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One-electron propagation in Fermi, Pasta, Ulam disordered chains with Gaussian acoustic pulse pumping

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In this work, we consider a one-electron moving on a Fermi, Pasta, Ulam disordered chain under effect of electron–phonon interaction and a Gaussian acoustic pulse pumping. We describe electronic dynamics using quantum mechanics formalism and the nonlinear atomic vibrations using standard classical physics. Solving numerical equations related to coupled quantum/classical behavior of this system, we study electronic propagation properties. Our calculations suggest that the acoustic pumping associated with the electron–lattice interaction promote a sub-diffusive electronic dynamics.

Keywords: Sub-diffusive spreading; electron–phonon coupling; wave packet dynamcis; nonlinearity.

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1. Introduction

The problem of electronic dynamics mediated by surface acoustic wave (SAW) has attracted an intense interest.[1–12] This research field, in broad terms, consists of a combination of solid-state theories including, e.g. Anderson localization theory,[13] electron–lattice interaction,[14–16] piezoelectricity[4] and general solid state physics.[17–22] An interesting experimental investigation of electronic transport induced by (SAW) was done in Ref. 1. The authors applied a surface acoustic wave through a GaAsAlGaAs two-dimensional (2D) electron gas. Moreover, Ref. 2 also reported

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experimental investigation on the electronic flux mediated by high frequency (SAW) in GaAsAlGaAs heterostructures. In Ref. 4, the authors moved a single electron along a wire in a kind of ping-pong game. Moreover, the possibility of using this "controlled motion" in the framework of quantum computing was pointed at, for example, to move a quantum 'bit' between two distant places.[4] This experimental setup consisted of trapping a single electron in a quantum dot and moving that particle along a channel by using a SAW. SAW usage in electron movement and in the construction of quantum bits has attracted interest from some solid-state physics specialists.[5–11] More recently, the dynamics of an initially localized wave packet in one-dimensional disordered harmonic chains under the effect of electron–lattice interaction and an acoustic wave pumping were investigated by numerical calculation.[12] They demonstrated the existence of sub-diffusive electronic transport mediated by the acoustic pumping using that method for solving equations.

In this paper, we investigate the competition between intrinsic cubic nonlinearity, on-site disorder and the pumping of an acoustic pulse. We consider noninteracting electrons moving on a nonlinear Fermi–Pasta–Ulam disordered chain under the effect of electron–phonon interaction and a Gaussian acoustic pulse's pumping. In our theoretical formalism, we apply quantum mechanics treatment for electron and classical physics for nonlinear atomic vibrations. The dynamics equations are solved numerically: A Taylor formalism is used for electronic propagation and a second-order Euler method is adopted to solve coupled quantum/classical equations. Our calculations suggest that the acoustic pumping associated with the electron–lattice interaction promotes a sub-diffusive electronic dynamics.

2. Model and Formalism

In our model, we consider a one-electron moving in a Fermi–Pasta–Ulam disordered chain of N masses. As previously stated, electronic dynamics is described by quantum Hamiltonian and the lattice vibrations characterized by classical mechanics. Total Hamiltonian is written as $H = H_e + H_{\text{lattice}}$, where[12,15,23]:

$$H_e = \sum_n \{\epsilon_n d_n^\dagger d_n + V_{n+1,n}(d_{n+1}^\dagger d_n + d_n^\dagger d_{n+1})\}$$

$$H_{\text{lattice}} = \sum_n \left\{ \frac{P_n^2}{2m_n} + \frac{1}{4}[(Q_{n+1} - Q_n)^2 + (Q_n - Q_{n-1})^2] \right.$$
$$\left. + \frac{\eta}{6}[(Q_{n+1} - Q_n)^3 + (Q_n - Q_{n-1})^3] \right\}, \quad (1)$$

where $d_n^\dagger$ and d_n are the creation and annihilation operators for the electron at site n. ϵ_n represents the on-site disorder distribution uniformly chosen within the interval $[-W/2, W/2]$. $V_{n+1,n}$ represents the electron's kinetic energy (the hopping term). P_n and Q_n are the momentum and displacement of the mass at site (n), respectively. m_n is a disordered distribution of masses generated by the following procedure: $m_n = e^{(\rho_n)}$, where ρ_n are random numbers uniformly distributed within the interval $[-W/2, W/2]$. η represents the strength of the cubic nonlinearity considered in our

model. The hopping elements $V_{n+1,n}$ depend on the relative distance between two consecutive molecules of the chain: $V_{n+1,n} = -e^{[-\alpha(Q_{n+1}-Q_n)]}$.[15] The quantity α defines the electron–lattice coupling strength. The time-dependent wave function $|\Phi(t)\rangle = \sum_n c_n(t)|n\rangle$ is obtained by numerical solution of the time-dependent Schrödinger equation. The Wannier amplitudes $(c_n(t))$ evolve in time as $(\hbar = 1)$:

$$i\frac{dc_n(t)}{dt} = \epsilon_n c_n(t) - e^{[-\alpha(Q_{n+1}-Q_n)]}c_{n+1}(t) - e^{[-\alpha(Q_n-Q_{n-1})]}c_{n-1}(t). \tag{2}$$

Lattice equation is written as

$$m_n\frac{d^2 Q_n(t)}{dt^2} = (Q_{n+1} - Q_n) - (Q_n - Q_{n-1})] + \eta[(Q_{n+1} - Q_n)^2 - (Q_n - Q_{n-1})^2]$$
$$+ \alpha\{(c_{n+1}^* c_n + c_{n+1}c_n^*)e^{[-\alpha(Q_{n+1}-Q_n)]}$$
$$- (c_n^* c_{n-1} + c_n c_{n-1}^*)e^{[-\alpha(Q_n-Q_{n-1})]}\}. \tag{3}$$

We consider the electron initially localized at site $n = 1$, i.e. $|\Phi(t = 0)\rangle = \sum_n c_n(t = 0)|n\rangle$, where $c_n(t = 0) = \delta_{n,1}$. For $t = 0$, we consider $Q_n(t = 0) = \dot{Q}_n(t = 0) = 0$, for n within the interval $[1, N]$. In addition, we consider the pumping of an acoustic Gaussian pulse at the extreme left side of chain (i.e. at the site $n = 0$):

$$Q_0(t) = e^{(-t^2/2\Delta t^2)}\cos(\omega t), \tag{4}$$

where ω represents the frequency of the gaussian acoustic pulse and $\Delta t = 1/\Delta\omega = 10$ is the width in time.

In order to solve numerically the quantum equations, we applied a Taylor expansion of time evolution operator $U(\delta t) = \exp(-iH_e\delta t) = 1 + \sum_{l=1}^{n_o}[(-iH_e\delta t)^l]/(l!)$.[24] The wave-function at time δt is $|\Phi(\delta t)\rangle = U(\delta t)|\Phi(t = 0)\rangle$. By employing recursion, we obtain the wave-function at time t. For classical equations, we used a prediction-correction second-order method.[25] This method consists of two steps: The first step consists of finding a initial prediction $Q_n(\delta t)^*$ at time δt, applying the formula below:

$$Q_n(\delta t)^* \approx Q_n(t = 0) + \delta t \frac{dQ_n}{dt}\bigg|_{t=0}. \tag{5}$$

In the second step, a correction formula is applied in order to get a better approximation to $Q_n(\delta t)$

$$Q_n(\delta t) \approx Q_n(t = 0) + \frac{\delta t}{2}\left[\frac{dQ_n}{dt}\bigg|_{t=0} + \frac{dQ_n^*}{dt}\bigg|_{\delta t}\right]. \tag{6}$$

This method (Eqs. (5) and (6)) is used recursively to obtain $Q_n(t)$. Our main calculations were carried out using $\delta t = 5 \times 10^{-3}$, and the sum of the Taylor expansion of time evolution operator was truncated on $n_o = 12$. It is worth mentioning that we dealt with border effects by considering a self-expanded chain. This method can be understood as follows: Whenever the probability of finding the electron or the atomic vibration at the right side of the chain exceeds 10^{-20}, 10 new sites will be added

to this position. Thus, we obtained the wave function norm with error $|1 - \sum_n |c_n(t)|^2| < 10^{-10}$ along the entire time interval. It is an important first check for the accuracy of our numerical procedure. Traditionally, the classical equation is solved by another method than the second-order Euler formalism (Eq. (3)). In recognition of this fact, we decided to perform a second check for accuracy employing a standard fourth-order Runge–Kutta (RK4)[25] to solve Eqs. (2) and (3). The results obtained using our numerical formalism showed no difference from those obtained using (RK4), a widely used method.

The physical properties are obtained through the calculations of some typical quantities, namely, mean position (centroid), mean square displacement and the Shannon entropy defined as [23,26]

$$\langle n(t) \rangle = \sum_n (n)|c_n(t)|^2, \tag{7}$$

$$\sigma(t) = \sqrt{\sum_n (n - \langle n(t) \rangle)^2 |c_n(t)|^2} \tag{8}$$

and

$$S(t) = -\sum_n |c_n(t)|^2 \ln[|c_n(t)|^2], \tag{9}$$

respectively. The centroid for a given time t represents the mean position of the electron. The mean square displacement and the Shannon entropy give some estimates of the number of sites in which the wave packet is spread at time t. For extended states in a chain with N sites, we have $\sigma(t \to \infty) \propto N$ and $S(t \to \infty) \propto \ln(N)$. For localized states, the situation changes drastically. In general, localized eigenstates occur in systems with uncorrelated disorder. Therefore, within the standard Anderson Localization theory $\sigma(t \to \infty) \propto l_0$ and $S(t \to \infty) \propto \ln(l_0)$ where l_0 is close to the largest localization length. Due to the presence of disorder, l_0 is of the order of a few sites and, therefore, both σ and $S(t)$ converge to small constants.

3. Results and Discussion

We start the numerical integration using a small chain (about $N(t = 0) = 200$ sites). During the integration, the $N(t)$ increases until 10^4 sites (or more). In our calculations, we will use $W = 2$. We emphasize that the mean value of the electronic hopping is about 1. Therefore, $W = 2$ represents an amount of disorder at the same order of the band width, i.e. an intermediate disorder in the one-dimensional (1D) model. We also emphasize that we adopted pumping at low-frequencies $\omega \ll 1$. High frequencies do not propagate easily within disordered systems.[27] A summary of our calculations for all quantities is shown in Figs. 1(a)–1(f). In plots (a) and (b), we have electronic Centroid, in ((c) and (d)) the mean Square displacement versus time t and
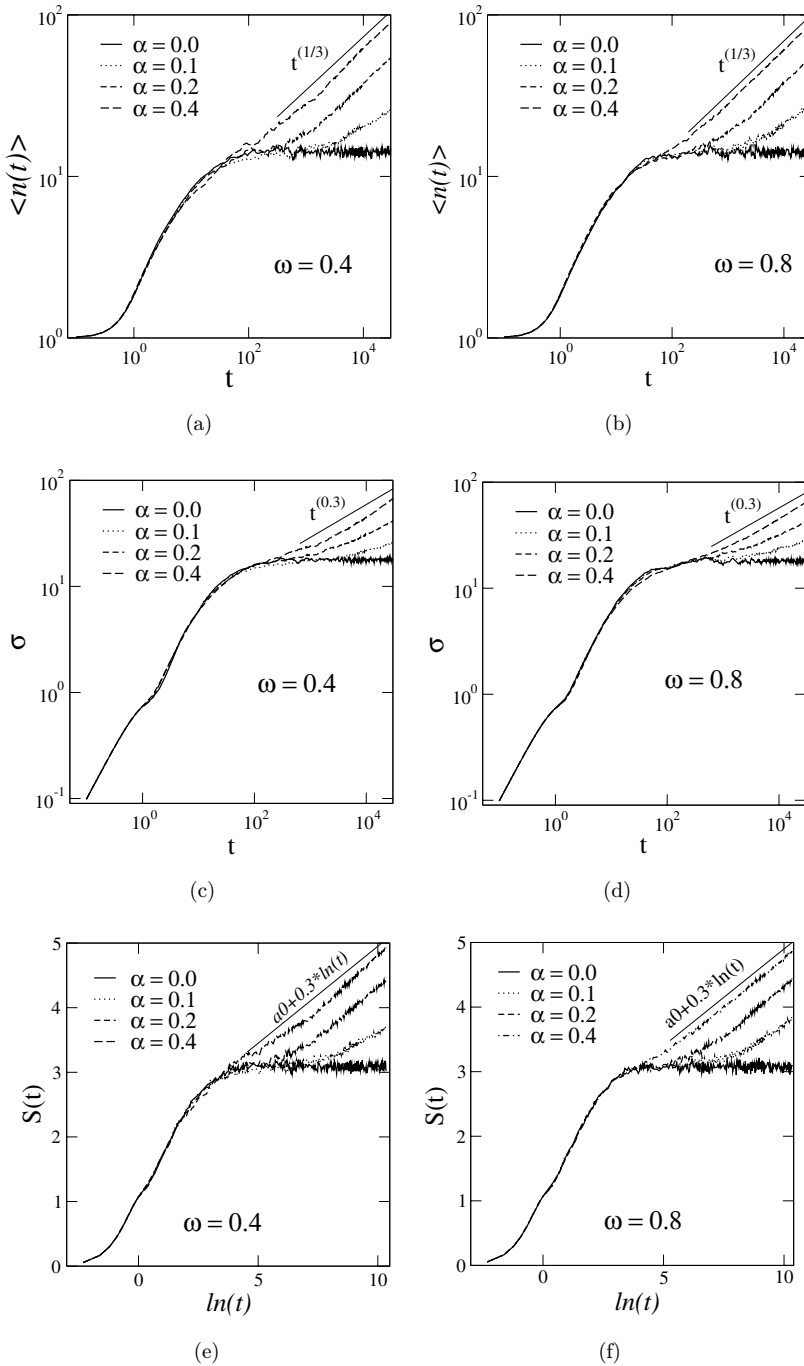
Fig. 1.   (a), (b) Electronic centroid, (c), (d) mean square displacement versus time t and (e), (f) Shannon entropy versus $\ln(t)$ for $W = 2$, $\omega = 0.4, 0.8$ and $\alpha = 0., 0.1, 0.2, 0.3$.

in ((e) and (f)) the Shannon Entropy versus $\ln(t)$ for $W = 2$, $\omega = 0.4, 0.8$ and $\alpha = 0., 0.1, 0.2, 0.3$.

We observe that for $\alpha = 0$ all quantities saturate for a long time. It is a direct consequence of the presence of disorder within our model. In 1D systems with uncorrelated disorder, all eigenstates are localized and therefore an initially localized wave-packet evolves to a finite region of the same order of the largest localization length.[13] The saturated behavior found in centroid, in mean square displacement and in the Shannon entropy is in good agreement with the previous statements.

As the electron-lattice parameter α increases, we notice a radical change of our results (see Figs. 1(e) and 1(f) for $(\alpha > 0)$. All quantities increase as the time evolves. The time-dependent behavior of $\langle n \rangle$, σ and $S(t)$ suggests that acoustic pumping interacts with electron-lattice coupling in a way to stimulate electronic transport along the chain (acoustic wave produces lattice vibrations on a small number of atoms in a short period of time, which seems to push electron to the right side of the alloy). Within the time-scale computed here, our analysis suggests that the electronic dynamics is sub-diffusive with $\langle n(t) \rangle \propto t^{1/3}$ and $\sigma \propto t^{0.3}$ (the Shannon Entropy follows a similar sub-diffusive trend with $S(t) \approx a_0 + 0.3 \log(t)$). In Figs. 2(a) and 2(b), we plot the wave function $|c_n(t)|^2$ versus n and t for $W = 2$, $\omega = 0.4$ and $\alpha = 0.0$(a) and $\alpha = 0.4$(b). This plot gives us a pedagogical overview of the electronic dynamics along the lattice. In the absence of electron–lattice interaction $(\alpha = 0)$, electron remains trapped around the initial position $(n = 0)$. For $\alpha > 0$, we observe that, despite the presence of uncorrelated disorder within the chain, electronic wave function gets spread. We emphasize that it is a clear breakdown of the standard Anderson localization theory.

Aiming to understand the electronic dynamics and its relation with the lattice dynamics better, we investigate some specificities of the lattice deformation in detail. So, we compute a kind of generalized probability of local deformation f_n. This quantity is obtained as follows: first, we compute the quantity: $x_n = (1 - e^{[-q_n + q_{n-1}]})$.[2] Second, we normalize x_n to get generalized probability of local deformation f_n, i.e.: $f_n = x_n / \sum_n (x_n)$. With this quantity, we can also compute the mean position of the lattice vibration $(\langle n_v \rangle = \sum_n n f_n)$ and also its dispersion
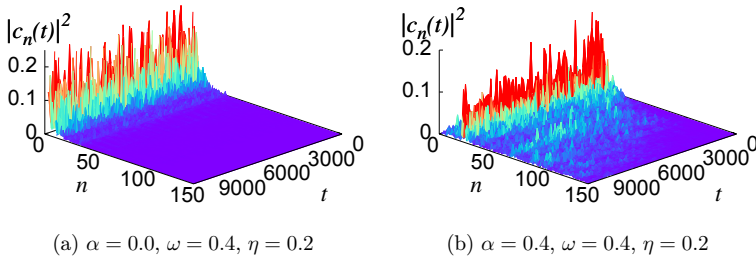

(a) $\alpha = 0.0$, $\omega = 0.4$, $\eta = 0.2$ (b) $\alpha = 0.4$, $\omega = 0.4$, $\eta = 0.2$

Fig. 2. (Color online) Wave function $|c_n(t)|^2$ versus n and t for $W = 2$, $\eta = 0.2$, $\omega = 0.4$ and $\alpha = 0$ (a) and $\alpha = 0.4$ (b). The presence of electron–lattice interaction promotes the spread of the electronic wave function.
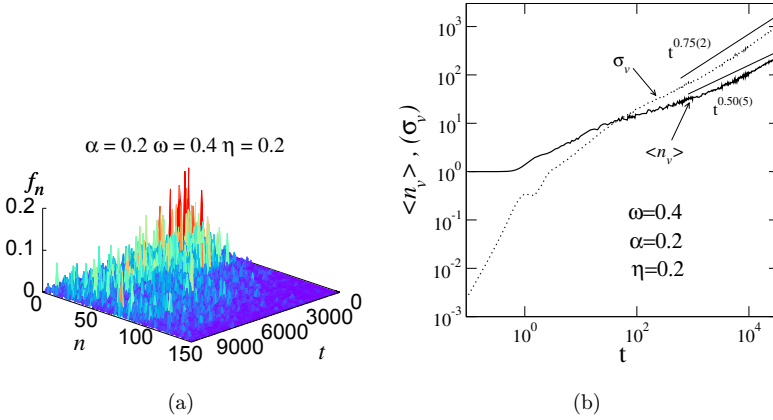
Fig. 3.   (Color online) (a) The generalized probability of local deformation f_n computed in a disordered chain with $W = 2$, $\omega = 0.4$ and $\alpha = 0.2$. (b) The mean position of the lattice vibration and its mean square displacement for the same case as in (a).

($\sigma_v = \sqrt{\sum_n (n - \langle n_v \rangle)^2 f_n}$). In Figs. 3(a) and 3(b), we show our numerical analysis about the vibrational energy propagation in this model succinctly. Figure 3(a) has a plot of the generalized probability of local deformation f_n versus n and t for a chain with $W = 2$, $\eta = 0.2$, $\alpha = 0.2$ and $\omega = 0.4$. We see that acoustic pumping clearly propagates along the chain in a similar trend, which was observed in Fig. 2(b). The results for $\langle n_v \rangle$ and σ_v are found in Fig. 3(b). Calculations were done for the same case as in Fig. 3(a). We observed that the mean position of the lattice vibration follows a diffusive dynamics. The mean square displacement of the energy wave-packet has a super-diffusive behavior. These results about the energy dynamics deserve a more detailed discussion. By revisiting Ref. 27, we know that the evolution of a initial localized momentum wave-packet within a classical disordered harmonic chain ($\eta = 0$) follows a similar super-diffusive trend.

First, we emphasize that the acoustic Gaussian pumping used here promotes a kind of continuous injection of momentum for the lattice. Therefore, in spite of the initial condition used here being formally distinct from the momentum injection used in Ref. 27, however, both contain the same nature: injection of momentum. Another important and new information in our calculations is the presence of super-diffusive dynamics in disordered nonlinear chains. We emphasize that our calculations were done for a classical lattice with quadratic and cubic ($\eta > 0$) interaction. Our results suggest that the cubic potential does not change the kind of energy propagation in the approximations used here.

Before the conclusion of our work, we show some brief results about nonlinearity and disorder dependence. In Figs. 4(a) and 4(b), we show our calculations for the mean position $\langle n \rangle$ and the Shannon entropy $S(t)$ versus time t for $\alpha = 0.2$, $\omega = 0.4$, $W = 2$ and $\eta = 0, 0.4, 0.8$. Our initial analysis shows that the mean positions and
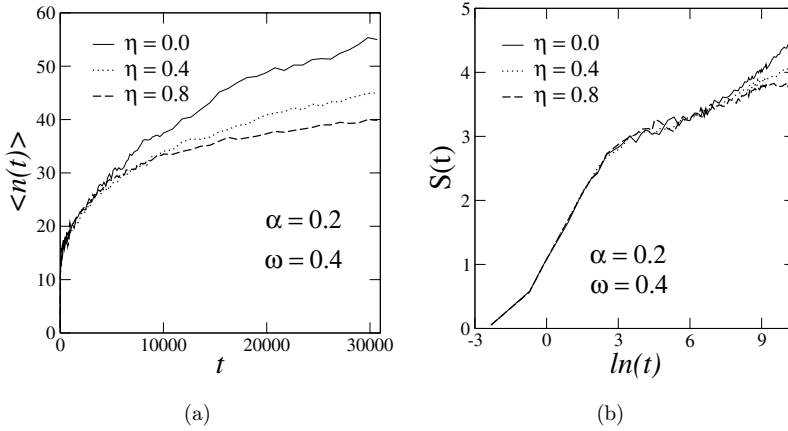
Fig. 4.   (a) Mean position $\langle n \rangle$ versus t and (b) Shannon entropy $S(t)$ versus $\ln(t)$ for $\alpha = 0.2$, $\omega = 0.4$, $W = 2$ and $\eta = 0, 0.4, 0.8$.

the Shannon entropy seem to decrease as the η is increased. Based on these calculations, the electron transport mediated by acoustic pumping seems to be more efficient in harmonic ($\eta = 0$) chains. However, we recognize that the range of η, we considered is not sufficiently wide to obtain, indeed, a more conclusive statement. We stress that as the magnitude of the cubic potential is increased within disordered chains, numerical instability increases and therefore it becomes complicated to solve the differential equations. This numerical difficulty could be overcome by using high order methods. However, computational time required to solve coupled equations increases in a considerable manner. We stress that we have used the RK4 method in order to find electronic dynamics. The computation time using RK4 was almost three times the computation time required using the Euler-Taylor formalism. In Figs. 5(a)
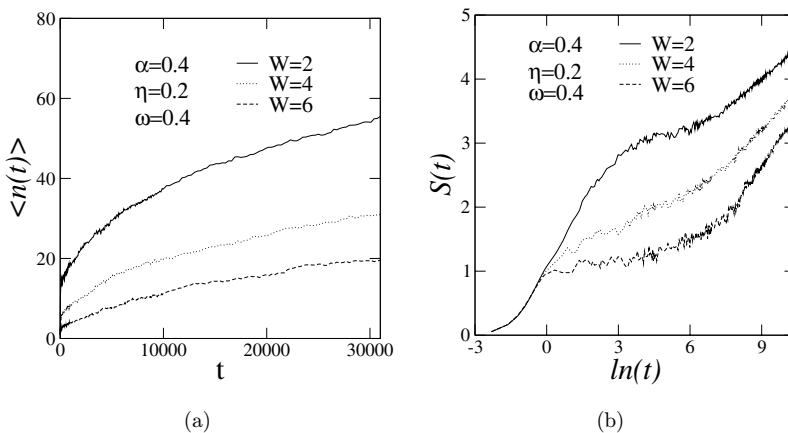

Fig. 5.   (a) Mean position $\langle n \rangle$ versus t and (b) Shannon entropy $S(t)$ versus $\ln(t)$ for $\eta = 0.2$, $\omega = 0.4$, $\alpha = 0.4$ and $W = 2, 4, 6$.

and 5(b), we plot the mean position $\langle n \rangle$ and the Shannon entropy $S(t)$ versus time t for $\alpha = 0.4$, $\omega = 0.4$, $\eta = 0.2$ and $W = 2, 4, 6$. We observe clearly that, in spite of the decreasing the magnitude of $\langle n \rangle$ and $S(t)$ with the increasing of W, the main result remains unchanged, i.e. a sub-diffusive dynamics is still obtained. We emphasize again that the strength of disorder we are using here ($W >$ electronic hopping) does not represent a weak disordered regime. In fact, our model with $W \geq 2$ represents a limit with intermediate/strong intrinsic disorder. Therefore, our calculations suggests that the electron–phonon coupling and the pumping of gaussian acoustic pulses can breakdown the Anderson localization in 1D systems even in the presence of an intense amount of disorder.

4. Summary and Conclusions

In this work, we studied the problem of electronic dynamics in a disordered nonlinear chain under effect of a Gaussian wave-packet pumping. By using a simplified model, we had the opportunity to investigate the competition between intrinsic cubic mass–mass interaction, on-site disorder and the pumping of an acoustic pulse. In our model, the electron was restricted to move on a nonlinear Fermi–Pasta–Ulam disordered chain. The effect of electron–phonon interaction was considered by assuming that the electronic hopping depends on the nearest-neighbor atomic distance. We also assumed that the position of the atom at the extreme left side of chain vibrates in a Gaussian pulse. Using this procedure, we simulated the pumping of a external acoustic mode. In our theoretical formalism, the electronic dynamics and the nonlinear atomic vibrations had two distinct formalisms: the former had a quantum mechanics treatment, while the latter was described by standard classic physics framework. We studied the electronic propagation by numerical analysis of the coupled quantum/classical equations. We applied a second-order Euler method to solve the classical dynamics and a Taylor formalism to solve one-electron equations. Our calculations showed that it is possible to move noninteracting electrons in 1D models with nonlinearity and disorder using an external acoustic mode of atomic vibration. We also investigated the vibrational energy dynamics within this mode. Our results suggests a standard super-diffusive dynamics even at the presence of nonlinear forces. We also did a brief comparison of our results with those obtained for an harmonic lattice. In our calculations, nonlinearity brings difficulties to the electronic transport. We hope that these calculations would stimulate further progress in the field of electronic transport mediated by acoustic wave pumping and electron–phonon coupling.

Acknowledgments

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