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Electronic transport in disordered chains mediated by interactions with acoustic waves

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ABSTRACT

We considered the dynamics of an initially localized wave packet in one-dimensional disordered chains under the effect of electron–phonon interaction and an acoustic wave's pumping. Our procedure consists of a quantum mechanics formalism for the electron transport and a classical Harmonic Hamiltonian model for lattice vibrations. We also introduce an electron–lattice interaction by assuming electron energy transfer between neighboring atoms as an exponential function of its effective distance. In our model, the electron was initially localized at the first site of the chain and we also added pumping of an acoustic wave at the zeroth site. We solved numerically the dynamic equations for the electron and lattice performing calculations for the spreading of an electronic wave-packet. We report numerical evidences with regard to the sub-diffusive transport.

1. Introduction

In the end of 1950s P.W. Anderson and co-workers demonstrated that extended eigenstates are completely absent in low-dimensional systems with uncorrelated disorder [1–7]. One of its consequences result in the saturation of the width of an initially localized wave-packet at a finite region around the initial position in the long time limit. Some years ago, it was demonstrated that the competition between nonlinearity and disorder plays an interesting role within the electronic transport [8–36]. By using a wide range of techniques, authors had shown that, even in the presence of disorder, nonlinearity can promote the appearance of a counter-intuitive electronic transport. From an experimental point of view, within the context of coupled waveguides patterned on an AlGaAs substrate, the presence of nonlinearity enhances the localization of linear modes whereas it induces the delocalization of nonlinear modes [13]. It is also interesting to emphasize the results of M.G. Velarde and co-workers [22–33] on the possibility of electronic transport mediated by a new type of electron–soliton pair.

Within the context of electron transport mediated by nonlinearity or electron–phonon interaction, the problem involving surface acoustic wave (SAW) has attracted an intense interest. In general lines, SAW has been used to control electronic dynamics in nano-devices. One of the best observations of electronic transport induced by SAW was experimentally done in Ref. [37]. The authors applied a surface acoustic wave through a GaAs–AlGaAs two-dimensional electron gas. In Ref. [38], an interesting investigation of the electronic flux mediated by high frequency (SAW) in GaAs–AlGaAs heterostructures was reported. In a recent excellent experiment [39], the authors moved a single electron along a wire to mimic a kind of ping-pong behavior. Moreover, it was pointed out that "controlled motion" might be used within the framework of quantum computing for moving a quantum 'bit' between two far from places [39]. The experimental setup consisted of trapping a single electron in a quantum dot and moved this electron around a channel by using a SAW. The authors obtained up to 60 shots with good quality. The possibility of using SAW to move electrons and construct quantum bits has attracted an intense interest [40–43].

We considered the dynamics of an initially localized wave packet in one-dimensional disordered chain under the effect of electron–phonon interaction and an acoustic wave's pumping. Our formalism consists of a quantum mechanics formalism for the electron transport and a classical harmonic Hamiltonian model for the lattice vibrations. We also introduce an electron–lattice interaction by considering electron energy transfer between neighboring atoms as an exponential function of its effective distance. In our model we made the electron initially localized at the first site of the chain and we added the pumping of an acoustic wave at the

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zero site. We solved numerically the dynamic equations for the electron and lattice performing calculations for the spreading of the electronic wave-packet. We report numerical evidences of the sub-diffusive transport.

2. Model and formalism

In our work the formalism consists of two Hamiltonians: the quantum electronic and lattice vibration dynamics. The electron Hamiltonian (H_e) and the lattice Hamiltonian $H_{lattice}$ are described, respectively, by

$$H_e = \sum_{m=1}^{N} \epsilon_m f_m^\dagger f_m + \sum_{m=1}^{N} \tau_{m+1,m}(f_{m+1}^\dagger f_m + f_m^\dagger f_{m+1}) \tag{1}$$

and

$$H_{lattice} = \frac{p_m^2}{2M_m} + \frac{1}{4}\sum_{m=1}^{N}\left[(x_{m+1}-x_m)^2 + (x_m - x_{m-1})^2\right], \tag{2}$$

where ϵ_m represents the on-site disorder distribution uniformly chosen within the interval $[-W/2, W/2]$, $\tau_{m+1,m}$ represents the energy transfer between the nearest sites, M_m represents the disordered distribution of masses and x_m and $p_m = M_m\dot{x}_m$ represents the atomic position and the momentum of the mth site. M_m is generated by using the following procedure: $M_m = e^{(\eta_m)}$ where η_m are random numbers uniformly distributed within a range $[-W/2, W/2]$. Electron–lattice interaction will be constructed by considering the electronic hopping term as $\tau_{m+1,m} = -e^{[-\alpha(x_{m+1}-x_m)]}$ where α represents, in units of the lattice spacing, the electron–phonon term. For small relative displacement we recover the Su, Schrieffer, Heeger approximation $\tau_{m+1,m} \approx -[1-\alpha(x_{m+1}-x_m)]$. The time-dependent wave function $\Phi(t) = \sum_m c_m(t)|m\rangle$ is obtained by numerical solution of the time-dependent Schrödinger equation. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as ($\hbar = 1$)

$$i\frac{dc_m(t)}{dt} = \epsilon_m c_m(t) - e^{[-\alpha(x_{m+1}-x_m)]}c_{m+1}(t) - e^{[-\alpha(x_m - x_{m-1})]}c_{m-1}(t). \tag{3}$$

The classical equations governing the lattice vibrations may be written as

$$\begin{aligned} M_m\frac{d^2x_m}{dt^2} = {} & x_{m+1} - 2x_m + x_{m-1} - \alpha\{e^{[-\alpha(x_{m+1}-x_m)]}(c_{m+1}^*(t)c_m(t) \\ & + c_{m+1}(t)c_m^*(t)) - e^{[-\alpha(x_m - x_{m-1})]}(c_m^*(t)c_{m-1}(t) \\ & + c_m(t)c_{m-1}^*(t))\}. \end{aligned} \tag{4}$$

We impose the electron initially localized at site $m=1$, i.e. $|\Phi(t=0)\rangle = \sum_m c_m(t=0)|m\rangle$, where $c_m(t=0) = \delta_{m,1}$. For $t=0$ we set $x_m(t=0) = \dot{x}_m(t=0) = 0$ for m within the interval $[1.N]$. Furthermore, we consider the pumping of an acoustic wave at the extreme left side of the chain (i.e. at the site $m=0$) given by the equation

$$x_0 = A_0\cos(\omega t), \tag{5}$$

where ω represents the frequency of the acoustic wave. We solve the set of quantum/classical coupled equations using combined high-order Taylor expansion and a second order finite-difference procedure. The former is employed to obtain a numerical solution of Schrödinger equation (Eq. (3)) via series expansion of the evolution operator $U(\Delta t)$ [44]:

$$U(\Delta t) = \exp(-iH_e\Delta t) = 1 + \sum_{l=1}^{n_o}\frac{(-iH_e\Delta t)^l}{l!} \tag{6}$$

where H_e is the one electron Hamiltonian. The wave function at time Δt is given by $|\Phi(\Delta t)\rangle = U(\Delta t)|\Phi(t=0)\rangle$. The method can be used recursively to obtain the wave-function at time t. Classical equations (Eq. (4)) are solved by using the latter approach on a discretized time. We write the second time derivative in Eq. (4) as

$$\frac{d^2x_m}{dt^2} \approx \frac{x_m(t+\Delta t) - 2x_m(t) + x_m(t-\Delta t)}{(\Delta t)^2} \tag{7}$$

Applying the previous formula to the classical equation we derive the following equation which can be solved numerically:

$$\begin{aligned} x_m(t+\Delta t) \approx {} & 2x_m(t) - x_m(t-\Delta t) + \frac{(\Delta t)^2}{M_m}\{x_{m+1}(t) - 2x_m(t) \\ & + x_{m-1}(t) - \alpha[e^{[-\alpha(x_{m+1}(t)-x_m(t))]}(c_{m+1}^*(t)c_m(t) \\ & + c_{m+1}(t)c_m^*(t)) \\ & - e^{[-\alpha(x_m(t)-x_{m-1}(t))]}(c_m^*(t)c_{m-1}(t) + c_m(t)c_{m-1}^*(t))]\}, \end{aligned} \tag{8}$$

Our calculations are made with step $\Delta t = 1\times10^{-3}$ and the sum of Eq. (6) is truncated at $n_o = 10$. Then we could keep the wave function norm within the following numerical tolerance: $|1 - \sum_m |c_m(t)|^2| < 10^{-10}$ along the entire time interval ($t_{max} \approx 3\times10^4$). After solving the dynamics equations, we computed some typical quantities which describe electronic transport on this disordered model, namely, mean position (centroid) and mean square displacement defined as [34–36]

$$\langle m(t)\rangle = \sum_m (m)|c_m(t)|^2 \tag{9}$$

and

$$\sigma(t) = \sqrt{\sum_m (m - \langle m(t)\rangle)^2 |c_m(t)|^2}, \tag{10}$$

respectively. The centroid for a given time t represents the mean position of the electron using the center of a self-expanded chain as the origin. The mean square displacement provides an estimate of the size of the wave packet at time t.

3. Results and discussion

We considered the electron fully localized at the left side of the chain (i.e. $\{c_m(t=0) = \delta_{m,1}\}$) and the pumping of an acoustic wave at the site $m=0$ i.e. $x_0 = A_0\cos(\omega t)$, where ω represents the frequency of the acoustic wave. We set $W=2$ for all calculations obtained in Figs. 1–3. Due to the presence of a mass disordered distribution in our model, we adopted pumping at low-frequencies $\omega \ll 1$. High frequencies do not propagate easily within disordered harmonic chains [45]. In our calculations we have used the self-expanding chain to minimize border effects; whenever the probability of finding the electron or the atomic vibration at the right side of the chain exceeded 10^{-20}, 10 new sites were added to the right side. Numerical convergence was ensured by checking the conservation of the norm of the wave packet at every time step; our results provide $|1 - \sum_m |c_m(t)|^2| < 10^{-10}$ for all times considered. In Fig. 1 we show results of several calculations for $\omega = 0.1, 0.2, 0.3$ and $\alpha = 0$ up to 0.5. For $\alpha = 0$ we detected clearly that the electron remains localized close to initial position. We emphasize that in the absence of electron–phonon coupling ($\alpha = 0$) our present model converged to the standard one-dimensional Anderson model with diagonal disorder of the same order of the bandwidth. Therefore, in this case the electronic behavior is characterized by exponentially localized eigenstates, thus promoting the saturation of σ and $\langle m(t)\rangle$ at long time limit. For $\alpha > 0$ we observed that the square root of the mean square displacement and the mean position increases with time. We also noticed that $\sigma \propto t^\zeta$ with $\zeta = 0.4 - 0.45$ i.e., a sub-diffusive behavior. The calculations in Fig. 1 suggest a disruption of the Anderson

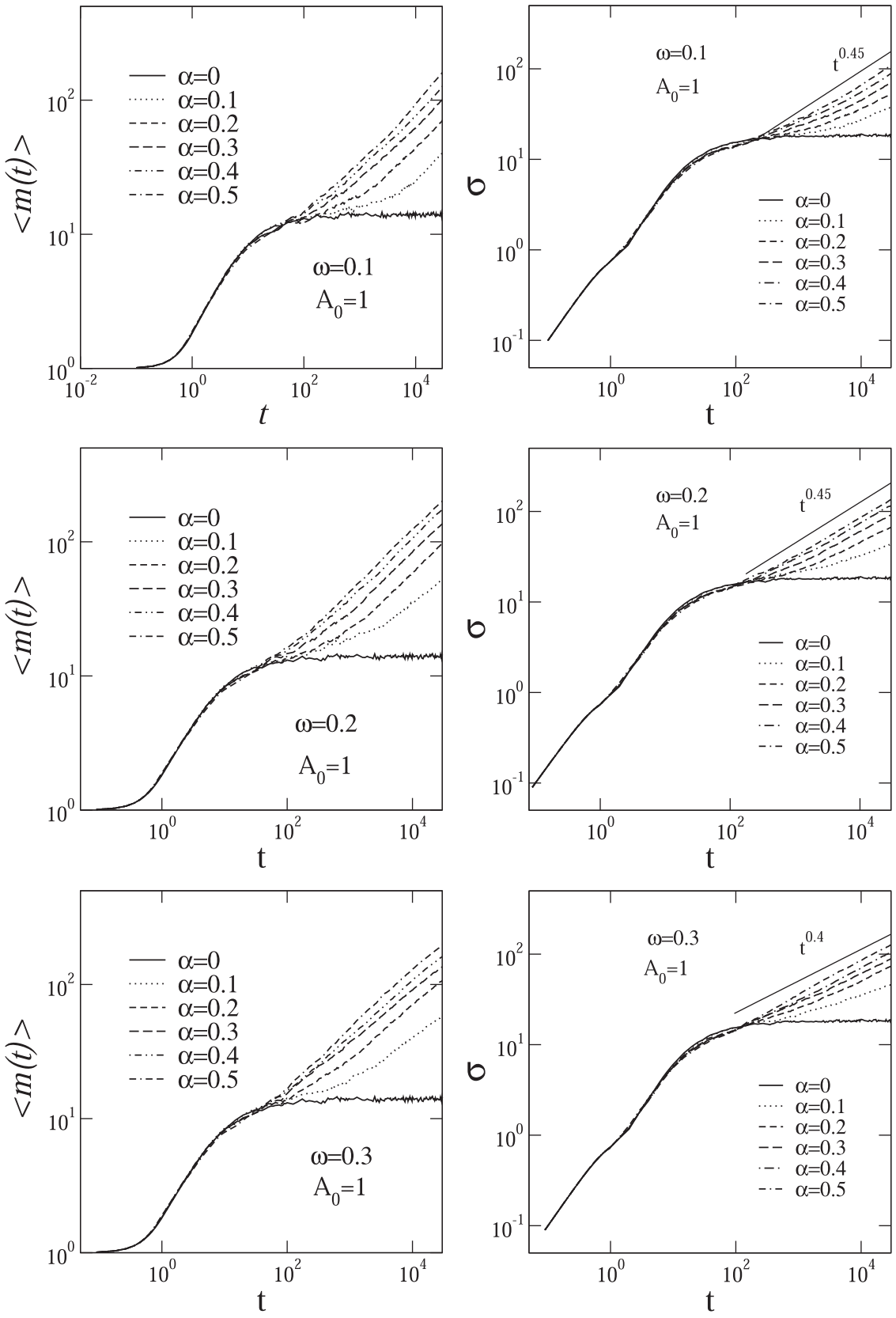

Fig. 1. The mean position and mean square displacement computed for $\omega = 0.1, 0.2, 0.3$ and $\alpha = 0$ up to 0.5. The amplitude of the pumping was set at $A_0 = 1$. For $\alpha > 0$ we can see that both $m(t)$ and $\sigma(t)$ increases along the time. Our calculations suggest that the coupling of the electron with the acoustic mode pumped in the left side of chain promotes the breakdown of the Anderson localization.

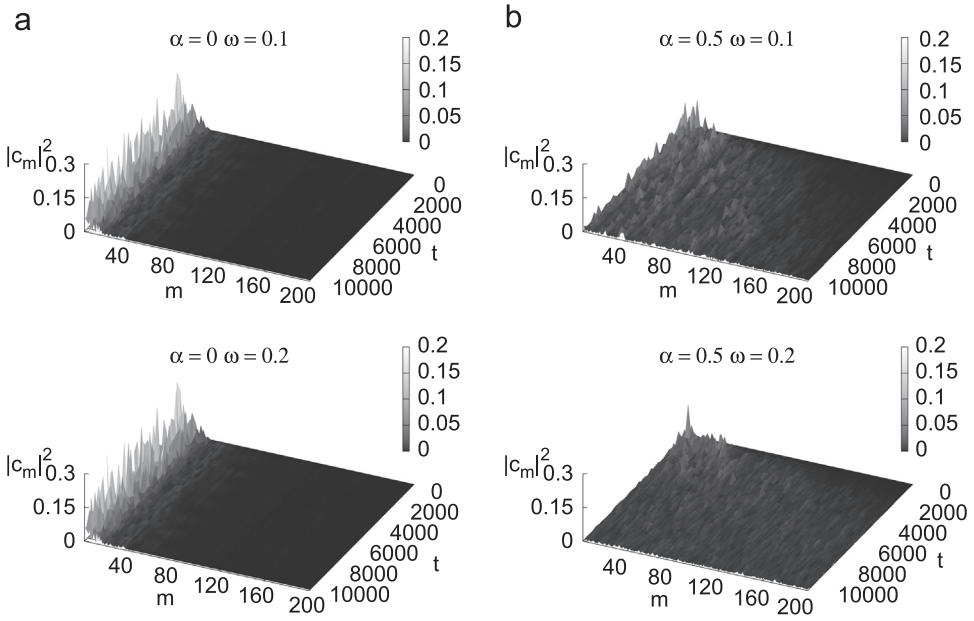

Fig. 2. $|c_m(t)|^2$ versus t and m for $\omega = 0.1, 0.2$ and $\alpha = 0, 0.5$.

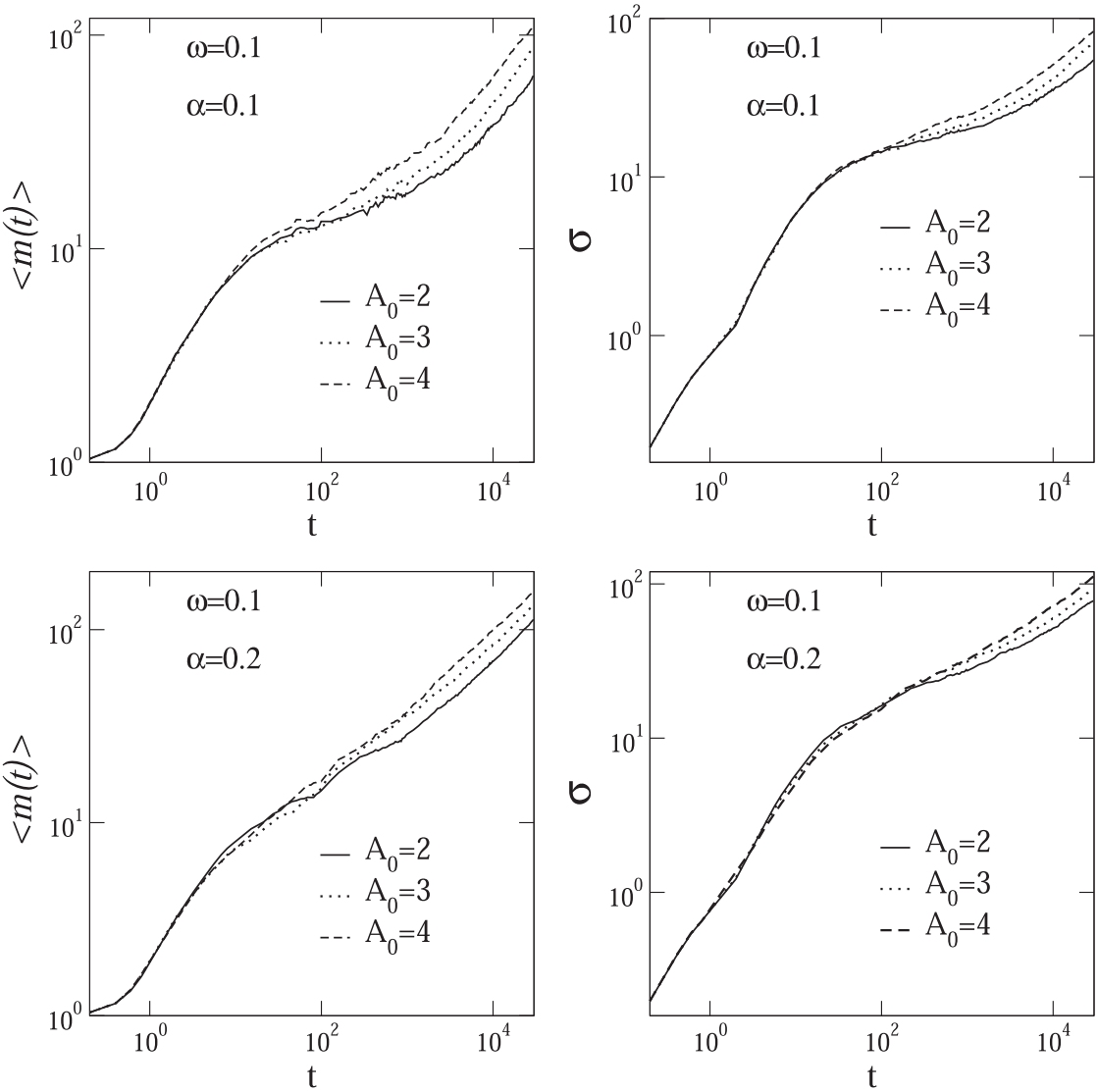

Fig. 3. The electronic centroid $\langle m(t)\rangle$ and the spread of the wave packet σ versus time for $\omega = 0.1$, $\alpha = 0.1, 0.2$ and $A_0 = 2, 3, 4$.

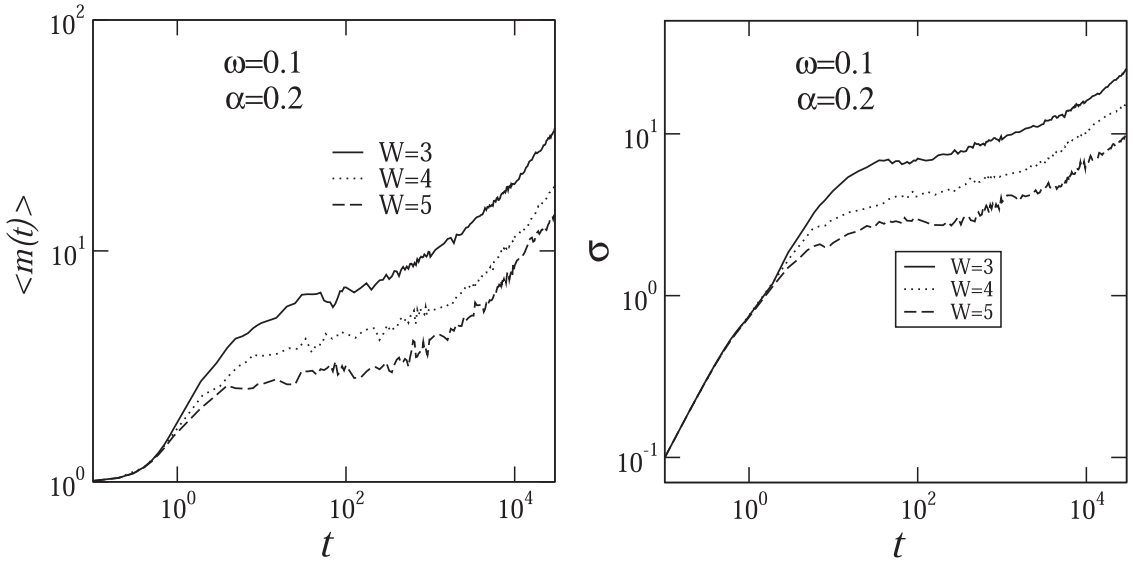

Fig. 4. The electronic centroid $\langle m(t)\rangle$ and the spread of the wave packet σ versus time for $\omega = 0.1$, $\alpha = 0.2$, $A_0 = 1$ and $W = 3, 4, 5$.

localization induced by the coupling with acoustic mode pumped in the left side of chain. It is an interesting result. In general lines, the injection of the acoustic wave in one of the ends of the chain associated with the electron–phonon coupling promotes the electronic propagation even at the presence of strong diagonal disorder. The acoustic wave seems to "push" the electron through the disordered chain. In Fig. 2 we plot $|c_m(t)|^2$ versus t and m for $\omega = 0.1, 0.2$ and $\alpha = 0, 0.5$. We noticed that for $\alpha = 0$ the wave-packet remains localized close to the left side of chain. For $\alpha = 0.5$ we observed that the wave-packet spreads along the chain. The results shown in Fig. 2 are in good agreement with Fig. 1 thus suggesting that the coupling between the electron and the acoustic mode developed electronic transport. In Fig. 3 we analyzed briefly the effect of the pumping amplitude A_0 on the electronic transport. We plotted the electronic position $\langle m(t)\rangle$ and the wave-packet width σ versus time for $\omega = 0.1$, $\alpha = 0.1, 0.2$ and $A_0 = 2, 3, 4$. Our calculations suggest a small increment of both quantities as the pumping amplitude A_0 increases. However, in general lines, the main results seemed to be qualitatively independent of the pumping amplitude A_0. Therefore the main summary of results shown in Figs. 1–3 suggests that, within the harmonic approximation, the coupling between the electron and a acoustic mode promote electronic dynamics. We emphasize that in our model we have considered a reasonable amount of disorder (W=2, i.e. the same order of the crystalline electronic bandwidth). We also emphasize that our results shown in the previous figures point out that even in the presence of intermediate amount of disorder, the acoustic wave mediates electron wave-packet dynamics along the chain. So this brings up the question: What happens at the limit of strong disorder? In Fig. 4 we included additional calculations for a more intense amount of disorder. We plotted the electronic position $\langle m(t)\rangle$ and the wave packet width for $\omega = 0.1$, $\alpha = 0.2$ and $W = 3, 4, 5$. We emphasize that this threshold can be considered a strong disordered limit in one-dimensional chains (in special W=5). Our results denote again that the electron transport is maintained even in this case. We observed that the diffusion constant in fact decreases as the disorder parameter increases. However, both quantities have shown a subdiffusive behavior similar to those obtained in the previous calculations.

4. Summary and conclusions

In this work we have considered the dynamics of an initially localized wave packet in one-dimensional disordered chain under effect of electron–phonon interaction and the acoustic wave's pumping. Our formalism consists of describing quantum electronic dynamics within the disordered chain and lattice vibration by two distinct Hamiltonians. The electron–lattice interaction was modeled by considering electron energy transfer between neighboring atoms as an exponential function of its effective distance. In our mathematical representation we set the electron initially localized at the first site of the chain and we add the pumping of an acoustic wave at the zero site. We solved numerically the dynamic equations for the electron and lattice performing calculations for the spreading of the electronic wave-packet. Our results point out that the electron–phonon coupling and the acoustic wave pumping promotes a breakdown of the Anderson localization. We analyzed the dependence of latter with the degree of disorder and we found that at the range of strong disorder, the electronic transport mediated by the electron–lattice coupling is still present. Our calculations were done describing the lattice by using a simplified harmonic theory. In general, nonlinear vibrations also play interesting roles within the context of electronic dynamics mediated by lattice vibrations. Our calculations demonstrated that, even within the harmonic approximation, the coupling with an acoustic wave propagating along the lattice can promote the charge transport. We hope that those calculations stimulate further studies in the field of electronic transport mediated by acoustic wave pumping and electron–phonon coupling.

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