Theoretical description of electron–phonon Fock space for gapless and gapped nanowires*

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We study the effect of electron–phonon (e–ph) interaction on the elastic and inelastic electronic transport of a nanowire connected to two simple rigid leads within the tight-binding and harmonic approximations. The model is constructed using Green's function and multi-channel techniques, taking into account the local and nonlocal e–ph interactions. Then, we examine the model for the gapless (simple chain) and gapped (PA-like nanowire) systems. The results show that the tunneling conductance is improved by the e–ph interaction in both local and nonlocal regimes, while for the resonance conductance, the coherent part mainly decreases and the incoherent part increases. At the corresponding energies which depend on the phonon frequency, two dips in the elastic and two peaks in the inelastic conductance spectra appear. The reason is the absorption of the phonon by the electron in transition into inelastic channels.

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1. Introduction

The current developments and advances in the nanostructures and molecular electronics have led to the creation of novel powerful and highly efficient electronic components with very small sizes.[1] Therefore, understanding the transport properties of such systems for their use in theoretical predictions and explanation of experimental results is crucial. This helps us in the fabrication of molecular/nanoscale thermal and electrical devices and improving the measurement methods in both application and research.[2,3] As is known, the thermal and electrical aspects of carriers are affected by each other. In particular, an electrical quantity such as conductance can be influenced by phonons via electron–phonon (e–ph) interaction leading to physical phenomena like thermoelectric,[4,5] superconductivity,[6] Peierls instability,[7,8], Jahn–Teller effect,[9] and so on. This may be the reason that some running theoretical and experimental research studies have been focused on the topic of e–ph interaction in nanostructures.[10–13] Numerous theoretical methods such as density functional theory,[14] semi-classical Boltzmann transport equation,[15] and Green's function technique[16] have been used to study this problem. In the weak coupling regime, usually the perturbative approaches are performed,[11,17] while in the strong coupling regime, the Fock space is a useful tool to consider the elastic and inelastic components of the system conductance separately. [18,19] In some special cases, this space can convert a one-channel many-body problem into a multi-channel one-body problem which is based on the concept of absorption and emission of phonon(s) due to e–ph interaction.

In this paper, we discuss the total electronic transmission coefficient as well as its elastic and inelastic components for a vibrating nanowire embedded between two uniform semi-infinite rigid leads. To this end, a model is suggested based on Green's function and multi-channel techniques within the nearest-neighbor tight-binding and harmonic approximations. The model gives simple analysis and comparison of local (Holstein model[20]) and nonlocal (Peierls-type model[21]) e–ph interaction effects on the conductance.[22] Also, it determines the contributions of elastic or inelastic parts in the total electronic transmission through the system depending on the tight-binding and interaction parameters. In this model, two types of simple and polyacetylene (PA) systems are examined to see the behaviors of tunneling and resonance conductances with respect to the type and strength of the e–ph interaction.

The paper is organized as follows. In Section 2, we present the framework of formalism by introducing the Green's function and multi-channels techniques. In this section, some expressions for computing the elastic, inelastic, and total electronic transmission coefficients at zero temperature are obtained. In Section 3, we perform the numerical calculation for six-atom uniform and PA-like nanowires as the examples of gapless and gapped systems, respectively. Comparison between the local and nonlocal as well as the elastic and inelastic regimes is given in this section. Finally, in Section 4, the concluding remarks of the paper are summarized.

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2. Model and formalism

We apply the zero temperature multi-channel technique to study the electronic transport properties of a vibrating simple chain including N atoms which is embedded between two simple rigid leads. Since at a special optical phonon mode the variations of the electronic hopping energies of the center wire can be maximum,[23] we limit ourselves to study only this polarized mode. Therefore, the Hamiltonian of the isolated central chain including the electronic, phononic, and e–ph interaction parts can be written as

$$H_{\rm W} = \sum_i \Big(\varepsilon_{\rm W} c_i^\dagger c_i + \hbar\omega b_i^\dagger b_i + \beta_{{\rm W},i}(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \Big(g c_i^\dagger c_i + \alpha(-1)^{i+1}(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)\Big)(b_i + b_i^\dagger)\Big), \quad (1)$$

where $b_i^\dagger$ and $c_i^\dagger$ are the phonon and electron creation operators at the i-th site, respectively, $\varepsilon_{\rm W}$ is the atomic electron on-site energy, $\beta_{{\rm W},i}$ is the electron hopping energy between the nearest neighbors which is intended as $\beta_{\rm W}$ for a simple chain and $\beta_{\rm s(d)}$ for the single (double) bond in a PA-like chain. Also, g and α denote the strengths of local and nonlocal e–ph couplings, respectively, which we suppose exist only in the center wire. Finally, ω indicates the phonon frequency of independent harmonic oscillators in the center chain. The term including the $(-1)^{i+1}$ coefficient refers to the fact that we choose a special optical mode in which the neighbor atoms oscillate against each other. The basis of the Fock space is specified as[24]

$$|i,n\rangle = c_i^\dagger \frac{(b_i^\dagger)^n}{\sqrt{n!}}|0\rangle, \quad (2)$$

where $|0\rangle$ represents the vacuum state, and n is the phonon quantum number. Then, the effective Hamiltonian of the center wire in terms of Fock states and in the presence of the electrodes is obtained as

$$\begin{aligned} H_{\rm W}^{\rm (eff)} = & \sum_i \sum_n \Big(\varepsilon_{\rm W} + n\hbar\omega + \Sigma_{\rm L}^{(n)}\delta_{i,1}\delta_{n,0} + \Sigma_{\rm R}^{(n)}\delta_{i,6}\Big) \\ & \times |i,n\rangle\langle i,n| + g\sqrt{n+1}\,|i,n\rangle\langle i,n+1| \\ & + \beta_{{\rm W},i}|i,n\rangle\langle i+1,n| \\ & + \alpha(-1)^{i+1}\sqrt{n+1}\Big(|i,n\rangle\langle i+1,n+1| \\ & + |i,n+1\rangle\langle i+1,n|\Big) + {\rm h.c.}, \end{aligned} \quad (3)$$

where $\delta_{i,j}$ is the Kronecker delta function, and $\Sigma_{\rm L(R)}^{(n)}$ is the chain self-energy of the n-th channel due to the existence of the rigid left (right) lead. In the nearest neighbor tight-binding approximation and in the absence of e–ph interaction in the whole system, this quantity obeys a standard formula ($n = 0$ in the following equation).[16] In the presence of e–ph interaction in the center wire, the electron absorbs n phonons and the band energy of the outgoing rigid lead will be shifted by $n\hbar\omega$.[25] Therefore, we can write

$$\Sigma_{\rm L(R)}^{(n)}(\varepsilon) = \frac{\beta_{\rm WL(R)}^2}{\beta_{\rm L(R)}} \exp\Big({\rm i}\cos^{-1}\Big(\frac{\varepsilon - \varepsilon_{\rm L(R)} - n\hbar\omega}{2\beta_{\rm L(R)}}\Big)\Big), \quad (4)$$

where ε is the electron energy, $\beta_{\rm WL(R)}$ is the hopping integral of the left (right) contact, and $\varepsilon_{\rm L(R)}$ and $\beta_{\rm L(R)}$ are the on-site and hopping energies of the left (right) lead, respectively. In Fig. 1, we present a scheme of multi-channel or electron–phonon Fock space according to Eq. (3). In this figure, the vertical and diagonal dashed lines indicate the e–ph coupling interaction effect on the electronic on-site (local) and hopping (nonlocal) energies, respectively. As it can be seen, there are maximum $N+1$ output channels (7 for Fig. 1) which refer to the linear form of the phonon part of the e–ph interaction term in Hamiltonian (1). By using Eq. (3), the effective Green's function of the center wire in the presence of the e–ph interaction and the left (right) lead is

$$G = \frac{1}{\varepsilon I - H_{\rm W}^{\rm (eff)}}, \quad (5)$$

where I is the unit matrix in the Fock space. Therefore, the Green's function in matrix form takes the dimension $d \times d$, where $d = N(N+3)/2$ is the number of intersections of the horizontal and vertical lines in the schematic picture of Fock space (27 for Fig. 1). Now, by evaluating the elements of the above mentioned Green's matrix, the electronic transmission coefficients from different channels can be determined. The analytic form of these elements is more complicated and the evaluation should be performed numerically. Specifically, the electronic transmission coefficient through a channel with no phonon absorption at the left lead and n phonon absorption by electron coming out at the right lead is given by[16,26]

$$T_{0,n} = 4{\rm Im}\,\Sigma_{\rm L}^{(0)}\,{\rm Im}\,\Sigma_{\rm R}^{(n)}\,\big|G_{1,n+N(N+1)/2}\big|^2, \quad (6)$$

where $G_{1,n+N(N+1)/2}$ is the first row and $(n+N(N+1)/2)$-th column element of the Green's function matrix in Fock space. By entering an electron from the left rigid lead into the vibrating region, n phonons are absorbed by the electron and it comes out from the n-th right channel. The matrix element of the Green's function corresponding to this travel is $1, n+N(N+1)/2$. Also, the following summation specifies the total transmission coefficient of the system as a function of incoming electron energy

$$T_{\rm tot}(\varepsilon) = \sum_{n=0}^{N} T_{0,n}, \quad (7)$$

which includes the elastic (without changing in the passing electron energy) and inelastic parts (including all phonon absorption channels) as

$$T_{\rm elastic}(\varepsilon) = T_{0,0}, \quad (8)$$

$$T_{\rm inelastic}(\varepsilon) = \sum_{n=1}^{N} T_{0,n}. \quad (9)$$

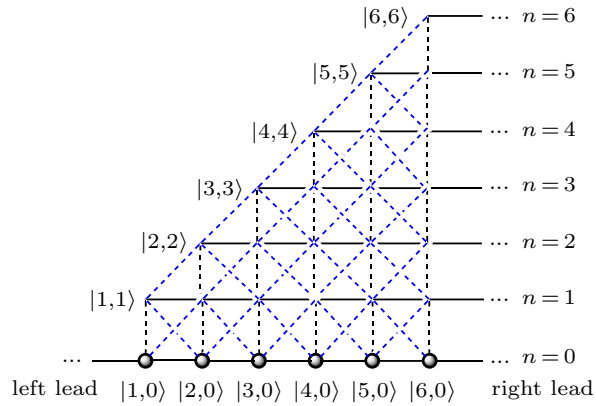


Fig. 1. (color online) Schematic picture of Fock space for electron–phonon states. The intersections of horizontal and vertical lines indicate the electronic sites and the corresponding phononic states. The solid lines refer to electronic hopping terms and the vertical and diagonal dashed lines are used to represent the local and nonlocal e–ph interactions, respectively.

3. Results

We consider a vibrating chain and a PA-like nanowire with six atoms which are connected to two semi-infinite simple rigid leads to calculate the elastic (Eq. (9)), inelastic, (Eq. (8)) and total (Eq. (7)) transmission coefficients. We study the mechanism of conductance and its comparison at the simple (gapless) and PA-like (including gap) chains in the local (Holstein) and nonlocal (Peierls-type) models. It is evident that each model can be considered separately by setting zero value for the corresponding e–ph coupling parameter of the other model (α for local and g for nonlocal). We have chosen the PA-like nanowire to find out how the electronic tunneling conductance can be influenced by the e–ph interaction at local and nonlocal regimes. Throughout the paper, the tight-binding parameters are set as $\beta_{\mathrm{W(L,R)}} = 1$ eV, $\beta_{\mathrm{WL(R)}} = 0.8$ eV, $\beta_{\mathrm{s}} = 0.8$ eV, $\beta_{\mathrm{d}} = 1.2$ eV, and $\varepsilon_{\mathrm{W(L,R)}} = 0$. We discuss the phononic and e–ph coupling parameters with the dynamic values.

Figures 2(a)–2(c) present respectively the variations of the elastic, inelastic, and total electronic transmission coefficients of the simple chain with respect to energy for several different local e–ph coupling strengths, $g = 0$ eV, 0.05 eV, 0.1 eV, and 0.15 eV. Here, we take the nonlocal e–ph coupling strength to be zero, which leads us to construct the Holstein model. Moreover, $\hbar\omega$ is chosen as 0.1 eV. It is first noted that in the presence of the e–ph interaction, the symmetry of the transmission function around the zero energy is missed. Due to the scattering of the transmitted electrons through the inelastic channels by increasing g, the elastic part of the transmission coefficient decreases while the inelastic part rises in most energies. According to Fig. 2(a), in the elastic transmittance spectra, there are two sharp dips which are produced by destructive interferences of electron wave-functions at different paths between initial and final channels of Fock space. At the corresponding energies where these dips occur, two peaks are observed in the inelastic component of the transmission coefficient (Fig. 2(b)), originated from scattering of electrons by phonons into the inelastic channels. The behavior of the total transmission coefficient (Fig. 2(c)) illustrates that the elastic contribution has overcome the inelastic one at these energies. Moreover, the Fano-resonance appearing at nearly 1.1 eV originates from the elastic part. At the valleys near the edges of the energy band as well as in the energy range [0.6 eV, 1.2 eV], the inelastic part will be overcome. Around the zero energy, the elastic and inelastic conductance components exhibit the constant and growing behaviors, respectively, when the hopping e–ph coupling strength increases. In other energies, especially at the resonance peaks, the elastic and inelastic regimes contribute equally to the conductance and neutralize the effect of each other.

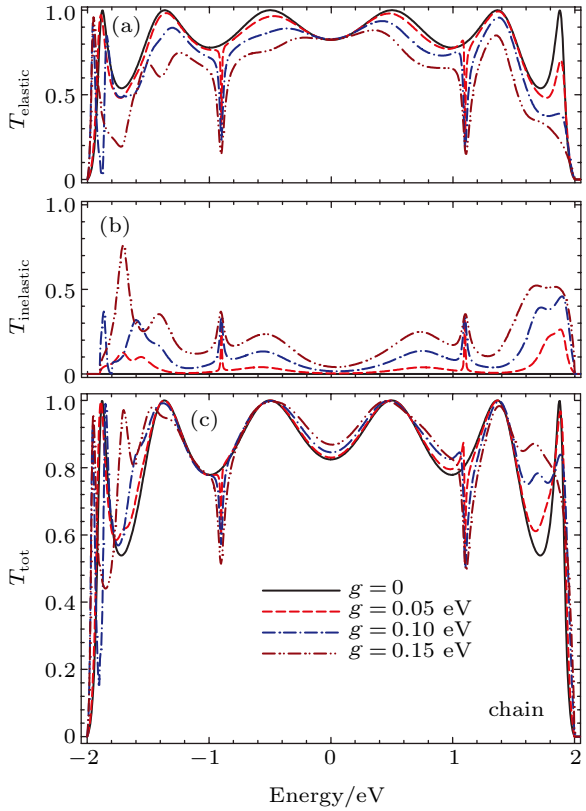


Fig. 2. (color online) (a) Elastic, (b) inelastic, and (c) total transmission coefficients of a six-atom vibrating chain connected to two rigid leads vs. energy for some different local e–ph coupling strengths. Here, we take $\beta_{\mathrm{L(R)}} = \beta_{\mathrm{W}} = 1$ eV, $\varepsilon_{\mathrm{W(L,R)}} = 0$, $\beta_{\mathrm{WL}} = \beta_{\mathrm{WR}} = 0.8$ eV, $\alpha = 0$, and $\hbar\omega = 0.1$ eV.

In order to examine the model for the tunneling conductance, we present in Figs. 3(a)–3(c), the elastic, inelastic, and total transmission coefficients of a six-atom PA-like chain as a function of energy for some different local e–ph coupling strengths. The numerical parameters needed to plot these figures are the same as those used in Fig. 2. By choosing the numerical values of 0.8 eV and 1.2 eV for β_{s} and β_{d}, respectively, the gap of the system lies in the range of $[-0.4\,\mathrm{eV}, 0.4\,\mathrm{eV}]$. In

this area, the behavior of the conductance is tunneling, while in other energies, it has the resonance mechanism. The figure demonstrates that the e–ph interaction helps the tunneling conductance (phonon-assisted tunneling effect[25,27]), while for the resonance conductance, the situation depends on the energy of the electron. In the PA-like nanowire, the e–ph interaction influences more specifically the anti-resonance dips compared with the simple chain (Fig. 2). Now, we simulate the Peierls-type model by putting the value of zero for g in the formalism. Figures 4(a)–4(c) respectively show the variations of the elastic, inelastic, and total electronic transmission coefficients of a six-atom vibrating chain confined between two similar simple rigid leads versus energy for some different nonlocal e–ph coupling strengths. Again, we take all needed numerical values the same as those used in the previous figures. First, by comparing between this figure and Fig. 2, it is seen that the effect of α is more important than g in the energies between the dips, while in other energies, the conductance variation is negligible, especially in the elastic and total ones. In the conductance spectra, the positions of peaks between two dips come close together by increasing α. Also, a Fano-resonance appears in the negative energies near -0.9 eV.

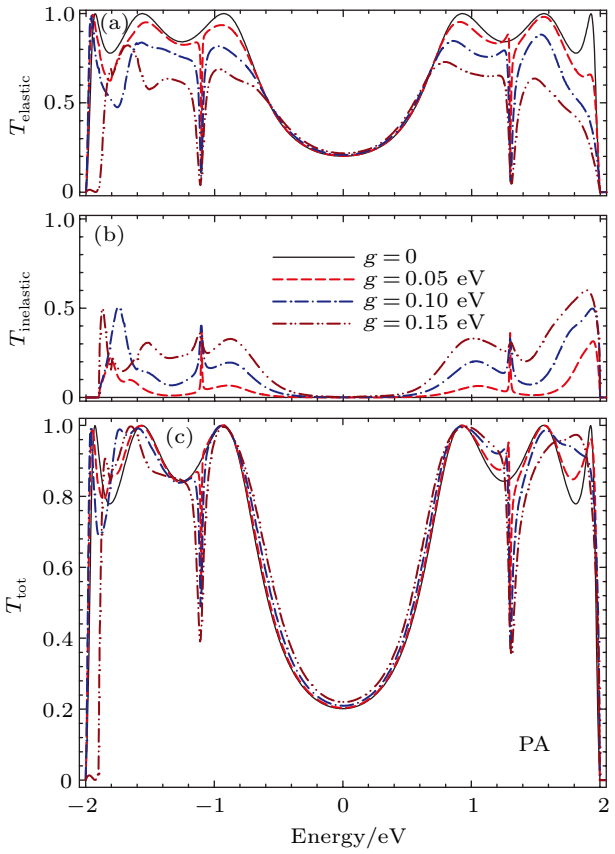


Fig. 3. (color online) (a) Elastic, (b) inelastic, and (c) total transmission coefficients of a six-atom PA-like chain embedded between two simple rigid leads vs. energy for some different local e–ph coupling strengths. Here, we set $\beta_{\rm L(R)} = 1$ eV, $\beta_{\rm s} = 0.8$ eV, $\beta_{\rm d} = 1.2$ eV, $\varepsilon_{\rm W(L,R)} = 0$, $\beta_{\rm WL(R)} = 0.8$ eV, $\alpha = 0$, and $\hbar\omega = 0.1$ eV.

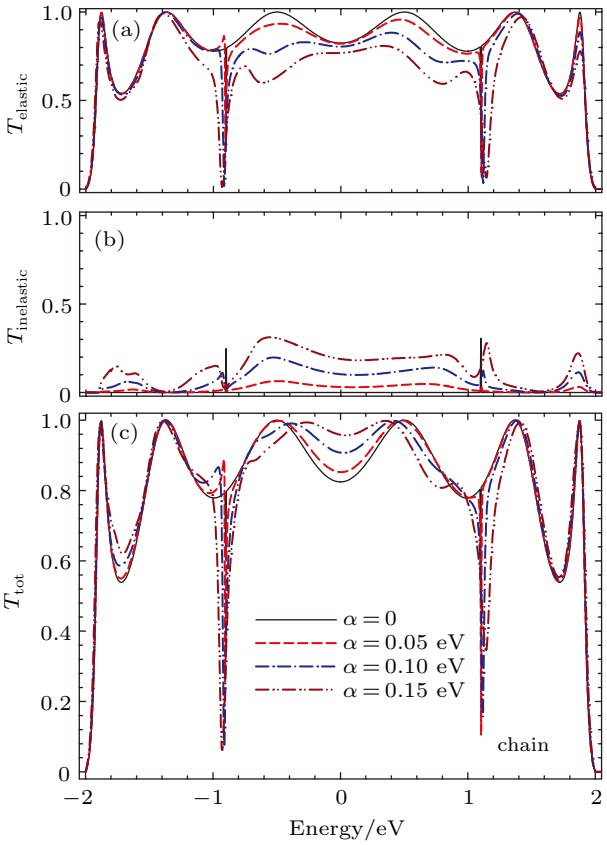


Fig. 4. (color online) (a) Elastic, (b) inelastic, and (c) total transmission coefficients of a six-atom vibrating chain connected between two simple rigid leads vs. energy for some different hopping e–ph coupling strengths. Here, we set $\beta_{\rm L(R)} = \beta_{\rm W} = 1$ eV, $\varepsilon_{\rm W(L,R)} = 0$, $\beta_{\rm WL(R)} = 0.8$ eV, $g = 0$, and $\hbar\omega = 0.1$ eV.

In Fig. 5, we plot $T_{\rm elastic}$, $T_{\rm inelastic}$, and $T_{\rm tot}$ for the six-atom PA-like nanowire under the conditions like Fig. 4. Again, the α parameter affects the conductance more than g (Fig. 3). In the area between two dips, the peak which is located in the positive energies is shifted to the left by a rising α, while the position of the peak which is located in the negative energies is fixed. At the end of the negative part of the energy band, a satellite peak appears at large values of α. The tuning of the total transmission coefficient at zero energy by values of g and α for simple and PA-like chains is studied in Fig. 6. Figures 6(a) and 6(b) are for the simple chain and figures 6(c) and 6(d) are for the PA-like nanowire. The model parameters are chosen as before. We observe that the conductance is influenced more by α with respect to g for both types of systems. Comparison of Fig. 6(a) with Fig. 6(c) shows that at a fixed α, when g varies, the conductance of the chain changes more than that of the PA-like nanowire. A similar situation occurs when g is fixed and α is varied.

Figures 7(a)–7(b) show respectively the total electronic transmission coefficients of the simple and the PA-like chains as functions of energy for several different $\hbar\omega$. We set the numerical parameters the same as those in the previous figures except that we fix $g = 0.1$ eV and $\alpha = 0$. By increasing $\hbar\omega$,

both conductance dips move to the right in the value of $\hbar\omega$. At the energies between the dips, the conductance for both chain and PA-like systems is independent of the phonon frequency. In the left edge of the energy band, the effect of this parameter is more observable than that in the right one.

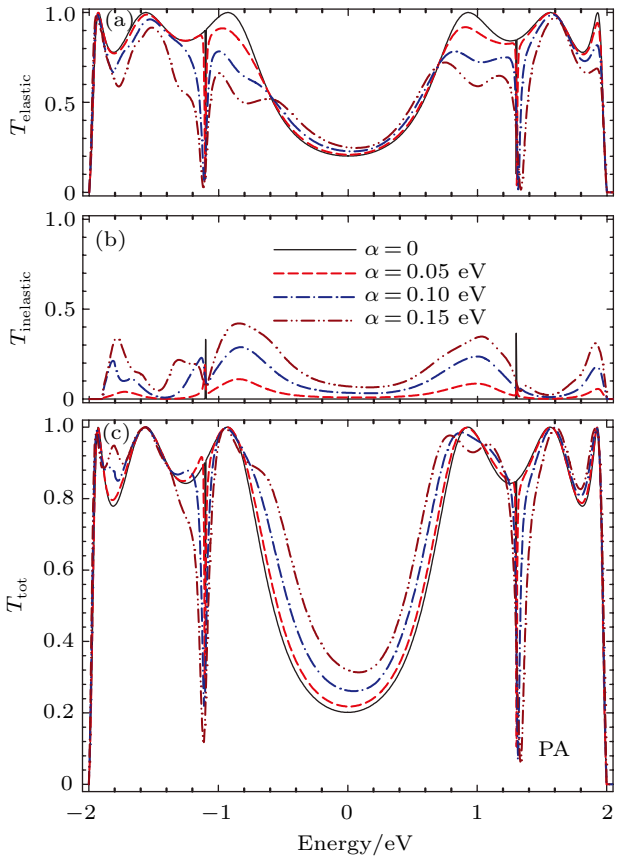


Fig. 5. (color online) (a) Elastic, (b) inelastic, and (c) total transmission coefficients of a PA-like nanowire confined between two simple rigid leads as functions of energy for some different nonlocal e–ph coupling strengths. Here, we set $\beta_{\rm L(R)} = 1$ eV, $\beta_{\rm s} = 0.8$ eV, $\beta_{\rm d} = 1.2$ eV, $\varepsilon_{\rm W(L,R)} = 0$, $\beta_{\rm WL(R)} = 0.8$ eV, $g = 0$, and $\hbar\omega = 0.1$ eV are chosen.

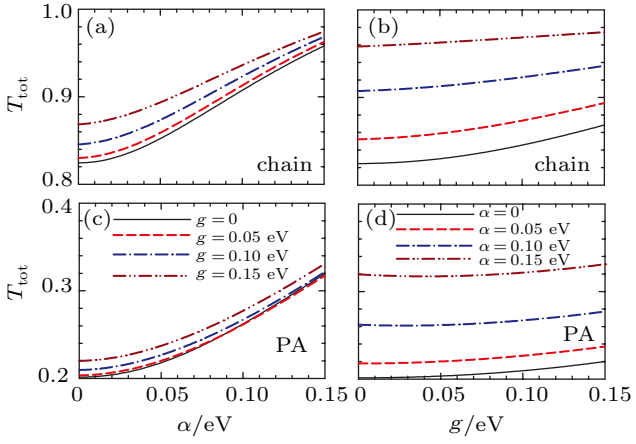


Fig. 6. (color online) (a) and (c) The total transmission coefficients of an extended simple chain and a PA-like nanowire, respectively, calculated at zero energy for some different local e–ph coupling strengths at $\alpha = 0$. (b) and (d). The same quantities for some different nonlocal e–ph coupling strengths at $g = 0$. The parameters to prepare this figure are chosen as $\beta_{\rm L(R)} = 1$ eV, $\beta_{\rm s} = 0.8$ eV, $\beta_{\rm d} = 1.2$ eV, $\varepsilon_{\rm W(L,R)} = 0$, $\beta_{\rm WL(R)} = 0.8$ eV, $g = 0$, and $\hbar\omega = 0.1$ eV.

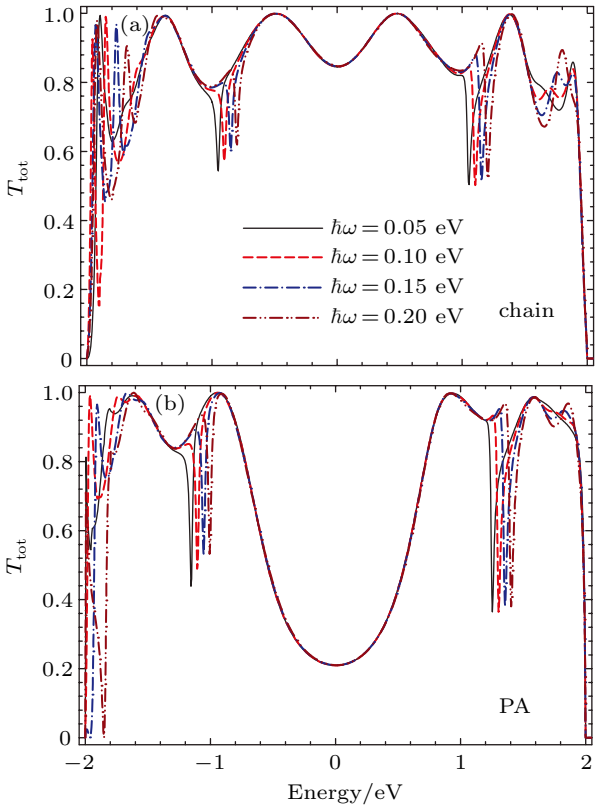


Fig. 7. (color online) The total transmission coefficients of (a) a six-atom simple chain and (b) a six-atom PA-like nanowire placed between two simple rigid leads as functions of energy calculated for some different phonon energies. In this figure, we choose $\beta_{\rm L(R)} = \beta_{\rm W} = 1$ eV, $\beta_{\rm s} = 0.8$ eV, $\beta_{\rm d} = 1.2$ eV, $\varepsilon_{\rm W(L,R)} = 0$, $\beta_{\rm WL(R)} = 0.8$ eV, $\alpha = 0$, and $g = 0.1$ eV.

4. Conclusion

We investigate the influence of both local (Holstein) and nonlocal (Peierls-type) e–ph interactions on the electronic transmission coefficient of an extended nanowire by using Green's function technique within the nearest neighbor tight-binding approximation. In the writing Hamiltonian, we suppose that there is a special optical phonon mode in the system. The Fock space for the systems is mapped by taking the electronic and phononic degrees of freedom into consideration. By using the model, we present our numerical results for the six-atom simple and PA-like chains in the local and nonlocal regimes. The results show that the electronic conductance is influenced more by the nonlocal e–ph interaction strength with respect to the local one. In general, the e–ph interaction in both regimes helps the tunneling conductance in the included gap systems. In the resonance region, the elastic conductance mainly decreases while the inelastic part increases by the e–ph interaction.

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