)$$

where Ω is a dimensionless frequency given by $\Omega = \omega/\omega_0$. The frequency ω_0 characteristic of the system is given by $\omega_0^2 = k(l, l')/m$, for l and l' nearest neighbors. $D(Z, \gamma_1, \gamma_2)$ is the dynamic matrix for the configuration described in Figure 1(a). I is the corresponding unit matrix. The complex factors $Z(\nu)$ determine the phase changes of the solution of (2) along the undoped polyacetylene chain. We can distinguish between two different types of solutions: those corresponding to $|Z(\nu)| = 1$, which describes propagating modes, and to $|Z(\nu)| < 1$, which describes evanescent modes. The diagonalisation of the matrix D for $Z = \exp(iaq_x)$ leads to the propagating eigenmodes Ω and the corresponding eigenvectors $U_l(\Omega, q)$ for the undoped chain. The resulting phonon dispersion curves are usually given as function of the wave vector $\varphi_x = aq_x$, where a is the interatomic distance and q_x the one-dimensional reciprocal lattice wave vectors along the x direction in the first Brillouin zone.

The study of the phonon scattering in the presence of the doped unit cell requires a detailed analysis of both the propagating modes and the evanescent solutions of the system. In the undoped transpolyacetylene chain, these modes are described by the phase factor doublets $\{Z(\nu), 1/Z(\nu)\}$, which are complex conjugate pairs that verify symmetrically the characteristic secular equations in each half space. The $\{Z(\nu), 1/Z(\nu)\}$ complex phase factors are the solution of (2). The determinant of the dynamical matrix vanishes leading to a characteristic secular equation, that is solved for a given system parameters at frequency Ω . For the transpolyacetylene chain in Figure 1(b), only physical acceptable solutions are retained, namely, the propagating and the evanescent modes. The evanescent modes do not transport any energy but are necessary for a complete description of the scattering problem, and to match the solutions on either side of the defect. The evolution of the absolute values of these phase factors $Z(\nu)$ may be given as a function of the normalized frequency Ω and the elastic force constant parameters of the system γ_1 and γ_2 . A more interesting alternative is to present the dispersion curves via 3D representation of Ω as a function of the Real and Imaginary parts of the phase factors $Z(\nu)$.

3. Scattering at the Doped Unit Cell

A number of methods exist to study the vibration dynamics and scattering properties of perturbed crystals. The matching procedure that we employ in this paper allows one to deal with both aspects of localized modes and of wave scattering, within the same mathematical framework. The reflection and transmission probabilities as well as the conductance of the doped unit cell in transpolyacetylene chain are calculated as a function of the phonon scattering frequency Ω in full accordance with the Landauer-Buttiker formalism for electron transport.

In the absence of inelastic scattering, for an incoming propagating phonon eigenmodes ν' , incident from the left to right of the doped unit cell along the x direction, at a frequency Ω , the resulting scattered fields are composed of the reflected and the transmitted parts. For sites l inside

the left semiinfinite transpolyacetylene chain (LW), the Cartesian components α of the displacement field $u_\alpha^-(l)$ may be expressed as the sum of the incident phonon field and a superposition of the eigenmodes of the undoped polyacetylene chain, that are backward scattered in reflection at the same frequency

$$u_\alpha^-(l) = u_{\alpha\nu'} [Z(\nu')]^m + \sum_\nu [Z(\nu)]^{-m} u_{\alpha\nu} R_{\nu\nu'}. \quad (3)$$

$R_{\nu\nu'}$ denotes the reflection amplitudes for the backward scattering of incident phonon ν' into the eigenmodes ν . The quantities $u_{\alpha\nu}$ denote the eigenvectors of the dynamic matrix at a frequency Ω , which are associated with the atomic displacements u_α for the mode ν . For sites l inside the right semi-infinite transpolyacetylene chain (RW), the displacement field $u_\alpha^+(l)$ may be expressed by another appropriate superposition of the eigenmodes that are forward scattered at the same frequency

$$u_\alpha^+(l) = \sum_\nu [Z(\nu)]^{-m} u_{\alpha\nu} T_{\nu\nu'}. \quad (4)$$

$T_{\nu\nu'}$ denotes the transmission amplitudes for the forward scattering of the incident phonon ν' into the eigenmodes ν . We denote by $[|R\rangle, |T\rangle]$ the basis vectors for the reflection and transmission in a constructed Hilbert space, and by $|U\rangle$ the vector composed of the displacement for sites in the doped unit cell. The equations of motion for atoms of the doped unit-cell boundary, coupled to the rest of the polyacetylene chains via the matching domains (LMD) and (RMD), may be written as

$$[\Omega^2 I - D_s][|U\rangle, |R\rangle, |T\rangle] = -|IH\rangle, \quad (5)$$

where $D_s(Z, \gamma_1, \gamma_2, \gamma_3, \gamma_4, \text{ and } \gamma_5)$ is a square-matched scattering matrix, and the column vector $-|IH\rangle$, mapped appropriately onto the basis vectors, regroups the inhomogeneous terms describing the incident phonon. The solution of (5) yields the displacements $|U\rangle$ of the irreducible set of atomic sites for the doped unit cell as well as the coherent reflection and transmission amplitudes $R_{\nu\nu'}$ and $T_{\nu\nu'}$ at the scattering frequency Ω .

The scattering is usually described in terms of the scattering matrix. Its elements are given by the reflection and transmission amplitudes at the scattering frequency Ω . When the scattering domain is connected to external reservoirs by phonon wave-guides with open channels, as is the case in the presence of doped transpolyacetylene chain, the reflection and transmission probabilities, $r_{\nu\nu'}$ and $t_{\nu\nu'}$, are related to the elements of the scattering matrix, by

$$r_{\nu\nu'}(\Omega) = \left(\frac{v_{g\nu'}}{v_{g\nu}} \right) |R_{\nu\nu'}|^2, \quad t_{\nu\nu'}(\Omega) = \left(\frac{v_{g\nu'}}{v_{g\nu}} \right) |T_{\nu\nu'}|^2. \quad (6)$$

In order to satisfy the unitary requirements of the scattering matrix, the scattered waves have to be normalized with respect to their group velocity, $v_{g\nu'}$. It is taken equal to zero for evanescent eigenmodes. Summing over all outgoing

channels, we obtain the reflection and transmission probabilities for a given eigenmodes ν' at the frequency Ω

$$r_{\nu'}(\Omega) = \sum_{\nu'} r_{\nu\nu'}(\Omega), \quad t_{\nu'}(\Omega) = \sum_{\nu} t_{\nu\nu'}(\Omega). \quad (7)$$

Further, in order to describe the overall phonon transmission or reflection of the doped transpolyacetylene chain, it is possible to sum over all input and output channels. This allows one to obtain the system phonon reflectance and the system phonon conductance at any scattering frequency Ω , as

$$r(\Omega) = \sum_{\nu'} \sum_{\nu} t_{\nu\nu'}(\Omega), \quad t(\Omega) = \sum_{\nu'} \sum_{\nu} r_{\nu\nu'}(\Omega). \quad (8)$$

The transmission probabilities $t_{\nu'}(\Omega)$ per eigenmodes ν' and the phonon conductance $t(\Omega)$ are important quantities to calculate since each corresponds to an experimentally measurable observable. They play an essential role in the calculation, for example, of the net heat current across the defect between the two domains held at different temperatures.

4. Numerical Resultants and Discussion

Numerical calculations are carried out using the mathematical framework of the matching procedure in the harmonic approximation with a fixed ratio $\gamma_1 = k_1/k = 0.5$ and $\gamma_2 = k_2/k = 0.8$ for the undoped transpolyacetylene chain. Those model parameters used in this work are those generally chosen for transpolyacetylene [29].

By solving (2), one can determine the normalized frequency (Ω) of the waves as a function of their wave number (also called wave vector) (q_x), where $q_x = 2\pi/\lambda$. The relationship between Ω and $\varphi_x = aq_x$ may then be plotted in the form of a dispersion relation. One important parameter that can be found from the dispersion relation is the group velocity (v_g) of the phonons, which is the slope of the branch on the dispersion relation.

The resulting phonon dispersion curves $\Omega(\varphi_x)$ far from the doped unit cell in each half-space are given in Figure 2(a) over the first Brillouin zone, for $\varphi_x \in [-\pi, +\pi]$. In this case, the eigenmodes labelled $\nu \in \{1, 2, 3, 4\}$ are propagating modes in the following respective frequency intervals:

$$\begin{aligned} \Omega_1 &= [\Omega_{1,\min} = 0, \Omega_{1,\max} = 0.7067], \\ \Omega_2 &= [\Omega_{2,\min} = 0, \Omega_{2,\max} = 1.4233], \\ \Omega_3 &= [\Omega_{3,\min} = 1.2267, \Omega_{3,\max} = 1.7889], \\ \Omega_4 &= [\Omega_{4,\min} = 1.5735, \Omega_{4,\max} = 2.1695]. \end{aligned} \quad (9)$$

Note that the four modes are indexed from the bottom to the top in Figure 2(a). It should be emphasized that in the frequency intervals some of the modes are propagating phonons, the others are evanescent modes. Figure 2(a) shows two distinct phonon modes in the dispersion curves. The two lower modes are called the acoustic modes because the linear relationship $\Omega = v_g \varphi_x$ for low frequency is similar to that for

a sound wave. These modes correspond to two neighboring atoms moving in phase with one another. The two upper modes, called the optic modes, correspond to the case where two neighboring atoms are moving out of phase with one another; for low frequencies, these modes are characterized by a vanishing group velocity. Because the group velocity of the optic modes is small or equal to zero at low frequencies, these modes generally do not participate in the heat transport process.

The behavior of the eigenmodes can be illustrated graphically by the curves $\Omega(Z)$ on and inside the unit circle of the complex plane. The resulting dispersion curves in the complex Z plane are represented in Figure 2(b), with nearest and next nearest neighbor interactions k_1 and k_2 for the specific case of $\gamma_1 = 0.5$ and $\gamma_2 = 0.8$ for the system, showing typically the generalized functional behavior for the four eigenmodes. The propagating modes, namely, $|Z(\nu)| = 1$, are represented by the curves following the unit circle. Usually the latter is represented by the phonon dispersion curves as a function of the wave vector $\varphi_x = aq_x$, rather than as a function of the parameter $Z = \exp(iaq_x)$. The evanescent modes inside the unit circle are described for $|Z(\nu)| < 1$. The absolute values of the phase factors as a function of the normalized frequency Ω are given specifically in Figure 3(a). For completeness, we also present in Figure 3(b) the group velocities of the phonon eigenmodes over their frequency intervals of propagation, under the same conditions.

The phonon scattering properties of the doped transpolyacetylene chain are calculated using (7) and (8) with reference to wave incident from the left to the right of the doped unit cell, in Figure 1(b). Numerical results are obtained for a number of choices concerning the system force constants in the scattering domain. We have investigated the evolution of these results and found that it is interesting to present those for scattering from a set of system parameters $\gamma_3 = 0.9$, $\gamma_4 = 0.95$, and $\gamma_5 = 0.5$ in two cases of interest as regards the mass of atoms constituting the doped unit cell, namely, the potassium and sodium atoms.

In Figures 4(a)–4(d) and 5(a)–5(d), we present the phonon scattering frequency Ω dependency of the calculated transmission t_1, t_2, t_3 , and t_4 and reflection r_1, r_2, r_3, r_4 probabilities, owing to the scattering of phonon modes 1, 2, 3 and 4 respectively, in the cases of potassium- and sodium-doped unit cell in polyacetylene chain.

The results show that the transmission probabilities are a sensitive function of the scattering frequency Ω . As expected, the influence of the dopants is smallest at low frequency. At the Brillouin zone center, where Ω tends to zero, only acoustical modes 1 and 2 are excited. In this domain, the transmission probabilities approach the unity for these incident modes, which indicates that the doped unit cell does not influence the transmission for wavelengths much greater than the lattice constant. The presence of dopants in the transpolyacetylene chain leads, however, to a general decrease of the transmission probabilities with increasing the scattering energy Ω and becomes zero at the BZ boundaries. For high frequencies, only the optical modes 3 and 4 are excited. We note that the frequency interval correspond to the propagating phonon modes 1, 2, 3, and 4, indicated in

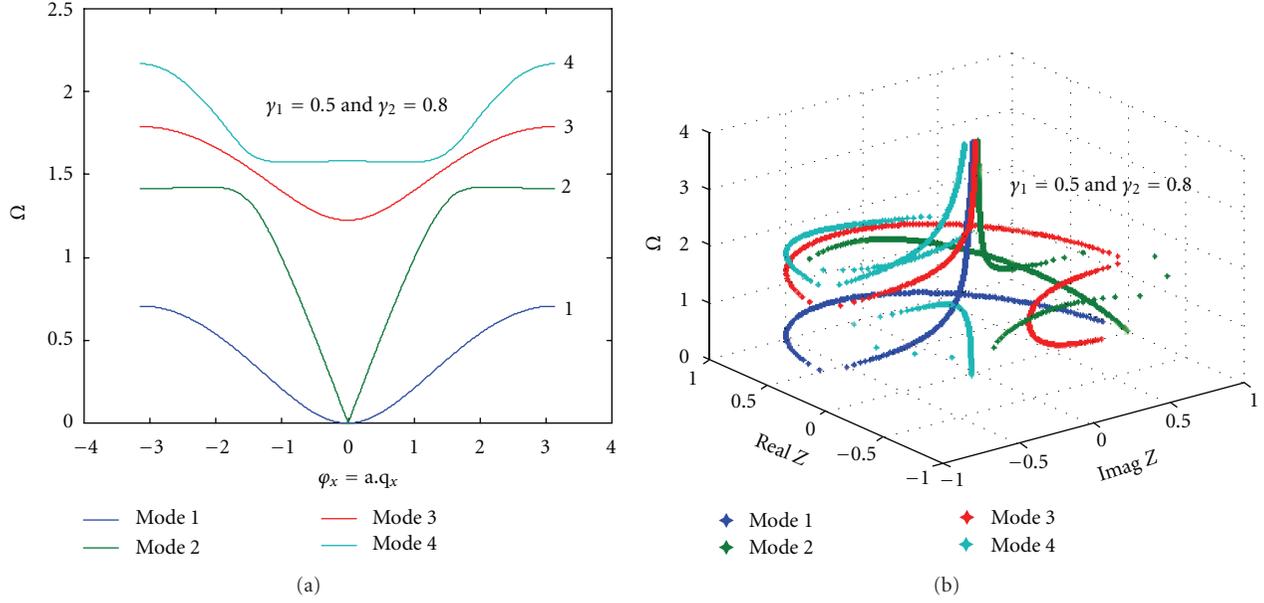


FIGURE 2: (a) A typical Phonon dispersion curve $\Omega(\varphi_x)$ for the considered undoped transpolyacetylene chain, with the ratio of $\gamma_1 = k_1/k = 0.5$ and $\gamma_2 = k_2/k = 0.8$ for the system. They are shown here over the interval $\varphi_x = [-\pi, +\pi]$ of the first Brillouin zone. (b) A three-dimensional view of the vibration eigenmodes $\Omega(Z_\nu)$ for the considered transpolyacetylene chain with nearest and next nearest neighbor interactions k_1 and k_2 for the specific case of $\gamma_1 = k_1/k = 0.5$ and $\gamma_2 = k_2/k = 0.8$; with Z_ν the phase factors, ν is taken here with the values 1, 2, 3, and 4.

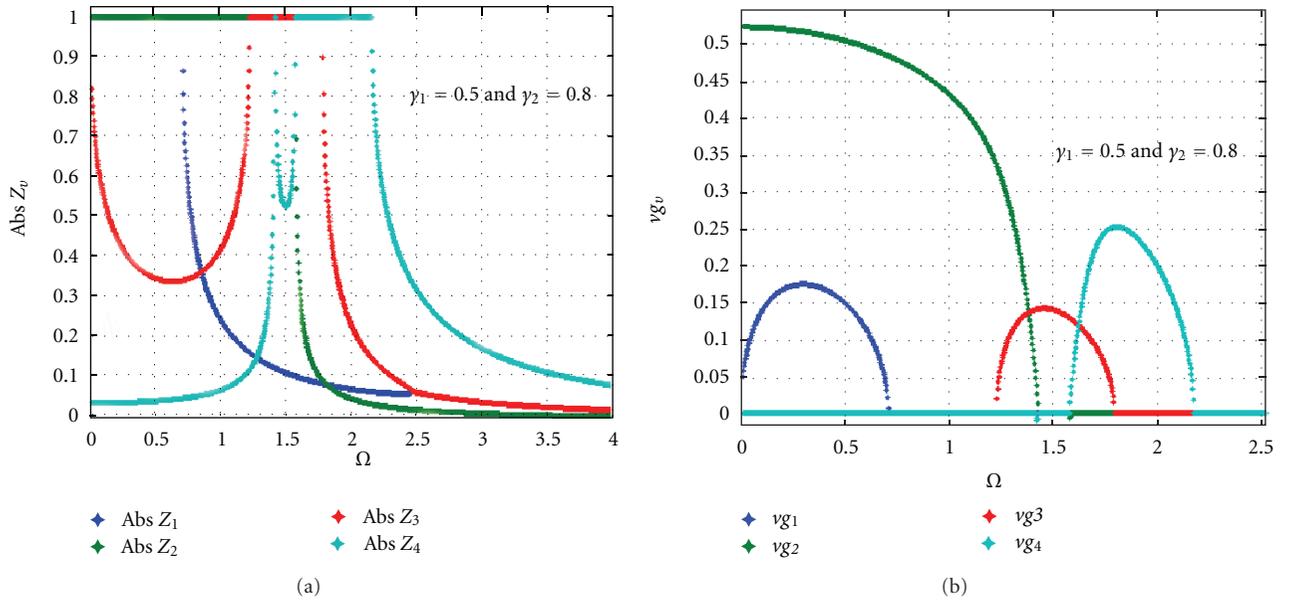


FIGURE 3: (a) Evolution of the absolute values of the complex phase factors Z_ν , as a function of the dimensionless frequency Ω , for the above γ_1 and γ_2 values. (b) Group velocity v_g for the different phonon eigenmodes as a function of the dimensionless frequency Ω , for the specific case of $\gamma_1 = k_1/k = 0.5$ and $\gamma_2 = k_2/k = 0.8$ of the undoped transpolyacetylene chain.

Figure 2(a). The upper and lower scattering frequency limits of the t_ν and r_ν spectra can be identified with reference to the dispersion curves of the undoped transpolyacetylene chain. The most striking consequence of these dopants is the appearance of resonance structures in the transmission

spectra as a function of the scattering frequency, which can be understood as Fano resonances, usually invoked to describe the coherent coupling between the propagating modes of the system and the localized vibration modes induced by the potassium atoms. The transmission and the

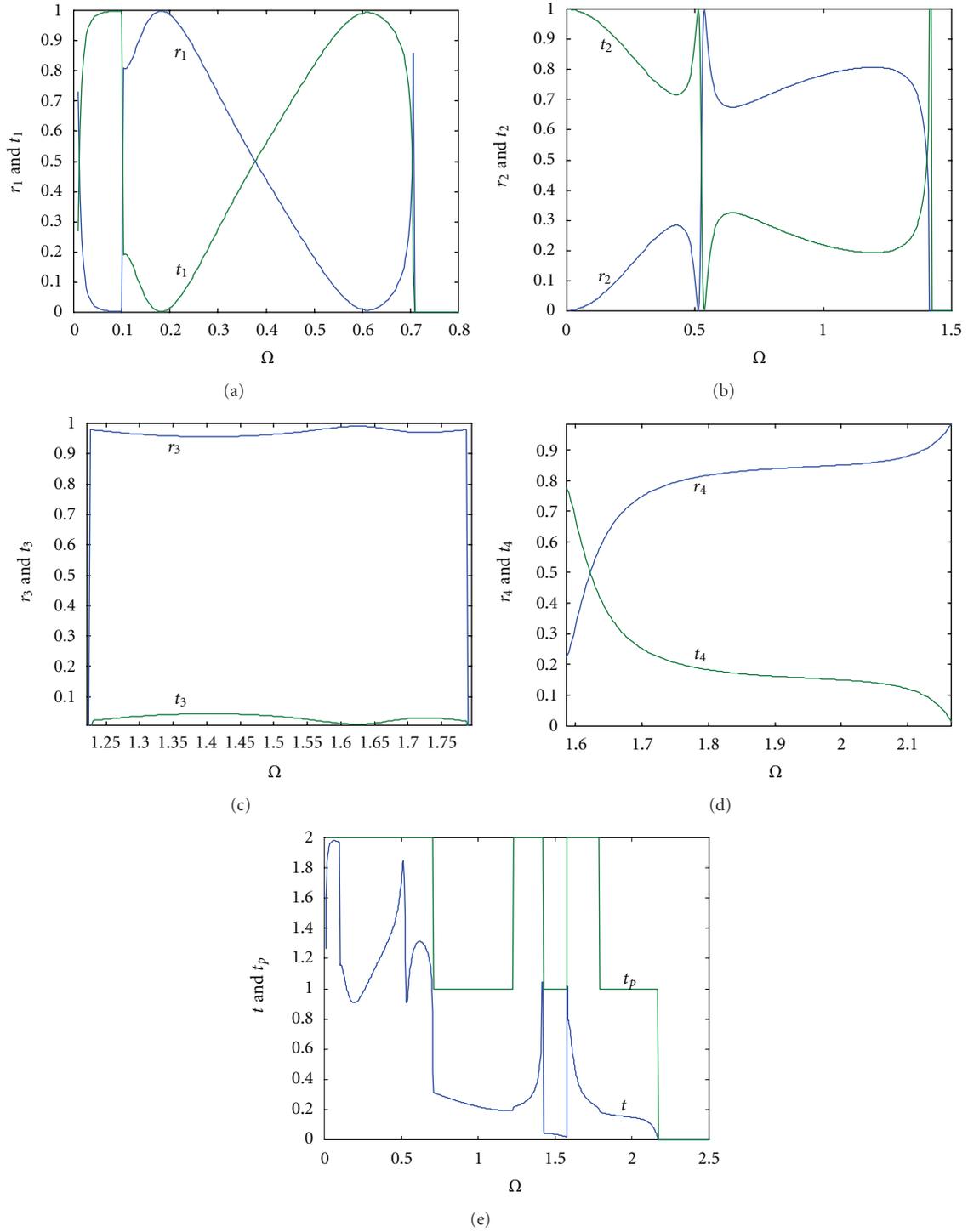


FIGURE 4: (a) The transmission t_1 and the reflection r_1 coefficients for phonon incident mode 1, (b) the transmission t_2 and the reflection r_2 coefficients for phonon incident mode 2, (c) the transmission t_3 , and the reflection r_3 coefficients for phonon incident mode 3, (d) the transmission t_4 and the reflection r_4 coefficients for phonon incident mode 4, and (e) the total transmission probability $t(\Omega)$ or phonon conductance of the doped transpolyacetylene chain and the total transmission probability $t_p(\Omega)$ or phonon conductance of the undoped transpolyacetylene chain as a function of the scattering frequency Ω in the case of potassium-doped transpolyacetylene chain with $e(K) = M/m = 4.54$.

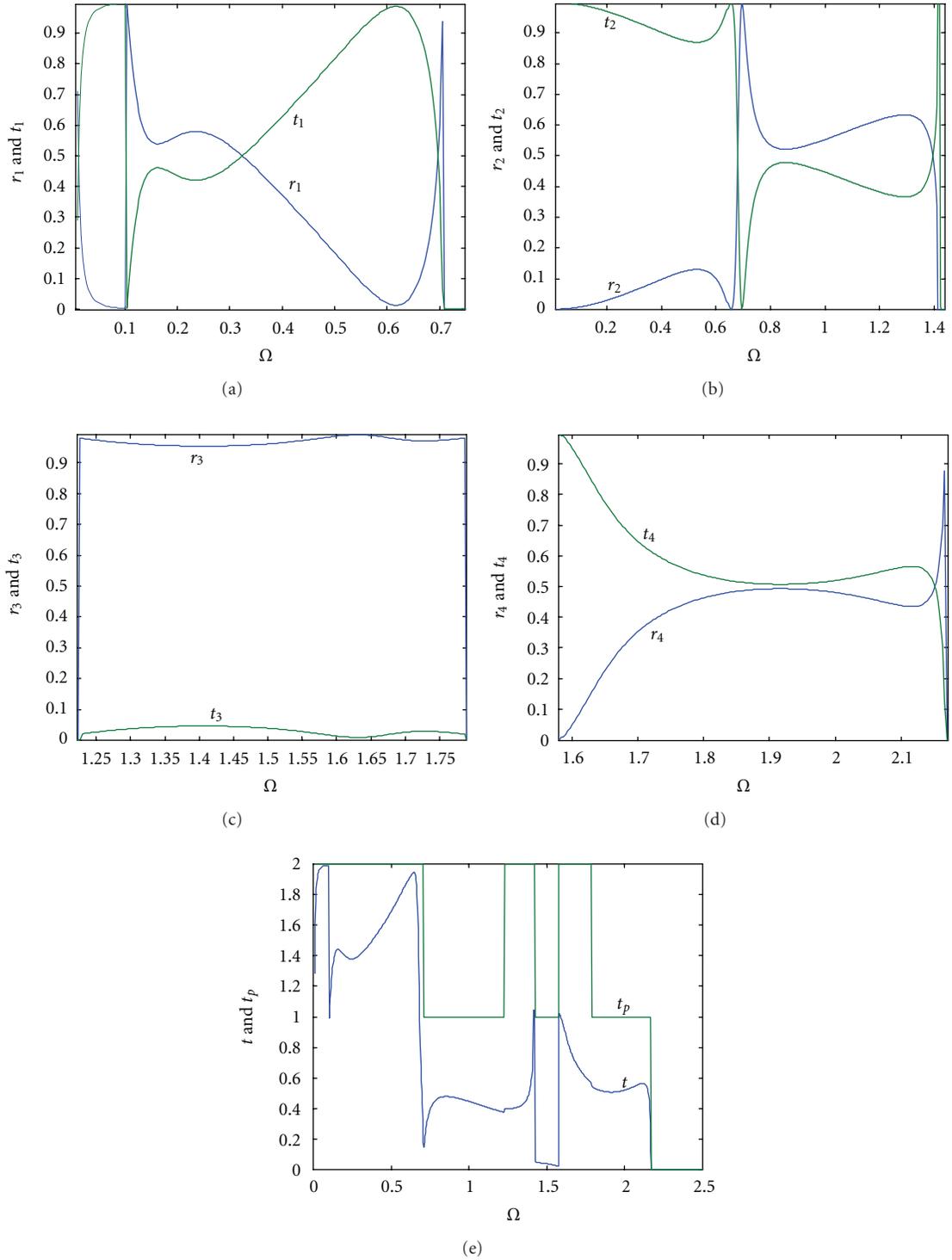


FIGURE 5: Similar to Figure 4 for the case of sodium-doped transpolyacetylene chain with $e(\text{Na}) = M/m = 2.69$.

reflection cross-sections verify the unitarity condition for the scattering matrix, and this is used throughout as a check on the numerical calculation.

In Figures 4(e) and 5(e), the total transmission probability $t(\Omega)$ or phonon conductance of potassium- and sodium-doped transpolyacetylene chain, respectively, and

the total transmission probability $t_p(\Omega)$ or phonon conductance of undoped transpolyacetylene chain, respectively, are presented as a function of the scattering frequency Ω . The phonon conductance of the system $t(\Omega)$ is useful to calculate, as it corresponds to an experimentally measurable quantity, for example, for thermal transport across such doped

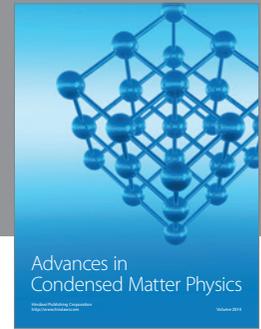
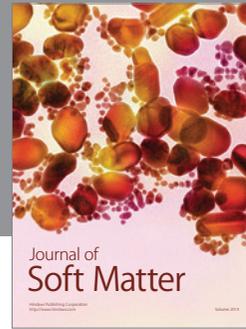
polymer. The histogram step of t_p in Figures 4(e) and 5(e) corresponds to the change in the number of propagating modes in the different frequency intervals.

In summary, we have studied theoretically the phonon dynamics and scattering properties in doped conjugated polymers such as potassium- and sodium-doped transpolyacetylene chain. The dispersion curves and group velocities as well as the phase factors of the propagating modes in undoped transpolyacetylene chain are calculated. Numerical results are obtained and graphically presented as function of the scattering frequency. We have also analyzed the dependence of the phonon transmission and reflection probabilities as well as the phonon conductance on the scattering frequency. This is done using the mathematical framework of the matching procedure in the harmonic approximation with nearest and next nearest neighbor elastic force constants. Our numerical results show that in spite of their special character, the scattering of phonons has some features in common with the scattering of electron waves, which can be described in terms of basically the same interference phenomena. The results show that the transmission probabilities and the phonon conductance, calculated in full accordance with the Landauer-Buttiker description of electron transport in mesoscopic systems are a strong function of the scattering frequency. The most striking consequence of this defect is the appearance of resonance structures in the transmission spectra as a function of the scattering frequency and system parameters. They are understood as Fano resonances, which are usually invoked to describe the coherent coupling between the propagating modes of the system and the localized vibration modes in the neighborhood of the dopants.

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