Solid State Communications 229 (2016) 22–27

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Fast-track Communication

# Electronic transport in disordered chains mediated by interactions with acoustic waves

A. Ranciaro Neto [a,b], M.O. Sales [a], F.A.B.F. de Moura [a,*]

[a] Instituto de Física, Universidade Federal de Alagoas, Maceió AL 57072-970, Brazil
[b] Faculdade de Economia, Administração e Contabilidade, Av. Lourival Melo Mota, s/n, bl. 14. Tabuleiro dos Martins 57072-970, Brazil

ARTICLE INFO

*Article history:*
Received 16 November 2015
F. Peeters
Available online 2 January 2016

*Keywords:*
wave-packet dynamics
disorder
acoustic waves
electron–phonon

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

* Corresponding author.
*E-mail address:* fidelis@fis.ufal.br (F.A.B.F.de. Moura).

http://dx.doi.org/10.1016/j.ssc.2015.12.004
0038-1098/

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 $\epsilon_m$ 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 $m$th site. $M_m$ is generated by using the following procedure: $M_m = e^{(\eta_m)}$ where $\eta_m$ 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 $\alpha$ 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 $\omega$ 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 $\Delta t$ 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 $\omega$ 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 $\sigma$ 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