Physica A 435 (2015) 15–21

Contents lists available at ScienceDirect

Physica A

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

Electronic transport in disordered chains with saturable nonlinearity

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HIGHLIGHTS

- Numerical solution of the Schrödinger equation with saturable nonlinearity.
- Sub-diffusive dynamics even in the presence of strong diagonal disorder.
- Electronic mobility in one-dimensional disordered systems.

ARTICLE INFO

Article history:
Received 12 February 2015
Received in revised form 22 March 2015
Available online 4 May 2015

Keywords:
Sub-diffusive spreading
Wave packet dynamics
Saturable nonlinearity
Nonlinear Schrödinger equation

ABSTRACT

In this work we study numerically the dynamics of an initially localized wave packet in one-dimensional disordered chains with saturable nonlinearity. By using the generalized discrete nonlinear Schrödinger equation, we calculate two different physical quantities as a function of time, which are the participation number and the mean square displacement from the excitation site. From detailed numerical analysis, we find that the saturable nonlinearity can promote a sub-diffusive spreading of the wave packet even in the presence of diagonal disorder for a long time. In addition, we also investigate the effect of the saturated nonlinearity for initial times of the electronic evolution thus showing the possibility of mobile breather-like modes.

1. Introduction

The works by P.W. Anderson and co-workers proved that extended eigenstates are absent in low-dimensional systems with uncorrelated disorder [1–5]. Therefore, the width of an initially localized wave-packet saturates at a finite region around the initial position in the long time limit. It was shown during the last two decades that extended states or a localization–delocalization transition can appear in low-dimensional systems with correlated disorder [6–25]. Moreover, the competition between nonlinearity and disorder has been investigated in Refs. [26–38]. In general lines, it has been found that the nonlinear aspects seem to be dominant over the disorder. In particular, it was observed a counter-intuitive sub-diffusive spreading of an initially localized wave-packet, without any indication of saturation for long time runs [27]. Experimentally, the competition between disorder and nonlinearity was investigated in coupled waveguides patterned on an AlGaAs substrate [31]. The authors reported that the presence of nonlinearity enhances the localization of linear modes whereas it induces the delocalization of nonlinear modes. Besides, the coupling between the lattice vibrations and the electronic dynamics has been shown that plays important roles on the effective electronic transports [26–38]. Some authors concluded that the superconducting state of several compounds is related to the strong electron–phonon coupling [39,40].

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http://dx.doi.org/10.1016/j.physa.2015.04.029
0378-4371/

Within the problems involving nonlinearity the presence of saturation within the nonlinearity distribution is an interesting issue. In Ref. [41] the existence of bistable solitons in materials with saturable nonlinearity was demonstrated. The discrete nonlinear Schrödinger (DNLS) equation with saturable nonlinearity was investigated in Ref. [42]. In Refs. [43,44] it was shown the existence of defect solitons in systems with saturable nonlinearity and parity–time symmetry. The authors in Ref. [45] investigated in detail the nonreciprocal diode-like behavior of an asymmetric dimer with saturable nonlinearity. It was found that the transmission band becomes wider and displaces to the higher input field intensities as the saturation coefficient increases. Despite numerous studies, this issue has not been completely understood yet.

In this paper, we report further progress along these above lines. One considers the problem of electronic dynamics in a disordered one-dimensional (1d) system with saturable nonlinearity. In our model we study the competition between diagonal disorder and saturable nonlinearity. We will solve numerically the nonlinear Schrödinger equation and compute the dynamics of an initially localized electronic wave-packet. Our calculations suggest that the saturable nonlinearity can promote a sub-diffusive dynamics even in the presence of diagonal disorder. Moreover, we also investigated the effect of the saturated nonlinearity for initial times of the electronic dynamics. Our results indicate the possibility of mobile breather-like modes.

2. Model and formalism

In order to describe the dynamical properties of a wave-packet within a tight-binding approach in the presence of disorder and saturable nonlinearity, we use the generalized discrete nonlinear Schrödinger equation given by

$$i\hbar\frac{dc_n}{dt} = c_{n+1} + c_{n-1} + \left[\epsilon_n + \frac{\chi|c_n|^2}{1+\zeta|c_n|^2}\right]c_n, \tag{1}$$

where ϵ_n are random number within the interval $[-W/2, W/2]$. χ and ζ are tunable parameters. ζ is the degree of saturation of the nonlinearity. In the present work, we solve the set of nonlinear coupled differential equations using a predictor–corrector Adams–Bashforth–Moulton formalism initialized by the Runge–Kutta method of order eight with time step $\Delta t = 0.005$ [46]. Our calculations for long times were done by using the tenth-order Adams–Bashforth as the predictor formula and eighth-order Adams–Moulton procedure as the corrector. The time step used here is sufficient to keep the wave-function normalization for long time ($|1 - \sum_n |c_n(t)|^2| < 10^{-10}$). We emphasize that we also have used the standard eighth-order Runge–Kutta method with $\Delta t = 0.005$ to entire integrations (not showed here). We have found exactly the same results within of the numerical tolerance. It is worth mentioning that the computational time required in the Runge–Kutta formalism is longer than the time required by the Adams–Bashforth–Moulton formalism. In order to characterize the dynamical behavior of an initially localized wave packet, i.e., $\{c_n(t=0) = \delta_{n,0}\}$, we will compute typical quantities associated with wave-packet spacial extension, namely the participation function and wave packet mean-square displacement which are defined as [36,37]:

$$\xi(t) = 1/\sum_n |c_n(t)|^4 \tag{2}$$

and

$$\sigma(t) = \sqrt{\sum_n [(n - \langle n(t)\rangle)^2]|c_n(t)|^2}, \tag{3}$$

$\langle n(t)\rangle = \sum_n n|c_n(t)|^2$. In the long-time regime, the scaling behavior of the last quantity can also be used to distinguish between localized and delocalized wave packets. Note that $\sigma(t)$ varies from 0, for a wave function confined to a single site, to a function which is proportional to the number of sites, for a wave uniformly extended over the whole system. In this work, the numerical calculations are performed with $t_{\max} \approx 10^6$.

3. Results and discussion

Our calculations were resulted from the time evolution of a wave-packet initially localized at the center of a self-expanding chain that is a simple trick to minimize the end effects. In particular, whenever the probability of finding the particle at the ends of the chain exceeded 10^{-40}, ten new sites are added to each end. The stability and convergence of the numerical computations are checked at every time step. We verify that the norm conservation, e.g., $|1 - \sum_n |\phi_n(t)|^2| < 10^{-10}$ is always satisfied during the simulation time. In our calculations the width of the diagonal disorder used was $W = 5$. Besides, for the purpose of preventing the effects of a specific disorder configuration, all calculations were averaged over 150 disorder configurations.

Within the standard theory of localization it is well known that in the absence of nonlinearity ($\chi = 0$) the wave-packet does not show any spreading [36]. In Fig. 1 we provide a detailed analysis of the wave-packet dynamics for several values of nonlinearity ($\chi = 1$, 2 and 3) and saturation parameter $\zeta = 0$ up to $\zeta = 30$. The initial wave-packet it was considered $c_n(t=0) = \delta_{n,n_0}$ where n_0 is the center of the self-expanding chain we have used. By examining both the participation function and the mean square displacement we observed that the wave-packet exhibits a sub-diffusive dynamics for long

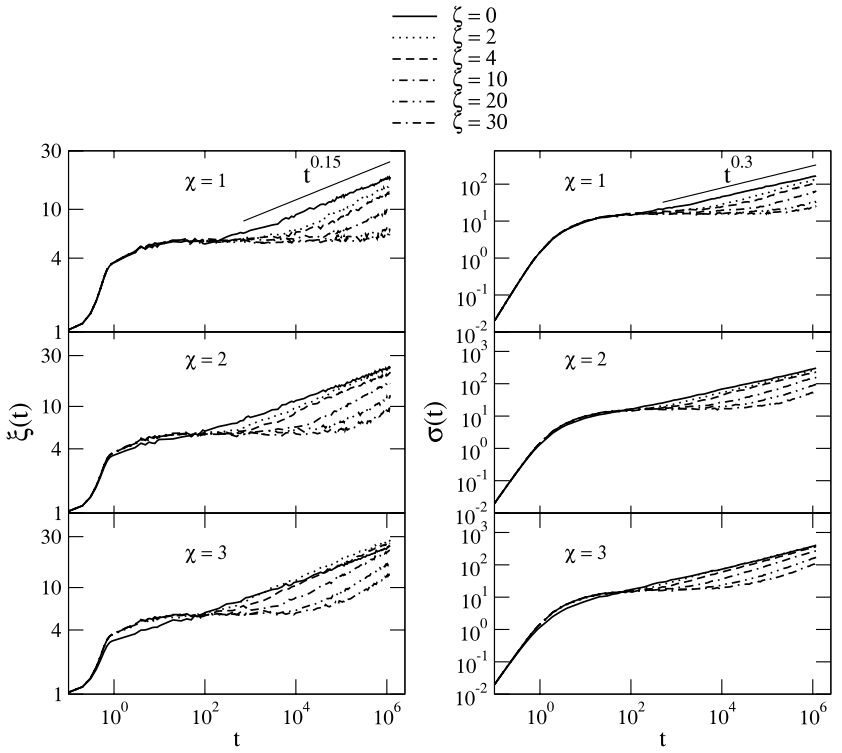

Fig. 1. The dynamics of an initially localized wave-packet in 1d disordered chain with saturable nonlinearity is studied. Two characteristic quantities associated with wave-packet spacial extension are shown. Left panel: The participation number $\xi(t)$ versus time t when $\chi = 1, 2, 3$ and $\zeta = 0, 2, 4, 10, 20, 30$ for each value of χ. Right panel: Plot of the mean square displacement $\sigma(t)$ versus time t for the same cases of the left panel. Both these characteristics exhibit a slow dynamics, $\xi(t) \propto t^{0.15}$ and $\sigma(t) \propto t^{0.3}$, indicating a sub-diffusive electronic wave-packet spreading.

time. We can see clearly that both these characteristics exhibit a slow dynamics ($\xi(t) \propto t^{0.15}$ and $\sigma(t) \propto t^{0.3}$) thus suggesting the presence of a sub-diffusive electronic wave-packet spreading. Also, we observe that for the strong saturation degree (i.e. $\zeta \gg 0$), there is an intermediate regime in which that both quantities shown a slower dynamics. In fact, for intermediate times and strong ζ the electron seems to stay almost trapped. For long-time, even for strong ζ, the wave-packet starts again to spread. For strong nonlinearity ($\chi = 2$ or 3) the behavior mentioned above is more well defined. This is an unusual behavior, directly related to the presence of saturable nonlinearity. We can provide some arguments that explain qualitatively this new electronic dynamics. For the intermediate times, the electronic wave-packet is localized around the center of chain, hence: $|c_{n^*}|^2 > 0$ with $(n_0 - L_c/2) < n^* < (n_0 + L_c/2)$ where n_0 is the center of chain and L_c is the mean width of the wave-packet for intermediate times (L_c is of the order of few sites). Therefore, at this stage and for large ζ, the nonlinear term is weak and the on-site disorder plays the major/key roles thus slowing the electronic dynamics. For the long-time limit, $|c_{n^*}|^2$ decreases, L_c increases a little and, even for large ζ, the cubic nonlinear term can compete with the diagonal disorder thus promoting the sub-diffusive dynamics.

In order to verify whether the phenomenology above is robust, we will re-consider the same problem but with another type of initial condition. To this end, we will perform the time evolution of an initial Gaussian wave packet with velocity defined by

$$c_n(t = 0) = A(\Sigma)\mathrm{e}^{(\mathrm{i}kn)}\mathrm{e}^{[-(n-n_0)^2/4\Sigma^2]}, \tag{4}$$

where Σ is the variance of the initial wave packet, $A(\Sigma)$ is the normalization constant and k is the wave-vector. In a pure chain with hopping is equal to one, k is related to the one-electron energy as $E = 2\cos(k)$. In Fig. 2 we plot the participation function and the mean square displacement versus time for $\chi = 1$ and several values of ζ. Here, we have taken $\Sigma = 1$ and two different values of $k = \arccos(E/2)$ with $E = 0.0$ and 1.99 which correspond to the center and the edge of crystalline band. From the numerical results, we can see that independent of the initial velocity of the wave-packet, the electronic wave-packet exhibits the same sub-diffusive trend. Moreover, for large ζ and intermediate times, we obtain a slower dynamics similar to that found in Fig. 1. Therefore, our results suggests that the presence of saturable nonlinearity promotes the emergence of sub-diffusive dynamics. However, it is necessary to emphasize that for strong values of saturation (large ζ), the wave-packet remains almost localized for intermediate times and starts its spreading for long-times.

Before finishing our work we will provide an additional analysis of the electronic dynamics at the initial stage of evolution. To this end, we only need to consider a short chain with $N = 100$ sites. In the absence of saturation and disorder the electronic dynamics in nonlinear crystalline chains is well established. In general, independent of the topology of system,

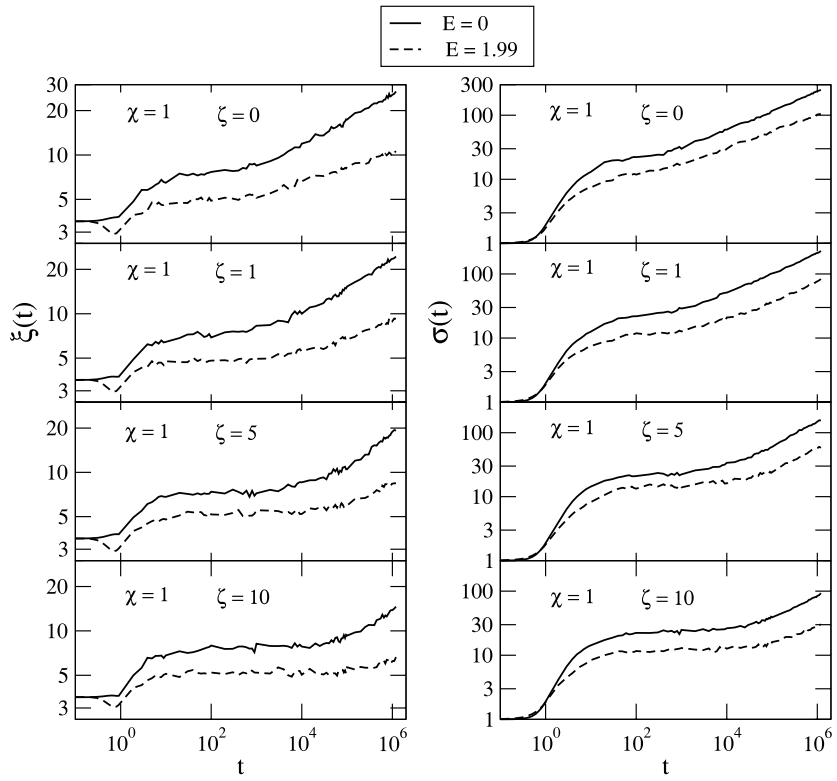

Fig. 2. The time evolution of an initial Gaussian wave packet with $\Sigma = 1$ is investigated. Plots of the participation number $\xi(t)$ and the mean square displacement $\sigma(t)$ versus time t for $\chi = 1$ and $\xi = 0, 1, 5, 10$ at the center ($E = 0.0$) and the edge ($E = 1.99$) of crystalline band. These results again confirm that the saturable nonlinearity induce the sub-diffusive spreading of the wave packet.

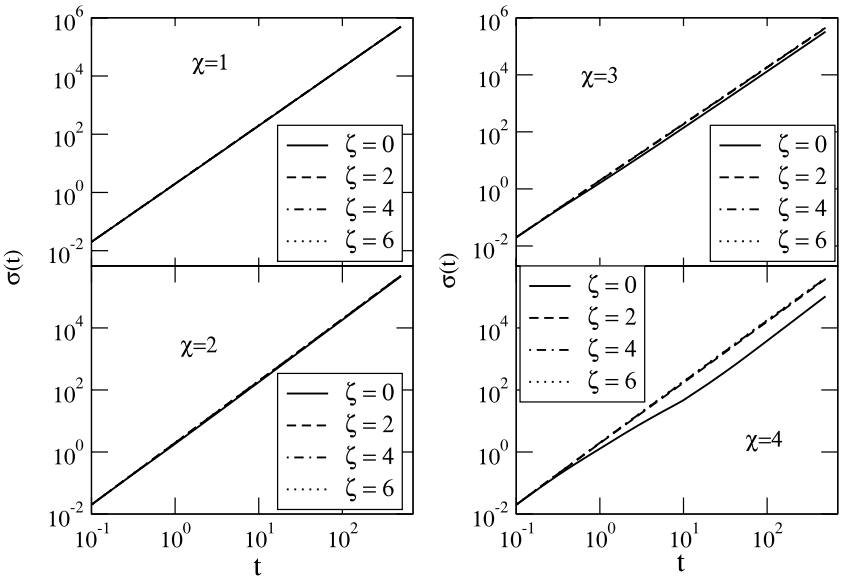

Fig. 3. Time evolution of an initially localized wave-packet in clean systems ($W = 0$) when $\chi = 1, 2, 3, 4$ for $\zeta = 0, 2, 4, 6$. We can see clearly that the electron exhibits a ballistic dynamics ($\sigma(t) \propto t$) even for strong saturation.

the presence of strong nonlinearity ($\chi > 4$) can trap the one-electron wave-packet around the initial position. In contrast, for weak nonlinear interaction ($\chi \leq 4$), the wave-packet remains extended. We investigate first the effect of saturated nonlinearity on the wave-packet spreading in the absence of disorder, $W = 0$. In Fig. 3 we show our numerical results for time evolution of an initially localized wave-packet in systems with $\zeta = 0, 2, 4$ and 6 when $\chi \leq 4$. We can see clearly that

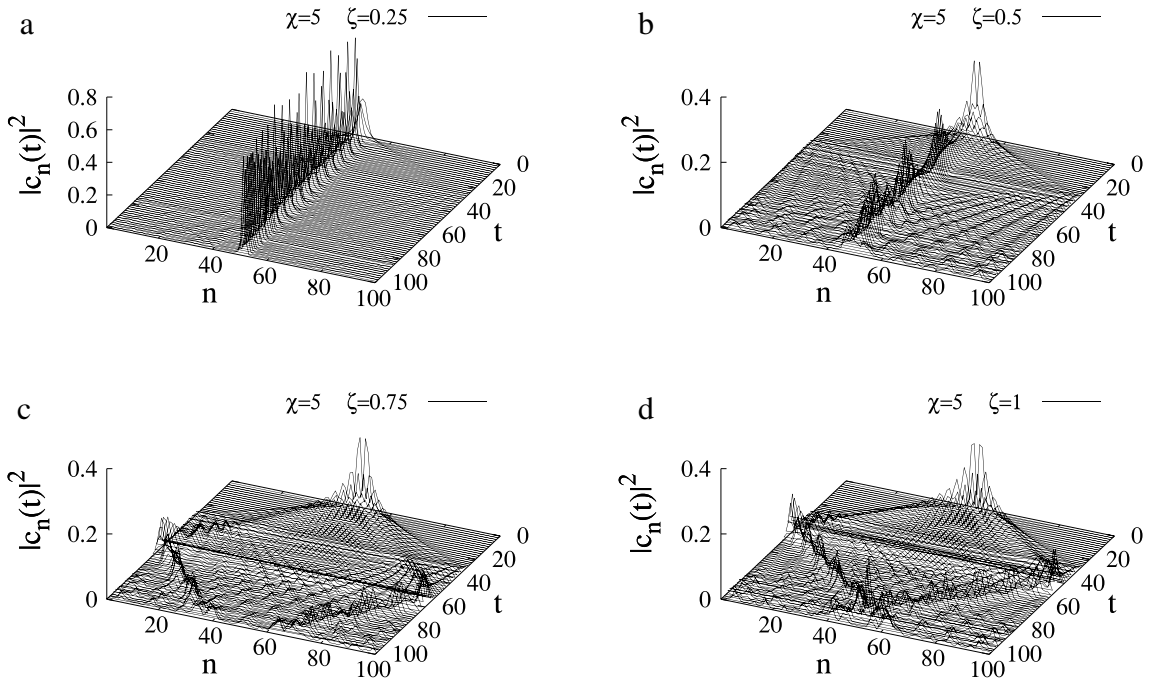

Fig. 4. Time-dependent wave-function profile $|c_n(t)|^2$ versus n and t for $\zeta = 0.25, 0.5, 0.75$ and 1 when $\chi = 5$, $W = 0$. The numerical results show that the self-trapping behavior could be destroyed even in the presence of a weak saturation, thus promoting the spreading of the wave-packet.

for weak nonlinearity, the saturation does not modify the initial dynamics of electron. The electron still exhibits a ballistic dynamics ($\sigma(t) \propto t$) even for strong saturation. Next, we will study the effect of saturation on the self-trapping state ($\chi > 4$). In Fig. 4 we plot the time-dependent wave-function profile $|c_n(t)|^2$ versus n and t when $\chi = 5$ for $\zeta = 0.25, 0.5, 0.75$ and 1. We can see that the saturation destroys the self-trapping state and promotes the spreading of the wave-packet. This indicates that an arbitrarily weak saturation also plays a major role within the electron dynamics. This detailed numerical analysis suggests that the self-trapping transition seems to be absent for strong saturated nonlinearity. Within this context, an interesting question we ask is what will happen to extremely strong nonlinearity? For the purpose of answering to this question, in Fig. 5, we plot the wave-function profile $|c_n(t)^2|$ versus n and t at different values of saturation parameter, $\zeta = 2, 4, 6$ and 8 when $\chi = 10$. We observe that for ζ about 2 the most part of the wave-packet remains trapped around the initial site. For $\zeta > 2$, however, the wave-packet spreads in two peaks that propagate along the chain. In fact, by examining the wave-function profile we observe that the intensity of both peaks display smooth fluctuations. This behavior seems to be a kind of breather mode that propagates along the chain. Soliton or breather modes are generally found in systems with nonlinear interaction. Finally, to finishing our analysis about the short-time electronic dynamics we introduced a diagonal disorder with strength $W = 5$ to the system under consideration. In Fig. 6 we summarize our calculations showing the wave-function profile $|c_n(t)|^2$ versus n and t when (a, b) $\zeta = 1, 2$ for $\chi = 1$ and when (c, d) $\zeta = 4, 6$ for $\chi = 5$. Our calculations suggest that for this initial stage of evolution, the wave-packet remains trapped around the initial position. The breather-like mode that was found, in the absence of disorder, does not appear when the disorder is taken into account. In fact, the scattering by disorder promotes initially the localization of wave-packet even in the presence of saturated nonlinearity.

4. Summary and conclusions

In this research, we have considered the coupling between lattice vibration and the diagonal on-site energy. Within the classical harmonic Hamiltonian and the Su–Schrieffer–Heeger approximation, a disordered Schrödinger equation is written with the presence of diagonal saturable nonlinearity. We solve the effective Schrödinger equation with nonlinear diagonal terms for an initially localized wave-packet using a predictor–corrector tenth-order Adams–Bashforth–Moulton method initialized by the Dormand–Prince Runge–Kutta method of order eight. From numerical analysis, we show that the saturable nonlinearity can promote a long-time sub-diffusive regime similar to that found in the models with a diagonal unsaturated nonlinearity [47]. However, our results reveal the existence of an intermediate region in which the wave-packet remains almost localized. In other words, the presence of saturation in the nonlinear term promotes the appearance of sub-diffusive dynamics however only for a long-time. Moreover, we also observed that as the saturation degree ζ is increased the time interval in which that the electronic wave-packet approximately trapped increases. Therefore, the presence of saturable nonlinearity promotes the appearance of a new time-scale in which the electronic wave-packet seems to be trapped. Aiming to support further these interesting behaviors, we provided a detailed analysis of this phenomenology for a more generalized

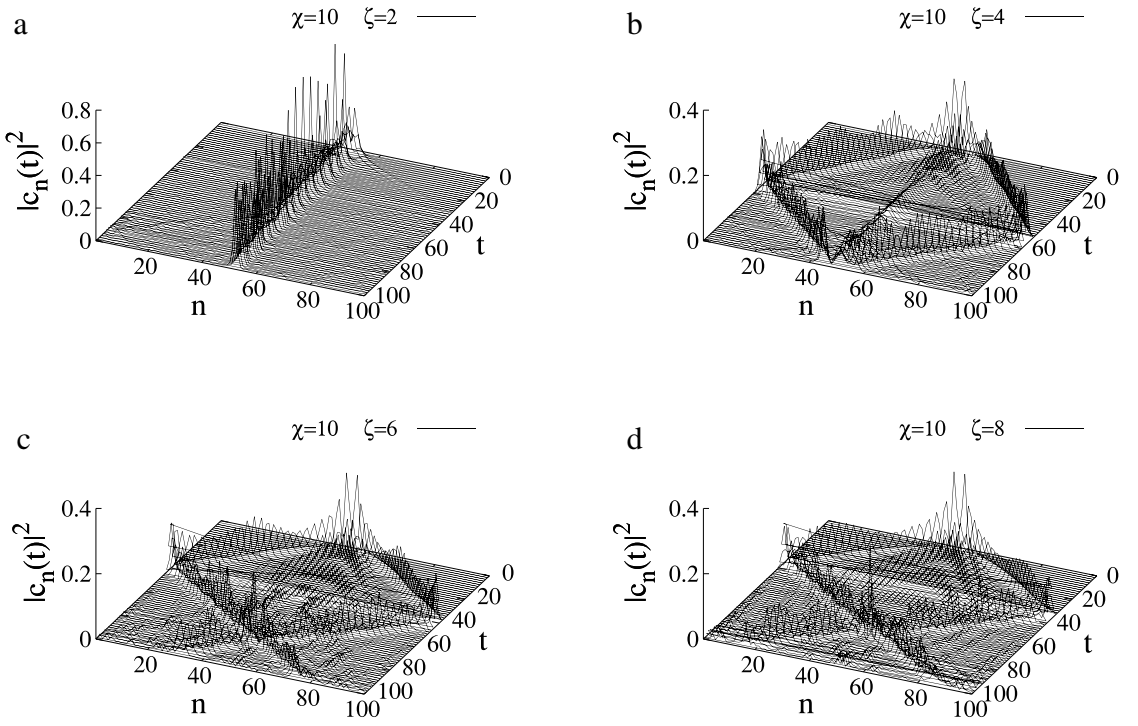

Fig. 5. The wave-function profile $|c_n(t)^2|$ versus n and t at different values of saturation parameter, $\zeta = 2, 4, 6$ and 8 in the limit of strong degree of nonlinearity ($\chi = 10$).

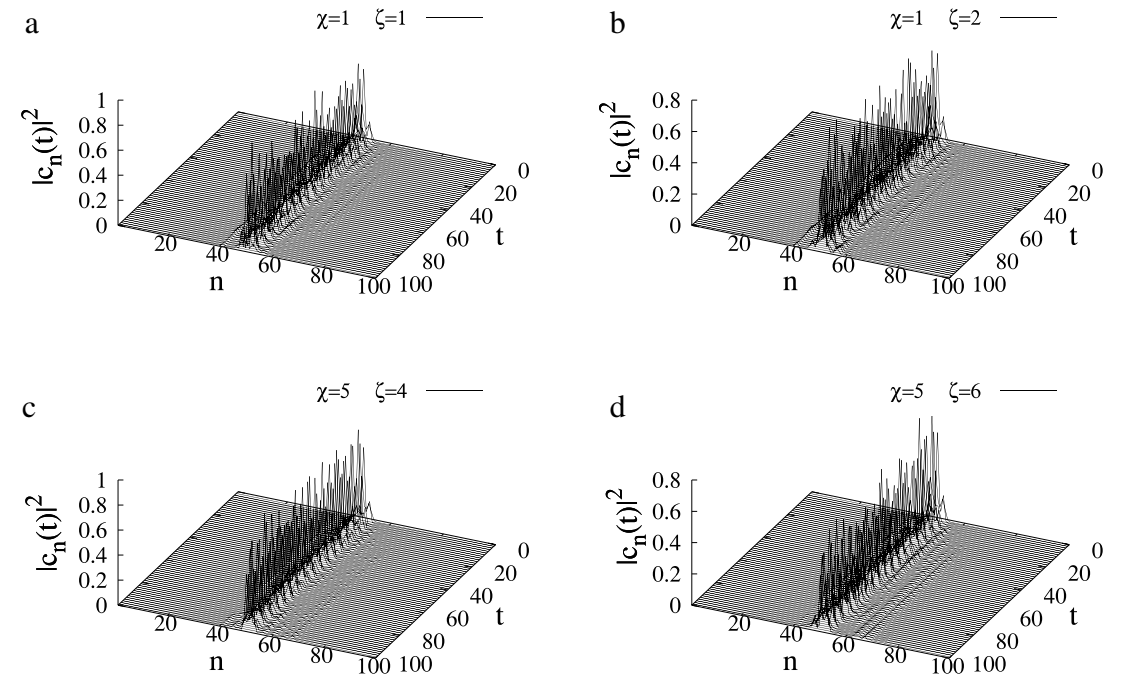

Fig. 6. The wave-function profile $|c_n(t)|^2$ versus n and t when (a, b) $\zeta = 1, 2$ for $\chi = 1$ and $W = 5$ and when (c, d) $\zeta = 4, 6$ for $\chi = 5$ and $W = 5$.

initial condition (a Gaussian) and also at the presence of initial momentum. Our calculations suggest that the behaviors are qualitatively the same: almost trapped for intermediate times and sub-diffusive for long-times. In addition, since saturation effect is usually important at the initial stage of evolution, we provided a detailed analysis of the electronic dynamics within this initial stage of evolution. We found that in the absence of disorder and for weak nonlinearity, the electron exhibits a ballistic dynamics ($\sigma(t) \propto t$) even for strong saturation. For nonlinearity χ slightly above the bandwidth, the saturation

destroys the self-trapping state and promotes the spreading of the wave-packet. Remarkably, for strong nonlinearity the wave-packet spreads in two peaks that propagate along the chain. This behavior seems to be a kind of breather mode that propagates along the chain. We also investigated the short-times behavior in the presence of diagonal disorder and saturated nonlinearity. Our results indicate that the breather-like mode is absent. We hope that our paper can stimulate discussion further along this line.

Acknowledgments

The research in Brazil was partially supported by the Brazilian research agencies CNPq, CAPES, INCT-Nano(Bio)Simes, as well as FAPEAL (Ala goas State Agency). B. P. Nguyen was supported by Vietnam's National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2014.10.

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