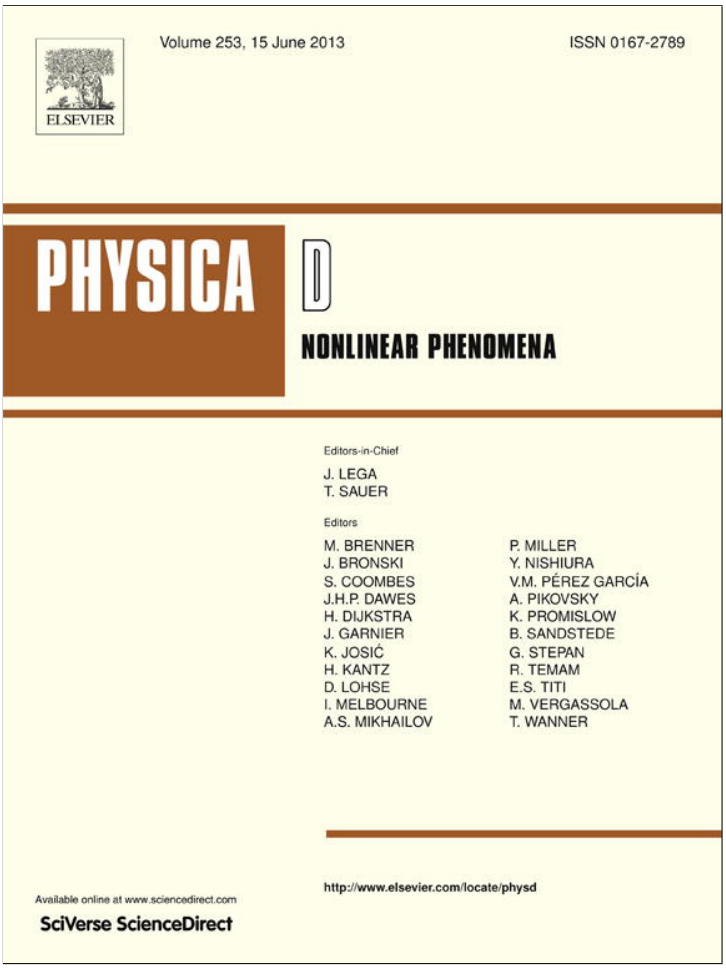

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Numerical evidence of electron–soliton dynamics in Fermi–Pasta–Ulam disordered chains

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HIGHLIGHTS

- The one-electron dynamics in a Fermi–Pasta–Ulam disordered chain.
- The competition between correlated disorder and nonlinearity.
- The existence of an electron–soliton pair.
- The electron transport mediated by solitonic excitations.

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ABSTRACT

In this paper, we study numerically the one-electron dynamics in a Fermi–Pasta–Ulam disordered chain. In our model the atoms are coupled by a random harmonic force and a nonlinear cubic potential. The electron–lattice interaction was considered such that the kinetic energy of the electrons depends on the effective distance between neighboring atoms. Basically, the hopping term will increase exponentially when the distance between neighboring atoms decreases. By solving numerically the equations describing the dynamics for the electron and lattice, we can compute the spreading of an initially localized electronic wavepacket. Our results suggest that the soliton excitation induced by the nonlinear cubic interaction present in the Hamiltonian can control the electron dynamics across the entire lattice. We report numerical evidence of the existence of a soliton–electron pair in Fermi–Pasta–Ulam disordered chains. We discuss in detail the conditions necessary for promoting the electron transport mediated by solitons in this model.

1. Introduction

In recent years the transport properties of nonlinear lattices have attracted significant interest from the solid state community as well as within the nonlinear science field [1–32]. In fact, it has been proposed by several authors [7–25] that the electron–phonon interaction plays a relevant role in transport and thermodynamics properties. As regards the electronic transport, the interaction between electrons and lattice vibrations leads to an effective nonlinearity [17–32]. Davydov [12–16] was one of the first to propose that this nonlinear character of the electron–lattice term can promote charge transport. The electrosoliton concept proposed by Davydov is based on the nonlinear combination of a linear electronic model and a soliton-bearing equation dynamically describing a linear lattice. Recently, other studies have considered systems in which either the lattice or the quantum particle interactions, or both, are themselves nonlinear. In particular, nonlinear discrete lattices are known to exhibit genuine intrinsic localized modes (solitons) or discrete breathers [17–19]. In Refs. [17–25], M.G. Velarde and co-workers demonstrated the existence of a *polaron–soliton* "quasiparticle" in nonlinear lattices, and have also emphasized its importance to the carrying of charge. The coupling of self-trapped states (polaron states) with the lattice solitons has been generally termed a *solectron* [17–25]. The solectron concept appears as a significant generalization of the original polaron concept, that can mediate non-Ohmic supersonic electric conduction [25]. Moreover, recently it was shown that in anharmonic one-dimensional crystal lattices, pairing of electrons or holes in a localized bisolectron state is possible due to the coupling between the charges and the lattice deformation that can overcome the Coulomb repulsion [7]. The dynamics of two interacting electrons in nonlinear models was also studied in Ref. [33]. By using numerical methods to solve the time-dependent nonlinear Schrödinger equation for an initially localized two-electron singlet state, it was shown that the magnitude of the electron–phonon coupling necessary for promoting the self-trapping of the electronic wavepacket decreases as a function of the electron–electron interaction.

The electron transport mediated by lattice vibration is a new phenomenon and it is strongly dependent on the kinds of atomic

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vibrational modes allowed. The nature of the vibrational modes in low-dimensional lattices depends on the kinds of atomic forces and also the lattice topology [34–48]. It is well known that the presence of anharmonicity promotes a richness of unusual vibrational modes. Moreover, the presence of nonlinear atomic interaction was pointed out as a key ingredient involved in the thermal conductivity in classical lattices [39–47]. One of the most well known properties of nonlinear chains is the presence of kink-soliton solutions. It is well known that the solitonic effect is damped by the presence of disorder. In fact, the scattering of solitons by disorder can be measured through the reduction of localized energy within the localization region, the time-dependent acceleration of the energy flux and the long-time behavior of the diffusion coefficient. The well known paper by Fermi, Pasta and Ulam was the first work that pointed out the importance of anharmonic forces in physics [48]. The dynamics of the energy in anharmonic chains was studied in detail and the manifestation of solitons was pointed out. Besides having shown the complexity of nonlinear systems [5], the FPU model also emphasized the value of computer simulations in the context of theoretical physics [5,48]. The competition between disorder and anharmonicity was studied in detail in Ref. [46]. It was numerically demonstrated that, while anharmonicity promotes energy transport through ultrasonic solitons, disorder decreases the propagation due to the well known Anderson localization [46]. The soliton dynamics in a Toda lattice with randomly distributed masses was studied in Ref. [47]. The disordered Toda model consists of a one-dimensional chain of disordered masses where each mass interacts with the others through a nearest-neighbor exponential potential. By using the inverse scattering transform, the effective equations for the decay of the soliton amplitude that take into account radiative losses were derived. It was shown that the soliton energy decays as $\propto N^{3/2}$ for small-amplitude solitons and $\propto \exp(2N)$ for large-amplitude solitons [47]. Moreover, in a more general context, the presence of nonlinearity in non-periodic solids represents a general challenge with a rich framework of non-intuitive phenomena.

In this work, we focus on the electron transport on non-periodic anharmonic classical lattices. We study numerically the one-electron dynamics in a one-dimensional alloy in which the atoms are coupled by a random harmonic force and also a nonlinear cubic potential. The harmonic elastic constants will be considered to follow a long-range correlated disorder distribution. By using a Fourier formalism we can generate several degrees of correlations by controlling a single parameter, γ. Our model for studying electronic transport is based on a Hamiltonian where the electron transport is treated quantum mechanically over the alloy in a tight-binding approximation and the longitudinal vibrations of the lattice are described by using a classical formalism. The electron–lattice term was considered in an intuitive way. The transfer integral for neighboring atoms, also called the hopping term, represents the electron kinetic energy and depends on the effective distance between neighboring atoms. Basically, the hopping term will increase when the distance between neighboring atoms decreases. We will follow M.G. Velarde and co-workers [9–11] by considering an exponential form of the electron–lattice interaction. Due to the presence of nonlinearity in the lattice, the present exponential form works better than the linear Su–Schrieffer–Heeger [49] approximation used previously [27–29]. By numerically solving the equations for the dynamics of the electron and lattice, we can compute the spreading of an initially localized electronic wavepacket. Our results suggest that at the strong correlation limit $\gamma \geq 2$, the soliton excitation induced by the nonlinear cubic interaction existing in the Hamiltonian can control the electron dynamics across the entire lattice. We report numerical evidence of the existence of a soliton–electron pair in Fermi–Pasta–Ulam disordered chains. We compare the mobile trapped electron wavepacket obtained with the energy spatial distribution, thus obtaining support for our finding. For the weak correlation limit $\gamma < 2$, our calculations indicate the absence of electron transport mediated by solitons. However, our calculations reveal a super-diffusive wavefunction spread, in contrast to the sub-diffusive behavior obtained previously in harmonic lattices [26].

2. Theory and numerical calculation

We consider one electron moving in a 1D anharmonic lattice of N masses. The complete Hamiltonian for one electron coupled to the vibrations of a nonlinear chain can be written as

$$H = \sum_n h_n + \sum_n V_{n+1,n}(c_{n+1}^{\dagger} c_n) + \sum_n \epsilon_n c_n^{\dagger} c_n \tag{1}$$

where $c_n^{\dagger}$ and c_n are the creation and annihilation operators for the electron at site n. V_n is the bare hopping amplitude and ϵ_n is the on-site energy of site n. $h_n(t)$ represents the classical energy of the mass at site (n) given by

$$h_n(t) = \frac{P_n^2}{2m_n} + \frac{1}{4}\Big[\beta_n(Q_{n+1} - Q_n)^2 + \beta_{n-1}(Q_n - Q_{n-1})^2\Big] + \frac{\eta}{6}\Big[(Q_{n+1} - Q_n)^3 + (Q_n - Q_{n-1})^3\Big]. \tag{2}$$

Here P_n and Q_n define the momentum and displacement of the mass at site (n). Here we will consider all masses identical, with $m_n = 1$ and the on-site term $\epsilon_n = 0$. The harmonic elastic constants β_n will be considered to follow a rule given by

$$\beta_n = b_0 + a_0 \tanh\theta_n, \tag{3}$$

where b_0 and a_0 are constants with $b_0 > a_0$ and θ_n is a long-range correlated disorder distribution. One of the simplest ways to numerically generate a long-range correlated sequence θ_n is to write its Fourier decomposition as follows [50]:

$$\theta_n = C_\gamma(N) \sum_{k=1}^{N/2} \frac{1}{k^{\gamma/2}} \cos\left(\frac{2\pi nk}{N} + \phi_k\right). \tag{4}$$

Here, the ϕ_k are $N/2$ independent random phases uniformly distributed within the interval $[0, 2\pi]$, and C_γ is a normalization constant. The hyperbolic transformation of the series yields the advantage of bounding the interval of the random variable without changing its asymptotic correlation function. We will keep the mean value of the sequence θ_n equal to zero (i.e., $\langle\theta_n\rangle = 0$) and choose C_α to keep the variance size independent $\left(\sqrt{\langle\theta_n^2\rangle - \langle\theta_n\rangle^2} = 1\right)$. The long-range nature of the correlations results from the power-law dependence of the amplitudes on the wavevector characterizing each Fourier component. In the case $\gamma \to 0$, one recovers an uncorrelated random sequence. For the opposite limit $\gamma \to \infty$, θ_n is analogous to a harmonic function. Intermediate values of γ give rise to a long-range correlated sequence. All calculations in this work will be done for $b_0 = 1$ and $a_0 = 0.25$. The reason behind this choice is simple: we are interested in following Ref. [51], keeping the mean value of the harmonic spring constants equal to unity and dealing with the intermediate disorder limit $\left(\sqrt{\langle\beta_n^2\rangle - \langle\beta_n\rangle^2} < \langle\beta_n\rangle\right)$. In our calculations, we assume that there is no disorder in the anharmonic contribution. For $\beta_n = \text{const}$, Eq. (2) is the Fermi–Pasta–Ulam (FPU) α model [48].

Following M.G. Velarde and co-workers [7–11,17–25], the interaction between the electron and the vibrational modes will be considered in our model by relating the electronic parameters $V_{n+1,n}$ with the displacements of the molecules from their equilibrium positions. The hopping elements $V_{n+1,n}$ will depend on

the relative distance between two consecutive molecules on the chain, following the expression

$$V_{n+1,n} = -V_0 \exp[-\alpha(Q_{n+1} - Q_n)]. \quad (5)$$

The quantity α will define how the hopping term $V_{n+1,n}$ will depend on the relative displacement of lattice units, or in other words, it determines the electron–lattice coupling strength. Following Refs. [7–11,17–25], we would like to stress that the exponential form of the electron–lattice interaction works for both small and large relative displacements, thus going beyond the range of harmonic interaction considered in previous papers [26,29]. For small relative displacements we recover the Su–Schrieffer–Heeger approximation $V_{n+1,n} \approx -V_0[1 - \alpha(Q_{n+1} - Q_n)]$. In our calculations we will use units such that $V_0 = 1$.

We will follow the time evolution of an initially localized one-electron wavepacket. The time-dependent wavefunction $\Phi(t) = \sum_n c_n(t)|n\rangle$ will be obtained by numerical solution of the time-dependent Schrödinger form. We consider the electron initially localized at site $N/2$, i.e. $|\Phi(t = 0)\rangle = \sum_n c_n(t = 0)|n\rangle$ where $c_n(t = 0) = \delta_{n,N/2}$. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as ($\hbar = 1$)

$$i\frac{dc_n(t)}{dt} = -\exp[-\alpha(Q_{n+1} - Q_n)]c_{n+1}(t) - \exp[-\alpha(Q_n - Q_{n-1})]c_{n-1}(t). \quad (6)$$

Moreover, the lattice equation can be written as

$$\frac{d^2Q_n(t)}{dt^2} = \beta_n(Q_{n+1} - Q_n) - \beta_{n-1}(Q_n - Q_{n-1}) + \eta[(Q_{n+1} - Q_n)^2 - (Q_n - Q_{n-1})^2] - \alpha\left\{\exp[-\alpha(Q_{n+1} - Q_n)](c^*_{n+1}c_n + c_{n+1}c^*_n) - \exp[-\alpha(Q_n - Q_{n-1})](c^*_n c_{n-1} + c_n c^*_{n-1})\right\}. \quad (7)$$

Our numerical formalism will be based on the precise numerical solution of the previous form, Eqs. (6) and (7). Both equations for the dynamics will be solved by using a standard Dormand–Prince eighth-order Runge–Kutta method with monitoring of local truncation error [52] with time step $dt \approx 10^{-3}$. The spatial and temporal evolution of the lattice vibrations will be described via the energy $h_n(t)$ of the mass at site (n). Aiming to characterize the dynamic behavior of the wavepacket, we computed a typical quantity that can yield information about the electronic transport in this nonlinear model, namely, the participation function, which is defined as [53,54]

$$\xi(t) = 1/\sum_n |c_n(t)|^4. \quad (8)$$

The participation function gives an estimate of the number of base states over which the wavepacket is spread at time t. In particular, the asymptotic participation number becomes size independent for localized wavepackets. On the other hand, $\xi(t \to \infty) \propto N$ corresponds to the regime where the wavepacket is uniformly distributed over the lattice [53,54].

3. Results and discussion

We obtained the time evolution of a wavepacket initially localized at the center of a self-expanding chain (i.e. $\{c_n(t = 0) = \delta_{n,N/2}\}$) numerically. Following Ref. [46], an initial impulse excitation ($P_n = \delta_{n,N/2} Q_n = 0$) was used in our calculations. The self-expanding chain was used to minimize end effects; whenever the probability of finding the electron at the ends of the chain exceeded 10^{-30}, ten new sites were added to each end. Numerical convergence was ensured by checking the conservation of the norm of the wavepacket at every time step; our results provide

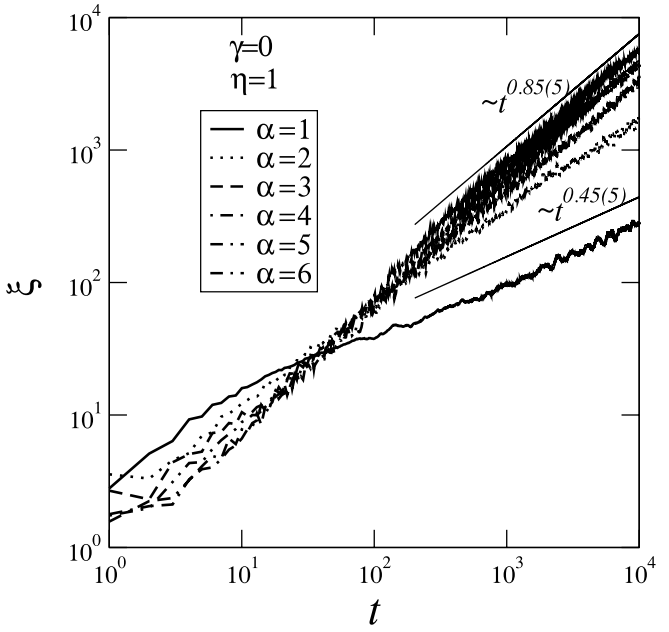

Fig. 1. Participation number $\xi(t)$ versus time for $\gamma = 0$, $\eta = 1$ and $\alpha = 1$ up to 6. Our results suggest that the electron propagation increases as the electron–lattice interaction is increased.

$|1 - \sum_n |c_n(t)|^2| < 10^{-10}$ for all times considered. All calculations were averaged over 20 disorder configurations. We plot in Fig. 1 the participation number $\xi(t)$ versus time for $\gamma = 0$, $\eta = 1$ and $\alpha = 1$ up to 6. Let us stress that for $\gamma = 0$ and $\eta = 1$ we are dealing with an α-Fermi–Pasta–Ulam chain where the harmonic constants exhibit an uncorrelated random distribution. Our calculations indicate that as the electron–lattice interaction is increased, the electron propagation also increases. We can see this by examining the time evolution of the participation number, i.e., $\xi \propto t^{0.45(5)}$ for $\alpha = 1$ and $\xi \propto t^{0.85(5)}$ for $\alpha = 6$. The increase of the electron spread induced by electron–phonon coupling was reported previously for harmonic systems in Refs. [26,29]. Our calculations indicate numerically that a similar framework can be obtained for anharmonic systems with uncorrelated disorder. We need to stress that with the present anharmonic model, the super-diffusive propagation obtained was significantly larger than that for the sub-diffusive rule ($\xi \propto t^{0.3}$) obtained for harmonic systems previously [26]. Now we will include the effect of long-range correlated disorder into this model. We consider now $\gamma > 0$. We plot in Fig. 2 the participation number $\xi(t)$ versus time for $\eta = 1, \gamma = 1$ up to 4, and $\alpha =$ (a) 1, (b) 2 and (c) 3. Our calculations reveal a nontrivial phenomenon. For $\gamma < 2$ our calculations are in good agreement with Fig. 1, i.e., the electron spread increases as the electron–lattice interaction is increased. However, for $\gamma \geq 2$ we obtain am unexpected result: the participation number decreases substantially. In fact, the electron wavefunction seems to be trapped in a small fraction of the lattice. Aiming to elucidate the possibility of electron mobility in this nonlinear chain, we will compute the mean position (centroid) defined as [53,54] $\langle n(t)\rangle = \sum_n n|c_n(t)|^2$. In Fig. 3 we plot $\langle n(t)\rangle$ versus time t for $\gamma = 3$, $\eta = 1$ and $\alpha = 3$. We can see that, in spite of the width of the wavefunction remaining finite (see Fig. 2), the wavepacket centroid evolves with time. These results suggest the possibility of electron transport. In order to understand what is happening here, we will examine the time-dependent wavefunction profile. In Fig. 4(A)–(D) we plot $|c_n|^2$ versus t and n for $\eta = 1, \gamma = 3$ and $\alpha = 4, 6, 8, 10$. Calculations were done using a finite lattice with $N = 600$ sites. We can see clearly that, in good agreement with previous results shown in Fig. 2, the wavefunction

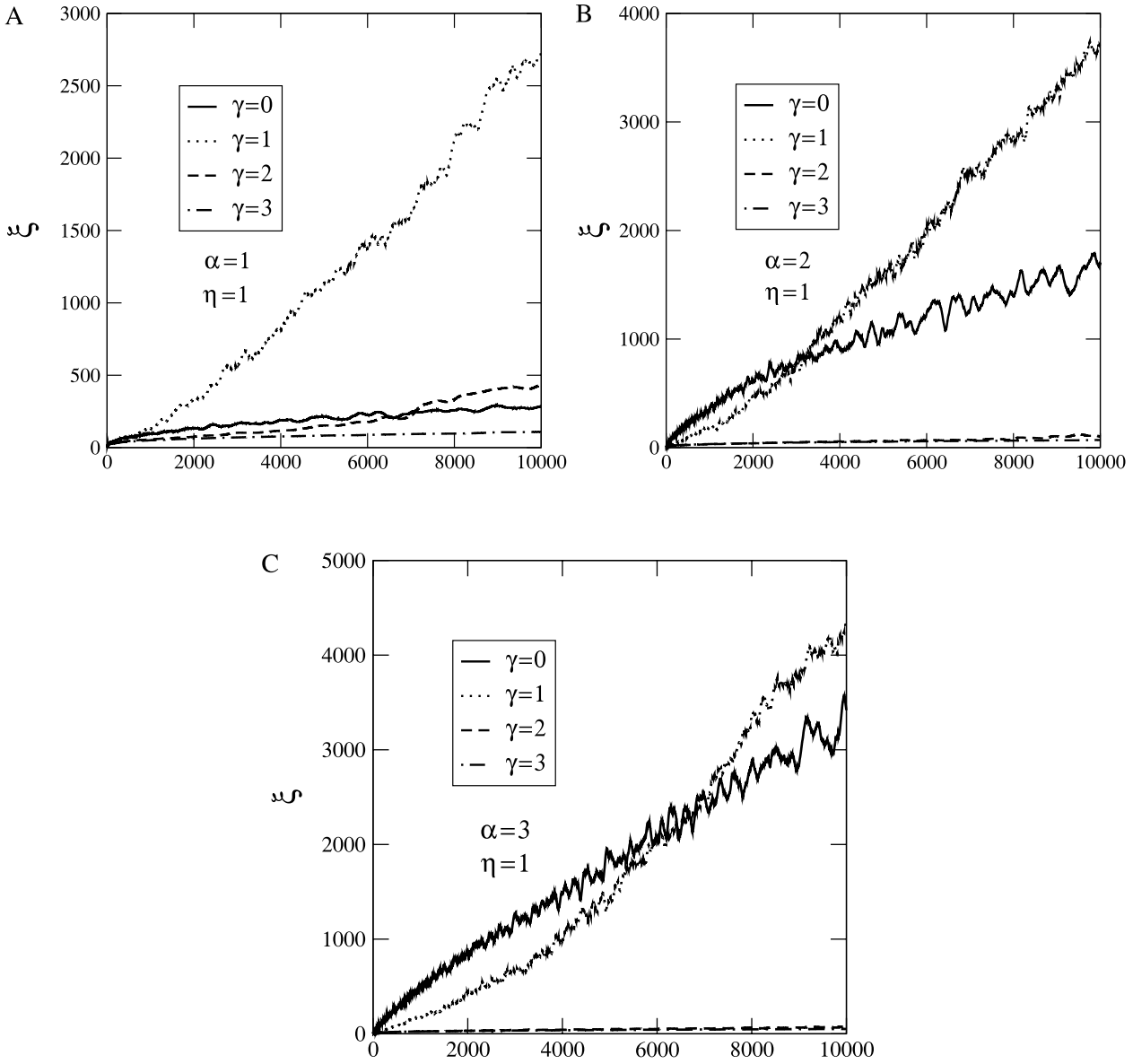

Fig. 2. Participation number $\xi(t)$ versus time for $\eta = 1$, $\gamma = 1$ up to 4 and $\alpha =$ (a) 1, (b) 2 and (c) 3. For small γ our calculations are in good agreement with Fig. 1, i.e., the electron spread increases as the electron–lattice interaction is increased. For $\gamma \leq 2$ the electron wavefunction seems to be trapped in a small fraction of the lattice.

remains trapped in a finite fraction of the lattice. Moreover, we can also see that the localized electronic wavepacket is moving along the chain. The dynamics of the localized wavefunction shown in Fig. 4(A)–(D) explain the centroid behavior obtained in Fig. 3. We need to understand the mechanism behind this electronic dynamics. We are dealing with a disordered nonlinear chain. For $\gamma \geq 2$ the harmonic spring constants are a long-range correlated sequence. It was numerically demonstrated that the low-frequency modes of a harmonic model with correlated disorder display an extended behavior. On the other hand, the cubic nonlinearity considered here promotes the appearance of soliton modes. However, solitons are scattering due to the presence of disorder, thus reducing the localized energy within the localization region, the time-dependent acceleration of the energy flux and the long-time behavior of the diffusion coefficient. The competition between disorder and anharmonicity was studied in detail in Ref. [46]. It was numerically demonstrated that, while anharmonicity promotes energy transport through ultrasonic solitons, disorder decreases the propagation due to the well known Anderson localization [46]. Here, the competition between correlated disorder and nonlinearity seems to maintain the soliton modes. Moreover, the electron–lattice interaction considered here promotes the appearance of a kind of electron–soliton pair. In order to give more information about this key point, we will study the spatial and temporal evolution of the energy of the lattice vibrations described in terms of the energy $h_n(t)$ of the mass at site (n). The spatial–temporal shape of $h_n(t)$ was previously used, both from analytical and numerical points of view, to detect the presence of solitonic waves in anharmonic periodic and disordered systems [45,46]. We plot in Fig. 5 $h_n(t)$ times t and n for an anharmonic chain with long-range correlated harmonic terms ($\gamma = 3$) and cubic nonlinearity with $\eta = 1$. We have used an initial impulse excitation located at site $n_0 = N/2$. Our results have shown that the initial excitation propagates along the chain in a soliton-like mode. Within our numerical precision, the energy intensity of this soliton-like mode seems to remain constant. We can see that the picture shown in Fig. 5 is in good agreement with the wavefunction dynamics obtained in Fig. 4(A)–(D). Therefore, our results in fact suggest that the coupling between the electron and this nonlinear lattice promotes the appearance of a mobile

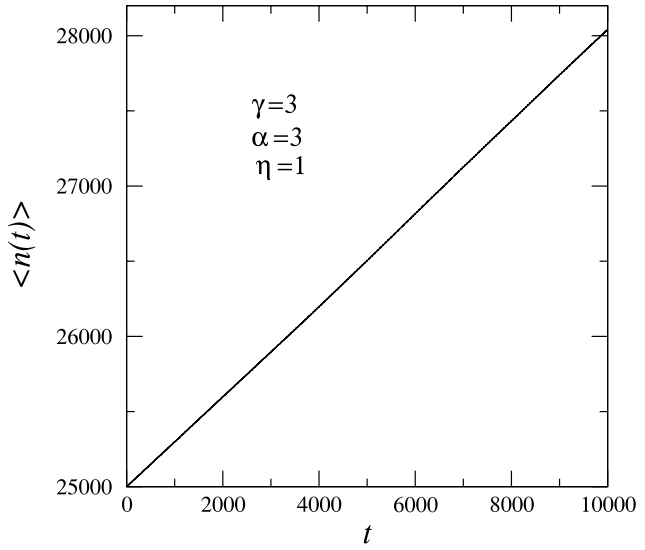

Fig. 3. The electron mean position (centroid) defined as $\langle n(t)\rangle = \sum_n n|c_n(t)|^2$ versus time t. We can see that the wavepacket centroid evolves with time, thus suggesting the possibility of electron mobility.

electron–soliton pair. We can observe that as the electron–lattice term α is increased, the soliton mode can come to trap the initial electronic wavepacket completely. Therefore, the electron–soliton pair becomes more well defined, almost completely focused at a single point. We would like to emphasize that the existence of an electron–soliton pair like the one found here favors the electron transport even in the presence of disorder. In Refs. [7–11,17–25], the electronic transport in a nonlinear Morse lattice was also mediated by an electron–soliton particle, called the *solectron* by the authors. Here, we have considered a distinct type of nonlinearity and also included the effect of static disorder. We demonstrated numerically the possibility of electron–soliton pair formation even in disordered nonlinear chains. We would like to stress that the calculations shown here, in spite of having been made for $\eta = 1$, are valid for other values of $\eta > 0$. In fact, the degree of nonlinearity can change some specificities of solitons; however, the existence of an electron–soliton pair becomes unchanged. The main point here was the possibility of electron transport mediated by solitons in disordered nonlinear Fermi–Pasta–Ulam chains.

4. Conclusions

In summary, we studied the electronic dynamics on non-periodic anharmonic classical lattices. We have studied numerically the one-electron dynamics in a modified α-Fermi–Pasta–Ulam case with long-range correlated disorder in the harmonic terms. In our model the electron transport was treated quantum mechanically over the alloy in a tight-binding approximation and the longitudinal vibrations of the lattice were described by using a classical formalism. The electron–lattice term was considered such that the transfer integral for neighboring atoms was dependent on the effective distance between neighboring atoms. We have used an exponential for the electron–lattice interaction [9–11]. By using a high-precision Runge–Kutta formalism for solving the equations for the dynamics of the electron and lattice, we can compute the spreading of an initially localized one-electron wavepacket. Our main results can be separated into two parts: (1) For disordered nonlinear chains with weak correlations ($\gamma < 2$) we find the electronic dynamics to display a sub-diffusive behavior for weak electron–phonon interaction ($\alpha \approx 1$) and a super-diffusive behavior for strong electron–lattice interaction ($\alpha > 1$). These results are a generalization of the previous calculations [26,29] concerning one-electron transport in disordered harmonic chains with electron–phonon coupling. The novel feature that we point out here is

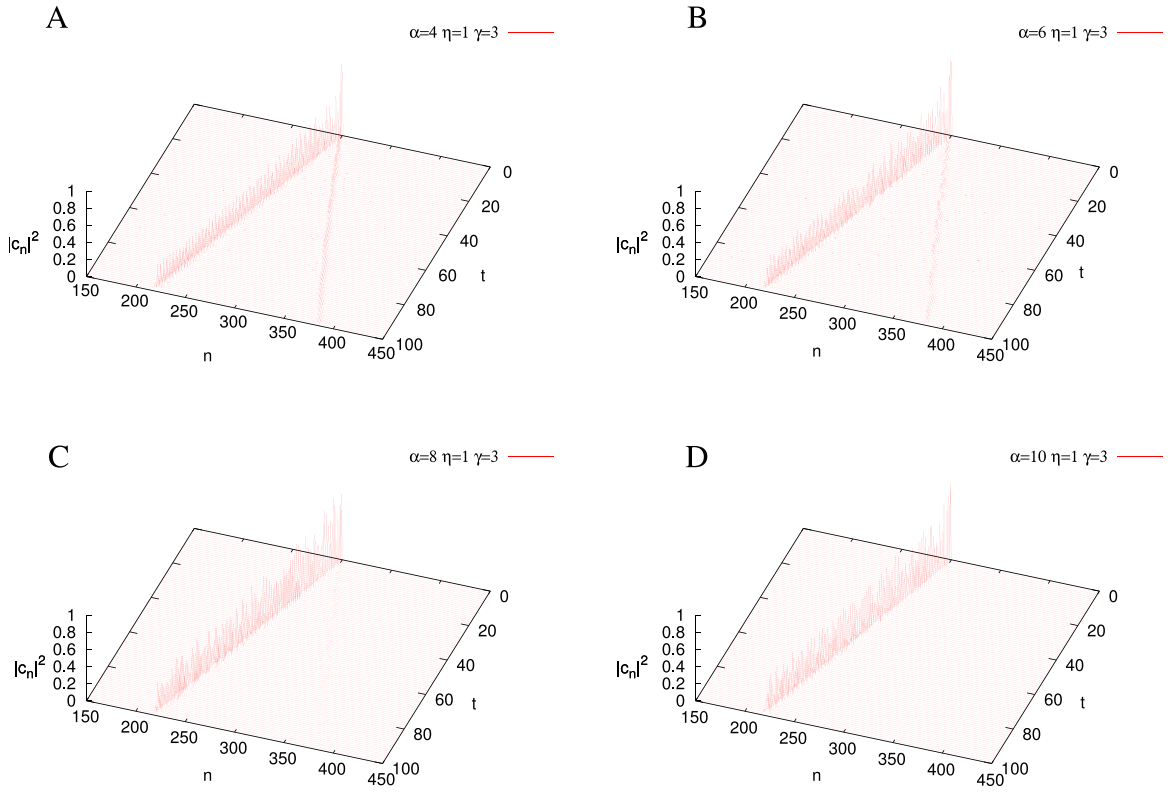

Fig. 4. The square wavefunction component $|c_n|^2$ versus t and n for $\eta = 1$, $\gamma = 3$ and ((A)–(D)) $\alpha = 4, 6, 8, 10$. Calculations were done for a lattice with $N = 600$ sites. The wavefunction remains trapped in a finite fraction of the lattice and is moving along the chain, thus suggesting the presence of an electron–soliton pair.

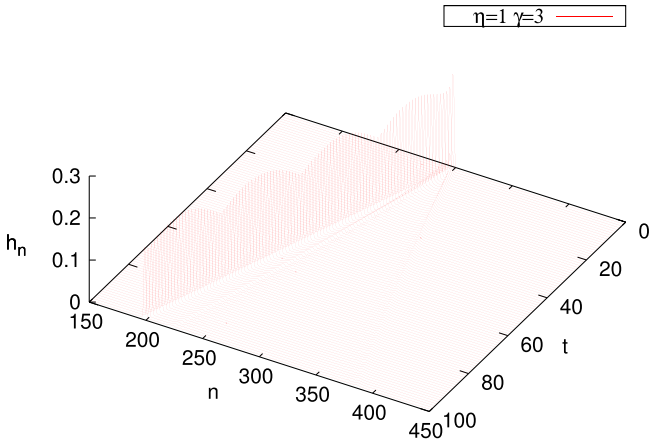

Fig. 5. The amount of energy at site n ($h_n(t)$) times n and t for $\eta = 1$ and $\gamma = 3$. The initial excitation had $P_n = \delta_{n,N/2}$ and $Q_n = 0$. Our results have shown the presence of a soliton mode that propagates along the chain.

the presence of nonlinearity in the lattice that increases the electronic spread along the disordered chain. We would like to stress that it was numerically proved that in disordered harmonic lattices [26,29] the electron–phonon coupling can promote only a sub-diffusive spreading. (2) At the strong correlation limit ($\gamma \geq 2$), our calculations suggest the appearance of an electron–soliton pair. Our results revealed a kind of trapped electronic state moving along the chain. The electron–soliton pair obtained here becomes well defined as the electron–lattice coupling is increased. We numerically demonstrate the possibility of electron transport mediated by solitons even in disordered nonlinear chains. Our results at the strong correlation limit ($\gamma \geq 2$) are in good agreement with recent works by M.G. Velarde and co-workers [7–11,17–25] concerning the existence of a new *particle* that arises from the trapping of an electron by a genuine solitonic mode. However, we stress that our results were obtained in α-Fermi–Pasta–Ulam chains with cubic nonlinearity, while in the case of Refs. [7–11,17–25], the electron–soliton pair was obtained by considering the Morse potential. We hope that our paper can stimulate discussion along these lines.

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