



Fast-track communication

Influence of lattice vibrations on the field driven electronic transport in chains with correlated disorder

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ABSTRACT

We investigate electronic transport in a one-dimensional model with four different types of atoms and long-ranged correlated disorder. The latter was attained by choosing an adequate distribution of on-site energies. The wave-packet dynamics is followed by taking into account effects due to a static electric field and electron-phonon coupling. In the absence of electron-phonon coupling, the competition between correlated disorder and the static electric field promotes the occurrence of wave-packet oscillations in the regime of strong correlations. When the electron-lattice coupling is switched on, phonon scattering degrades the Bloch oscillations. For weak electron-phonon couplings, a coherent oscillatory-like dynamics of the wave-packet centroid persists for short periods of time. For strong couplings the wave-packet acquires a diffusive-like displacement and spreading. A slower sub-diffusive spreading takes place in the regime of weak correlations.

1. Introduction

Electronic transport in disordered lattices has been a subject of long standing scientific interest over several decades [1–14]. Based on the Anderson scaling theory, it is well established that there are no extended eigenstates in low-dimensional systems for any degree of uncorrelated disorder. However, it has been shown that low-dimensional disordered systems can support extended states or a localization-delocalization transition in the presence of short or long-range correlations in the disorder distribution [15–34].

Several works on electronic dynamics in systems with correlated disorder have been developed so far by considering a uniform distribution of site energies in a finite range $[-W/2, W/2]$. However, a few models have been introduced where the on-site energy assumes only discrete values (e.g. binary and ternary models) [35–38]. The Anderson model with a long-range correlated ternary disorder sequence was studied in [35]. The authors demonstrated by numerical calculations that the system is an insulator if the ternary sequence is generated totally at random. Nevertheless, by creating a ternary diagonal disorder with long-range correlations, a localized-delocalized phase transition was observed [35]. The effect of long-range correlations in the sequence of capacitances of classical transmission lines (TL) was studied by Lazo and Diez [36,37]. To generate the ternary correlated distribution of capacitances, they used the Fourier filtering method [36] and also the Ornstein-Uhlenbeck (OU) process [37]. In both cases, a transition was observed from the non-conducting to the

conducting state of the TL induced by strong correlations. More recently, a one-dimensional classical ternary harmonic chain with mass distribution constructed from an OU process was studied by [38]. It was reported that only the zero frequency mode can propagate along the chain, thus contradicting previous works [35–37]. We highlight that the study of models with discrete correlated disorder exhibits considerable interest from the experimental point of view. The possibility to generate real systems with a discrete correlated disorder can be a feasible tool to make a comparison of theoretical and experimental procedures, also allowing for the design of new materials with adjustable properties.

In this work, we study the electronic transport in chains with a correlated quaternary disorder distribution. The term “quaternary disorder” represents a disorder distribution containing only four values $(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$. We aim to evaluate the effects of an electric field and its competition with the electron-lattice (i.e. electron-phonon) interaction. In the absence of electron-phonon coupling, the electric field induces wave-packet oscillations in the regime of strong correlations. We will show evidences that electron-phonon scattering degrades the Bloch oscillations. However, for weak electron-phonon coupling, the wave-packet centroid still exhibits a coherent oscillatory dynamics for short times. In the strong coupling regime, the wave-packet is carried diffusively by the external field. In contrast, a slower sub-diffusive wave-packet spreading will be characterized in the regime of weakly correlated disorder.

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2. Model and formalism

We construct a quaternary correlated sequence by performing the mapping of a continuous correlated series $\{V_n\}$ in a discrete sequence of four values $(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$. The continuous series $\{V_n\}$ will be obtained through a numerical procedure that generates the trace of a fractional Brownian motion [17–20],

$$V_n = \sum_{k=1}^{N/2} \frac{1}{k^{\gamma/2}} \cos\left(\frac{2\pi nk}{N} + \phi_k\right). \quad (1)$$

The sequence of values $\{V_n\}$ exhibits a power spectrum approximately $1/k^{\gamma/2}$, and ϕ_k represents random phases distributed within the range $[0, 2\pi]$. For $\gamma = 0$, the sequence is fairly uncorrelated. On the other hand, $\gamma > 0$ introduces long-range correlations in the continuous sequence $\{V_n\}$. According to the approach used in [17], we will perform a normalization process such that $\langle V_n \rangle = 0$ and $\sqrt{\langle V_n^2 \rangle - \langle V_n \rangle^2} = 1$. Once the correlated sequence $\{V_n\}$ has been built, we proceed to the construction of the quaternary correlated sequence $\{\epsilon_n\}$. The mapping definition is given by:

$$\epsilon_n = \begin{cases} \epsilon_1 & \text{if } V_n < -b \\ \epsilon_2 & \text{if } -b < V_n < 0 \\ \epsilon_3 & \text{if } 0 < V_n < b \\ \epsilon_4 & \text{if } V_n > b. \end{cases} \quad (2)$$

The parameter b shown in (2) controls the probability for each of the four values $(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$ to appear on the quaternary distribution. Here, we choose $b \leq 2$, once 2 is approximately the largest value of the V_n sequence after the normalization process. Moreover, we will use the following representative values for on-site energies: $\epsilon_1 = -2$, $\epsilon_2 = -1$, $\epsilon_3 = 1$ and $\epsilon_4 = 2$.

2.1. Electron-lattice interaction

Most of the previous works concerning electronic transport in random systems investigated the nature of the electronic wave-function and its dependence on the type of intrinsic disorder. Moreover, the widely used approach considered the atomic lattice to be “frozen”, i.e. the atoms are stopped (also known in the literature as the Born-Oppenheimer approximation). By contrast, we will study the electronic dynamics considering the presence of atomic vibrations. In other words, we will consider the presence of an electron-phonon coupling. This topic has been the subject of many studies [39–42]. We recall that the electron dynamics will be described by the Anderson Hamiltonian, and that the lattice will be addressed considering that the interaction among nuclei is harmonic. Thus, the complete Hamiltonian can be written as:

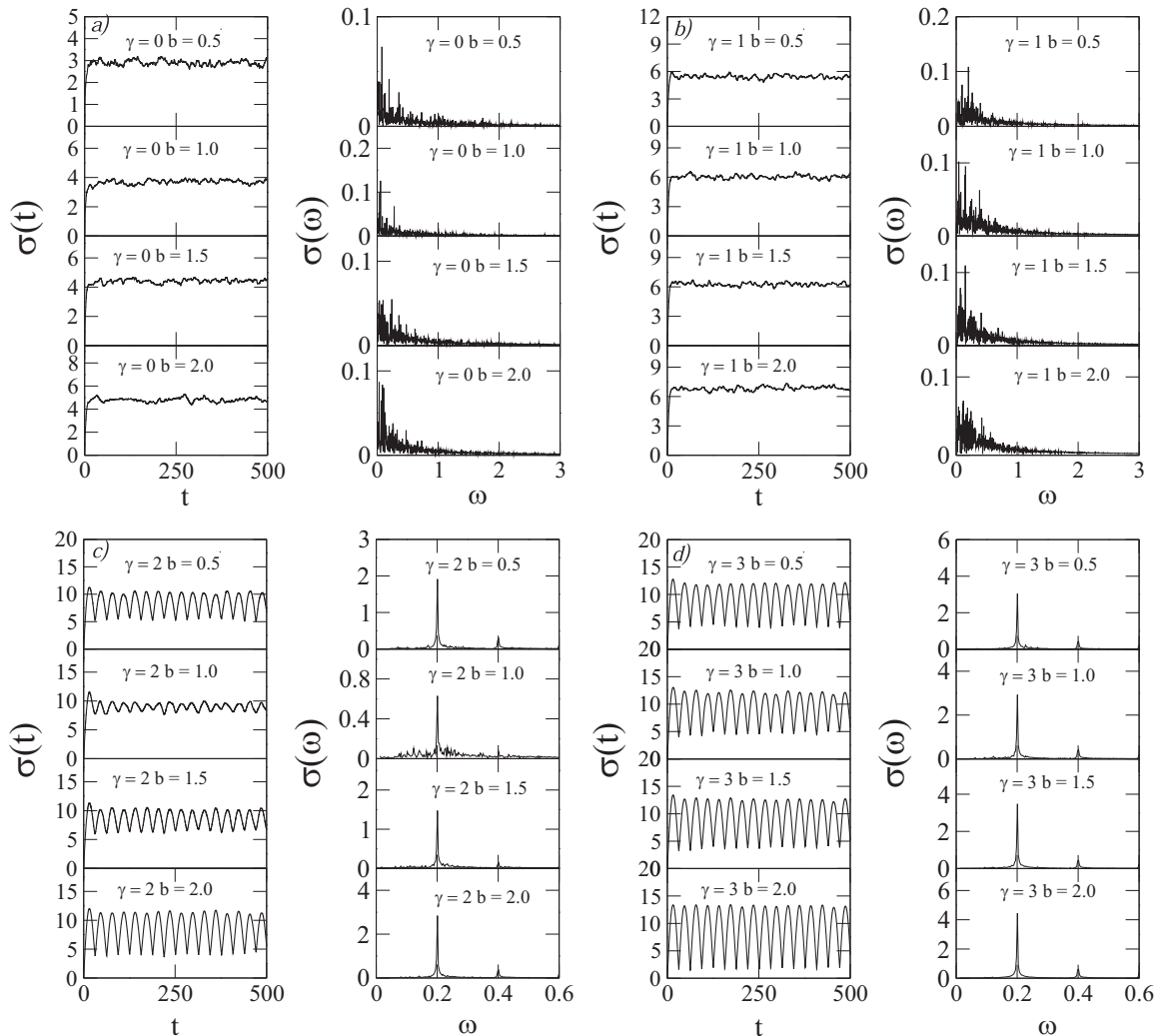


Fig. 1. Average width $\sigma(t)$ of the electronic package versus time t (left panel) and its Fourier transform $\sigma(\omega)$ (right panel) with $\alpha = 0$, $N = 500$, $F = 0.2$ and b ranging from 0.5 up to 2.0. We observe in (a) ($\gamma = 0$) and (b) ($\gamma = 1$), the absence of coherent oscillations in $\sigma(t)$. In (c) ($\gamma = 2$), $\sigma(t)$ shows nearly coherent oscillations. In (d) ($\gamma = 3$), there is a well defined fundamental frequency $\omega \approx F$ for all values of b considered.

$$H = \sum_n \zeta_n |n\rangle\langle n| + \sum_n \tau_n (|n\rangle\langle n+1| + c.c.) + \sum_n \frac{P_n^2}{2m_n} + \sum_n \frac{1}{4} [\beta_n (Q_{n+1} - Q_n)^2 + \beta_{n-1} (Q_n - Q_{n-1})^2]. \quad (3)$$

The first and second terms represent the Anderson Hamiltonian for an electron with on-site energy ζ_n and hopping term τ_n . In the present model, we take into account the presence of a static electric field F parallel to the chain, besides the presence of a quaternary disorder distribution. Therefore, the on-site energy will be considered as: $\zeta_n = \epsilon_n + F(n - N/2)$ where ϵ_n is the correlated quaternary disorder defined previously, and $F(n - N/2)$ represents the potential energy due to the electric field. The third and fourth terms are, respectively, the kinetic and the potential energy of the lattice. Q_n represents the displacement and P_n is the momentum of the lattice element n . We also consider in our calculations the masses m_n of each atom, as well as the spring constants β_n , equal to unity. The coupling between the electron and the lattice will be carried out through the hopping energy τ_n . To introduce the electron-lattice coupling, we write the hopping term as:

$$\tau_n = -\exp[-\alpha(Q_{n+1} - Q_n)], \quad (4)$$

where α is a tunable parameter that controls the intensity of the electron-lattice interaction (the electron-phonon coupling). Analyzing Eq. (4), we notice that, if the atoms located at positions n and $n + 1$ are approached ($Q_{n+1} - Q_n < 0$), the hopping energy will be strong; otherwise it will be very weak when they are apart ($Q_{n+1} - Q_n > 0$). $\tau_n = -1$ corresponds to the typical scale of the hopping energy for atoms separated exactly by one lattice spacing. The approach presented in Eq. (4) is a generalization of that of Su, Schrieffer and Heeger (SSH)

[43]. For small vibrations, (4) retrieves the SSH model: $\tau_n = -\exp[-\alpha(Q_{n+1} - Q_n)] \approx -[1 - \alpha(Q_{n+1} - Q_n)]$ [43]. The time-dependent Schrödinger equation $H|\Psi\rangle = i\hbar \frac{d|\Psi\rangle}{dt}$ can be easily written considering the state $|\Psi\rangle = \sum_n f_n |n\rangle$. The classical part of Hamiltonian (3) does not operate in the state $|\Psi\rangle$, and the hopping energy is defined by Eq. (4). Therefore, we have:

$$i\hbar \frac{df_n}{dt} = \zeta_n f_n - [e^{-\alpha(Q_{n+1}-Q_n)}] f_{n+1} - [e^{-\alpha(Q_n-Q_{n-1})}] f_{n-1}. \quad (5)$$

In order to follow the time evolution of the lattice deformation, we will use the standard Hamilton formalism. From the point of view of classical mechanics, Hamilton's equation for the moment P_n is written, in this problem, as $\dot{P}_n = -\frac{\partial(H)}{\partial Q_n}$, where $\langle H \rangle = \langle \Psi | H | \Psi \rangle$. The equation that governs the lattice vibrations can be displayed in the form:

$$\dot{P}_n = \beta_n (Q_{n+1} - Q_n) - \beta_{n-1} (Q_n - Q_{n-1}) + \alpha [e^{-\alpha(Q_{n+1}-Q_n)} (f_n^\dagger f_{n+1} + f_n f_{n+1}^\dagger) - e^{-\alpha(Q_n-Q_{n-1})} (f_{n-1}^\dagger f_n + f_{n-1} f_n^\dagger)]. \quad (6)$$

The Schrödinger Eq. (5) and the previous lattice Eq. (6) can be solved numerically through traditional numerical methods such as high-order Runge-Kutta [44]. For $\alpha = 0$, there is no electron-phonon coupling, and the equations are decoupled. For $\alpha > 0$, electron-phonon coupling introduces a time-dependent hopping energy τ_n . After the numerical solution of this set of equations, we compute the average position of the electron and the wave-packet mean-square displacement. The average position is defined by $\langle n(t) \rangle = \sum_n n |f_n(t)|^2$. Then, the width σ of the electronic packet is [45]:

$$\sigma(t) = \sqrt{\sum_n (n - \langle n(t) \rangle)^2 |f_n(t)|^2}. \quad (7)$$

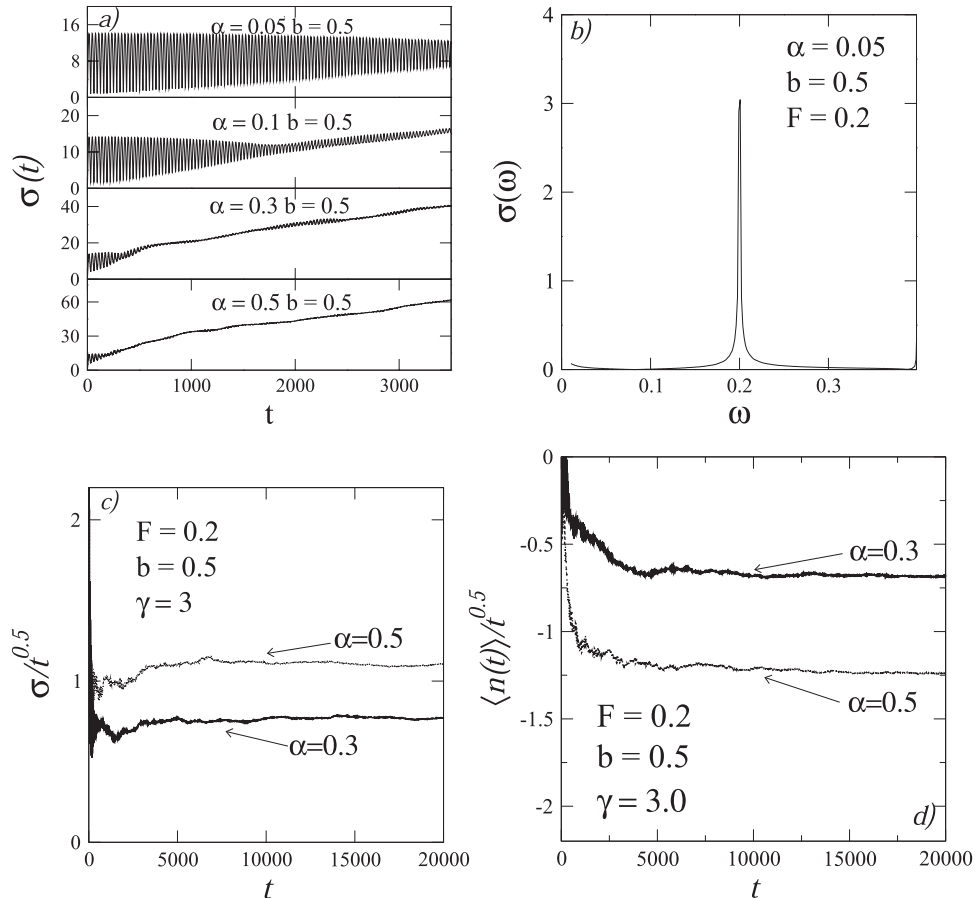


Fig. 2. (a) Wave-packet width $\sigma(t)$ versus time t for $\gamma = 3$, $F = 0.2$ and $\alpha = 0.05, 0.1, 0.3, 0.5$. (b) The Fourier transform $\sigma(\omega)$ for $\gamma = 3$, $F = 0.2$ and $\alpha = 0.05$. (c) The rescaled mean wave-packet width $(\sigma(t)/t^{0.5})$ and (d) the rescaled mean position $(\langle n(t) \rangle / t^{0.5})$ versus t for $\gamma = 3$, $F = 0.2$, $b = 0.5$ and $\alpha = 0.3$ and 0.5 , characterizing a diffusive-like spreading.

which provides an estimate of the size of the wave-packet at time t .

3. Results and discussions

In the following, we present our main findings for the electronic dynamics in a chain with quaternary correlated disorder, with particular emphasis on the effect of electron-lattice interaction under the influence of an external electric field. Let us consider initially that the electron is fully localized in the center of the chain. Thus, the amplitude of the wave-function can be written as: $f_n(t=0) = \delta_{n,N/2}$. Solving the Eqs. (5) and (6) in the presence of electron-phonon coupling and a static electric field, we calculate the spread $\sigma(t)$ of the wave-packet as a function of time. The size of the chain was set at $N=500$, and the values of the correlation parameter were, in turn, $\gamma = 0, 1, 2, 3$. We choose for the parameter b values belonging to the interval 0.5 until 2.0. Let us consider first the case where there is no electron-lattice coupling ($\alpha = 0$). The results in Fig. 1 show the average spread $\sigma(t)$ of the electronic package versus time (left panel) and its Fourier transform (right panel). The electric field was considered $F = 0.2$. In the case of uncorrelated disorder [$\gamma = 0$ shown in Fig. 1 (a)], the package does not present coherent oscillations. This observation is confirmed in the frequency diagram, where we observe a broad spectrum with several spikes. This result is similar to those obtained in Fig. 1 (b) for $\gamma = 1$ (weak long-ranged correlated disorder). Again, the absence of coherent oscillations is signalled by the broadness of the Fourier transform (see Fig. 1 (b)). For $\gamma = 2$ (Fig. 1 (c)), we observe the onset of nearly coherent oscillations and a frequency spectrum typical of Bloch's oscillations with a pronounced peak. We stress that the limit $b = 2$ represents a turning point, when the disordered quaternary distribution approaches to an almost non-random sequence. In Fig. 1 (d), we present our results with $\gamma = 3$, representing the case of strong long-range correlations leading to the emergence of delocalized states in the absence of an

external field. In this case, the field-driven oscillation pattern is quite coherent. We clearly see the presence of a fundamental frequency $\omega \approx F$ for all values of b considered. This result is a strong indication that the oscillatory behavior observed in the left frame is compatible with the Bloch oscillations scenario.

To analyze the influence of the coupling between the electron dynamics and lattice vibrations, we start by focusing attention to the case with strong correlations ($\gamma > 2$). In Fig. 2 we present the wave-packet width $\sigma(t)$ versus time for $\gamma = 3$, $b = 0.5$, and $\alpha = 0.05, 0.1, 0.3, 0.5$. We stress that the computational solution of the differential equations became extremely sensitive to the numerical precision for large α . The results presented here are within the range of values for which the numerical accuracy could be well controlled in the entire range of integration time. In Fig. 2 (a) for $\alpha = 0.05$ and 0.1, there is an oscillatory behavior for short times. We note that the coherent oscillation pattern disappears for intermediate and long times. The Fourier transform in Fig. Fig. 2b still signals the presence of a predominant frequency around $\omega = F$ reminiscent of Bloch oscillations. For larger electron-phonon coupling factors ($\alpha = 0.3$ and 0.5), these oscillations quickly vanish and the wave-packet width depicts a continuous growth. The underlying mechanism leading to this crossover is that the atomic vibrations are still small at short times. Consequently, the electric field term dominates the dynamics, thus imposing the initial oscillating pattern. For longer propagation times, the atomic vibrations become stronger, thus introducing a more intense randomness into the hopping energy. Therefore, this time-dependent disordered hopping distribution is likely to degrade the regular electronic oscillations. Formally, the Bloch oscillations for long times do not exist within this framework of quaternary correlated disorder and electron-phonon coupling. In Fig. 2c–d we show that the wave-packet width display a diffusive-like growth while its centroid is diffusively carried by the static field.

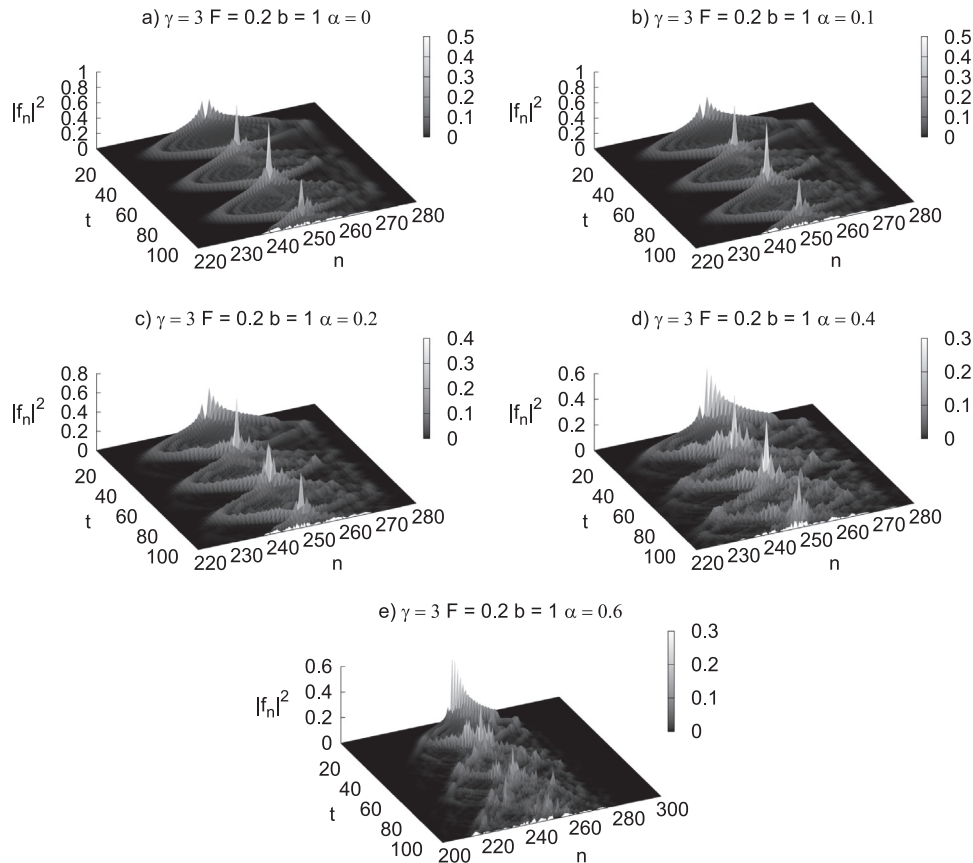


Fig. 3. Wave-function profiles for $\gamma = 3$, $F = 0.2$ and $\alpha = 0$ up to 0.6. Notice that increasing the electron-phonon coupling strength leads to a degradation of coherent oscillations.

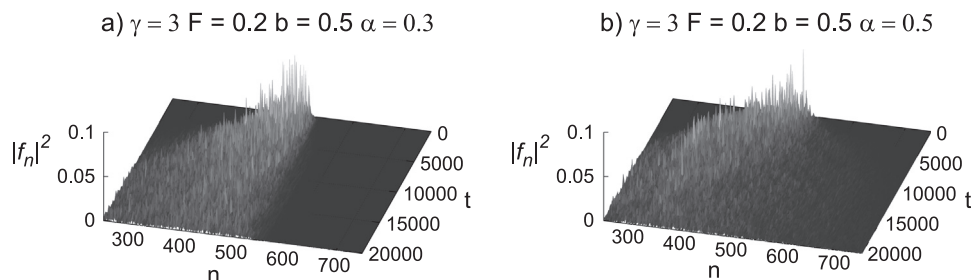


Fig. 4. Wave-packet profiles for $\gamma = 3$, $F = 0.2$ and $\alpha = 0.3$ (a) and 0.5 (b). Notice that after losing coherence, the wavepacket continues to spread while drifting.

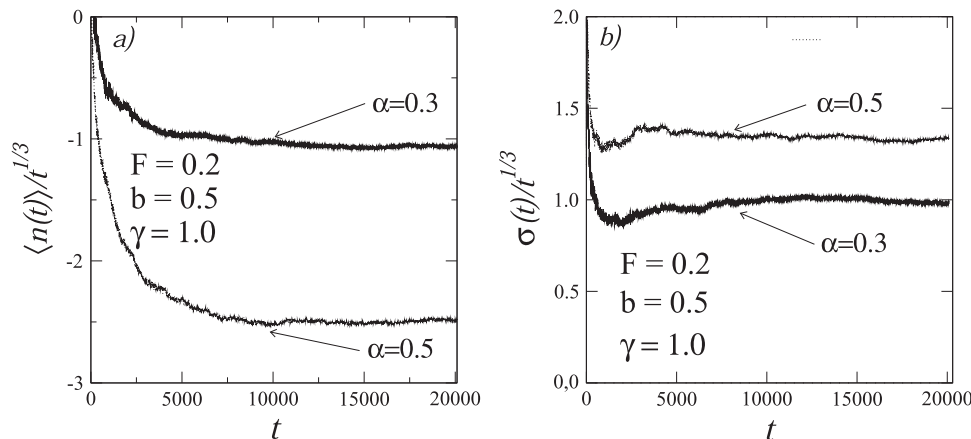


Fig. 5. (a) Rescaled mean position ($\langle n(t) \rangle / t^{1/3}$) versus t and (b) the rescaled wave-packet width ($\sigma(t) / t^{1/3}$) versus t for $\gamma = 1$, $F = -0.2$ and $\alpha = 0.3$ and 0.5 . In this case of weak long-range correlations ($\gamma < 2$) the wave-packet displays a sub-diffusive spreading and drifting.

In Fig. 3 (a–e) we plot the wave-function distribution $|f_n(t)|^2$ versus t and n for $\gamma = 3$, $F = 0.2$ and $\alpha = 0$ up to 0.6 . For $\alpha = 0$, the coherent electronic oscillation is well defined, in good agreement with the previous results shown in Fig. 1. However, for $\alpha > 0$, we verify the effect of scattering by atomic vibrations. We clearly observe the Bloch-like oscillatory profile for short times. However, as time evolves, the coherent oscillations are gradually degraded. In Fig. 4 we show a longer run for the cases of strong couplings which clearly illustrates the widening of the wave-packet while its centroid is driven by the external field. The above results unveils that the effective dynamic disorder associated with the coupling with lattice vibrations induces a diffusive-like dynamics of the electronic wave-packet on which both the centroid and width grow in time as $t^{1/2}$.

We also investigated the electron-lattice coupling in the regime of weak long-range correlations ($\gamma < 2$) on which the electronic states are all exponentially localized in the zero-coupling limit and no-Bloch oscillations are present. In this case (see Fig. 5), the action of the relevant static disorder together with the coupling-induced dynamic disorder results in a slower spreading of the wave-packet on which the width and centroid evolve sub-diffusively, roughly as $t^{1/3}$. This result is similar the one previously reported to take place for field driven wave-packets propagating in nonlinear chains [46].

4. Summary and conclusions

In summary, we studied the electronic wave-packet transport in quaternary systems with correlated disorder. Our goal was to understand the localization properties of the electronic wave-function. We employed a methodology that allowed us to include the electron-lattice interaction as well as the presence of an external electric field. In general, we considered a one-dimensional model with four kinds of atoms. The on-site diagonal energy at each of these atoms was given by $(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$. The distribution of these energies was chosen in order to exhibit long-range correlations, resembling the trace of a fractional

Brownian motion with power spectrum $S(k) \propto k^{-\gamma}$. Our analysis of the effects of the field and its competition with the scattering by lattice vibrations presented several instructive features. In the absence of electron-phonon coupling $\alpha = 0$, the presence of an electric field produces coherent oscillations if the diagonal disorder has strong long-range correlations (with spectral exponent $\gamma > 2$). When the electron is coupled to the lattice vibrations, phonon scattering degrades the Bloch oscillations. In the regime of strong long-range correlations, the electron-lattice coupling leads to a diffusive-like spread and displacement of the electronic wave-packet. In contrast, a slower sub-diffusive dynamics develops in a weak long-range correlated potential with $\gamma < 2$. It is important to stress that the present results have been obtained in the framework of non-interacting electrons. However, electron-electron interaction is known to strongly influence the nature of electronic states in disordered systems [47,48]. It would be valuable to have future efforts devoted to study the competition between electron-electron and electron-phonon interactions in random media. It is possible that the emergence of bounded two-electron states can suppress the coherence loss due to phonon scattering. We hope to address this relevant issue in a future contribution.

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