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Anderson localization in a disordered chain with a finite nonlinear response time

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Abstract. In this work, we investigate the competition of disorder, nonlinearity and non-adiabatic process on the wave packet dynamics in 1D. We follow the time evolution of the second moment of the wave packet distribution to characterize its spreading behavior. In order to describe the dynamical behavior of one-electron wave packets, we solve a discrete nonlinear Schrödinger equation which effectively takes into account a diagonal disorder and a nonlinear contribution. Going beyond the adiabatic regime, we consider that the nonlinearity relaxes in time according to a Debye-like law. In the adiabatic regime, it has been recently demonstrated that the interplay of disorder and nonlinearity leads to a sub-diffusive spread of the wave packet. Here, we numerically demonstrate that no sub-diffusive spreading of the second moment of the wave packet distribution takes place when the finite response time of the nonlinearity is taken into account.

1 Introduction

The study of the electronic properties in disordered system has been one of the most recurrent issues in condensed matter physics. The cornerstone result about the nature of the electronic states was done in a seminal work by Abrahams et al. [1] in which the authors claimed that all states in a disordered system with dimension $D \leq 2$ are localized in an absence of magnetic field and spin-orbit coupling. Originally developed in order to understand electronic transport in non-periodic structures, Anderson localization became an even stronger result since such prediction is still valid for every field described by a wave equation. For instance, Anderson localization in superlattice-graphene nanotubes and nanoribbons [2,3], of electromagnetic fields [4], water waves [5] and Bose-Einstein Condensates (BEC) [6] has been reported in the recent literature. The last issue has attracted an increased interest motivated by recent remarkable advances in experimental technologies. It is possible, for example, to create a one-dimensional (1D) disordered potential through of an optical lattice and verify evidences of Anderson localization of BEC [7–10]. One interesting aspect of BEC in a 1D disordered potential is that its dynamic is well described by the Gross-Pitaevskii equation [11] and the nonlinearity present in this equation leads to exciting new physical properties [12–14]. Nonlinearity in the Schrödinger equation also appears in the electronic context. It originates from interaction between the electron and lattice vibrations [15,16]. The presence of the nonlinearity in the electronic Schrödinger equation induces the phenomenon of self-trapping [17,18] in which an initially localized wave packet does not spread over the lattice. It occurs when the nonlinearity exceeds a critical value of the order of the bandwidth [15–18]. The interplay between nonlinearity and disorder has also been recently investigated. Nonlinear aspects seem to be more important than disorder effects in low-dimensional systems [19–22]. Pikovsky et al., for example, have studied the effects of the competition between disorder and nonlinearity in one and two-dimensional disordered systems [19,20,23]. In particular, they followed the wave packet spreading of an initially localized state. They observed that, for nonlinear strengths exceeding a critical value, there is a counter-intuitive sub-diffusive spreading of the wave function with no indication of saturation in long time runs. In this sense, a more realistic model that takes into account the electron-phonon interaction, supports the existence of states that are not exponentially localized in disordered low-dimensional system.

Experimentally the competition between nonlinearity and disorder has been investigated showing that, in coupled waveguides patterned on an AlGaAs substrate, the presence of nonlinear perturbations enhance the localization of the linear model while, on the other hand, they induce delocalization of the nonlinear modes [24]. It is worth to keep in mind that the study of wave propagation in nonlinear media is an important issue in many branch of physics. It has been investigated, for example, within the context of the propagation of electromagnetic waves in nonlinear disordered media [25,26]. The effects on localization of nonlinearity coming from anharmonic terms in phonon-phonon interaction have also been explored [27].

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In general, one assumes that the nonlinearity arisen from the electron-phonon interaction is instantaneous. However, this adiabatic approximation is very limited since the effective electron-phonon interaction is limited by the response time of the medium. In fact, models considering the relaxation of the effective nonlinearity have been reported in the literature [28–31]. It has been demonstrated that when relaxation process of the nonlinearity is taken into account in a two-level system, there is a stationary self-trapping regime and a coexistence of static and dynamical transitions depending on the degree of nonlinearity as well as on the relaxation time [28]. Recently, it was reported the influence of the non linear response time on the one-electron wave packet dynamics in linear chains [31]. Considering the delayed nonlinear term coupling the electronic wave function at time t with the electronic density at $t-\tau$, the authors reported that the tendency of self-trapping is reduced for long response times. On the other hand, it is the critical nonlinear strength needed to promote self-trapping that becomes smaller in the regime of small, although finite, nonlinear response times [31]. More recently, the effects of a Debye-like relaxation of the nonlinearity was considered [32]. It was shown that the delay of the nonlinear response potentializes the occurrence of self-focusing, thus strongly reducing the critical nonlinear strength above which the wave packet becomes localized.

In this work, we advance in the investigation of the influence of the non-instantaneous character of the nonlinear coupling on the electronic wave packet dynamics on linear chains. We investigate the combination of the above three ingredients, namely, disorder, nonlinearity and non-adiabatic process. We follow the time evolution of the second moment of the wave packet distribution in order to characterize its spreading behavior. The wave packet dynamics will be considered to obey a discrete nonlinear Schrödinger equation which effectively takes into account a diagonal disorder and a nonlinear contribution arising from an underlying electron-phonon interaction in the limit of a non-adiabatic coupling. Our calculations numerically reveal that the sub-diffusive spreading of the second moment of the wave packet distribution does not take place beyond the adiabatic regime where a finite nonlinear response time has to be considered.

2 Model and formalism

We effectively take the non-adiabatic behavior of the electron-phonon interaction into account by introducing a relaxation function in the nonlinear Schrödinger equation, following the same lines developed in references [28,29]. In this approximation, the dynamics is governed by the nonlinear Schrödinger equation given by:

$$i\dot{\psi}_n(t) = \varepsilon_n\psi_n(t) + V(\psi_{n+1}(t) + \psi_{n-1}(t)) + \beta f_n(t)\psi_n(t) \quad (1)$$

where we consider $\hbar = 1$. ε_n's are the on site energies taken from a white noise distribution in the range $-\frac{W}{2} \leq \varepsilon_i \leq \frac{W}{2}$, V is the hopping overlap integral, which we set to be the energy unit, β is the nonlinearity strength and $f_n(t)$ is the function that introduces the relaxation in the nonlinearity. The Schrödinger equation must be solved concomitantly with the relaxation equation [28,29]:

$$\dot{f}_n(t) = -\frac{1}{\tau}\left(f_n(t) - |\psi_n|^2\right) \quad (2)$$

where τ is the relaxation time which is related with the time response of the medium. $\tau = 0$ corresponds to the adiabatic case because it implies in $f_n(t) = |\psi_n(t)|^2$ in order to have a finite evolution rate of the nonlinearity. The second equation describes the dynamics of the lattice vibrations. The nonlinear parameter β is proportional to the local electron-phonon coupling under an adiabatic approximation [28,29], which occurs when $f_n(t) = |\psi_n(t)|^2$ and/or $\tau = 0$. The delayed DNLSE model used here was derived following the assumptions put forward in reference [28]. The model starts by considering a set of $2N$ coupled equations. Half of them corresponds to the wave packet dynamics of the moving quantum particle. The other half corresponds to the motion equation of Einstein-like site oscillators. $f_n(t)$ is the displacement of the oscillator at site n, which has a typical frequency ω and is damped at a rate α. By assuming the oscillators to reach their equilibrium position much faster than the typical time scale for the quantum particle evolution, the time derivative of $f_n(t)$ can be disregarded, thus resulting in the well known adiabatic DNLSE with a nonlinear contribution to the on-site energy given by $|\psi_n(t)|^2$ [28]. In the strong damping regime the set of coupled equations reduces to the delayed DNLSE (Eqs. (1) and (2)) with $\tau = \omega^2/\alpha$. The non-adiabatic character is incorporating by explicitly solving the relaxation equation considering a finite response time $\tau \neq 0$. Systems with slow non linear response have large values of τ. In order to solve the above equations, we use seventh order Taylor expansion with time step $\Delta t = 0.01$ for both equations. This procedure allows us to achieve a precision of the order of 10^{-6} in the norm of the wave function for times up to 10^7. The quantity that we use to characterize the spreading of the wave function is the second moment of the probability function, defined as:

$$\sigma(t) = \sum_{n=1}^{N}(x_n - \bar{x}(t))^2|\psi_n(t)|^2 \quad (3)$$

where $\bar{x(t)} = \sum_i^N x_i|\psi_i(t)|^2$ is the centroid of the wave packet at the time t.

3 Results

We start solving equations (1) and (2) for an initially localized state at the center of the chain: $|\psi(t=0)\rangle = \sum_n \psi_n|n\rangle$, with $\psi_n = \delta_{n,n_0}$, where n_0 is the center of the chain. The non linearity and disorder strength are $\beta = 3$ and $W = 4$, respectively. It is important to stress that our results are still qualitatively valid for other parameter sets that we tested. In the adiabatic regime, the electronic wave packet starts the spreading following an initial

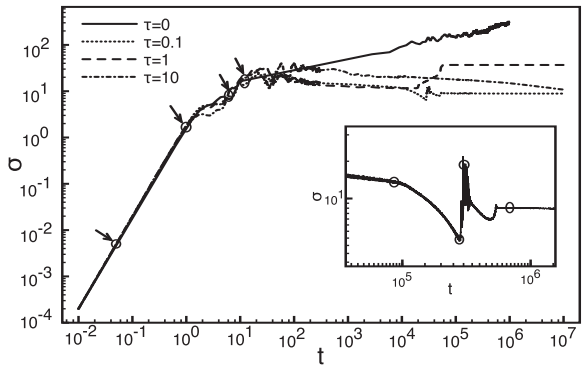

Fig. 1. Time dependence of the second moment of the probability distribution for disorder strength $W = 4$ and $\beta = 3$. Data are from a single disorder configuration. The continuous line is the second moment considering an instantaneous response. It shows a sub-diffusive spreading due to the interplay of disorder and nonlinearity. Delayed responses are shown for three different response times: $\tau = 0.1$ (dotted), $\tau = 1$ (dashed) and $\tau = 10$ (dotted-dashed). These curves show that the sub-diffusive spreading is destroyed when the nonlinear response is delayed. Circles and arrows indicate the points where the wave functions are shown in Figures 3 and 4. Inset: a dynamical instability present for $\tau = 0.1$ coming from the competition between disorder and nonlinearity.

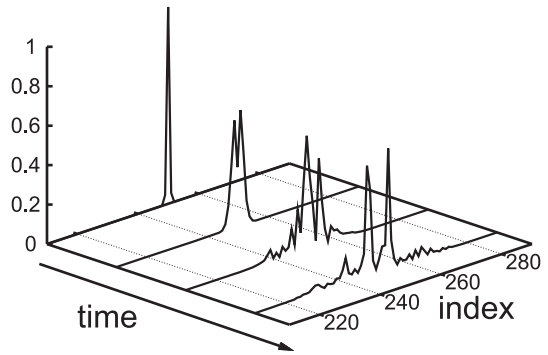

Fig. 2. Wave packet distribution calculated in a system with $W = 4$, $\beta = 3$, and $\tau = 0.1$ at four distinct instants: $t = 0.05$, $t = 1.02$, $t = 6.68$ and $t = 15.5$ (these times are indicated by arrows in Fig. 1). The first two are in the ballistic regime and the other two are in the sub-diffusive regime. One can see that the wave packet is spreading at these initial moments developing a structure with two peaks.

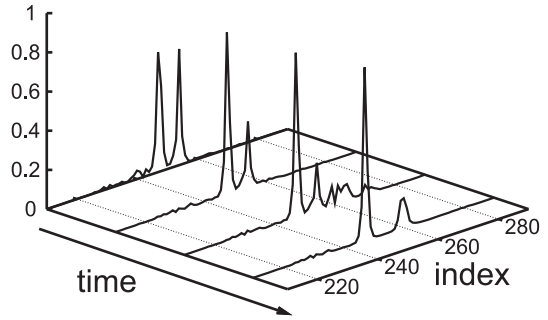

Fig. 3. Wave packet distribution calculated in a system with $W = 4$, $\beta = 3$, and $\tau = 0.1$ at four distinct instants: $t = 8610$, $t = 27\,780$, $t = 30\,650$ and $t = 68\,740$ (these times are indicated by circles at the inset of Fig. 1). These wave packet distributions are in the region of the dynamical instability shown in the inset of Figure 1. It can be seen that probability distribution initially depicts two similar peaks. One peak becomes unstable and starts to spread. Finally, it focuses again resulting in a quite asymmetric two peak distribution.

ballistic regime. As soon as the electron experiences the disorder, it goes through a crossover regime for a short period (between $t = 1$ and $t \sim 10$ and finally it achieves a sub-diffusive regime, in agreement with references [19,22]. This behavior is shown as a continuous line in Figure 1. On the other hand, when the relaxation process is taken into account, although the initial and intermediary spreading regimes of the electronic packet remain the same, the sub-diffusive spreading is replaced by a saturation of the wave packet width, signaling an ultimate localization. This behavior is shown in Figure 1 for three different response times: $\tau = 0.1$ (dotted), $\tau = 1$ (dashed) and $\tau = 10$ (dotted-dashed). It is noticeable that there is a strong indication that the wave packet remains localized and the sub-diffusive spreading does not take place for any value of τ. It is interesting to see that $\sigma(t)$ for $\tau = 0.1$ is almost equal to the adiabatic case up to $t = 10^2$, even within the sub-diffuse regime. However this behavior is destroyed and a localized regime takes place after a long run.

Figure 2 shows the wave packet at different times (indicated by arrows in Fig. 1). The first two are in the ballistic regime and the others are in the intermediary regime. One can see that the wave packet splits into two well localized peaks. Such splitting of the wave packet is strongly dependent of the particular disorder configuration around the initial wave packet position.

One interesting aspect coming from the nonlinearity is the emergence of some anomalous behavior where there would be an apparent stability. A representative case is found for $\tau = 0.1$ and reported in details in the inset of Figure 1. Such instability is associated to the interplay between the effective disorder (on site potential and the nonlinear term) and the relaxation process. A better understand can be gotten by looking the wave packet at the times indicated by circles in the inset of Figure 1. These are shown in Figure 3. Initially there are two peaks with roughly the same height. However, the relaxed nonlinear potential (not shown here) originates a strong disorder spur at the first peak enhancing the localization of the wave packet around this region. The second peak spreads out over a small region. Nevertheless, it localizes due to the disorder and keeps this configuration up to long time runs.

The results that we have been discussed up to here were obtained from a single disorder configuration. Quantitatively, those results are strongly dependent on the disorder configuration. However sub-diffusive spreading was not found for any disorder configuration that we have checked. Figure 4 shows the second moment of the probability distribution averaged over seven disorder configurations for three different response times: $\tau = 0.1$ (continuous), $\tau = 1$ (dotted) and $\tau = 10$ (dashed). One can clearly notice that there is no spreading of the wave packet up to $t = 10^7$ indicating that none of the disorder configurations

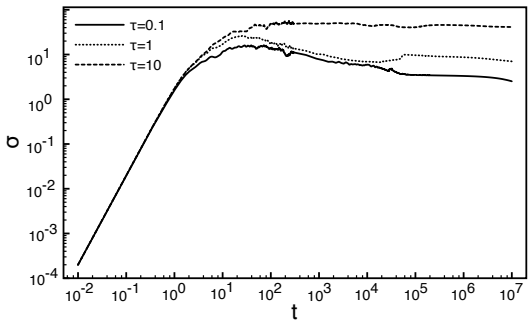

Fig. 4. The second moment of the wave packet probability distribution as a function of time, with $W = 4$ and $\beta = 3$. Data were averaged over seven different disorder configurations. Three distinct response times are shown in this figure: $\tau = 0.1$ (continuous), $\tau = 1$ (dotted) and $\tau = 10$ (dashed). The absence of sub-diffusion, even on the average, indicates that wave packet localization is achieved for any disorder configuration.

supports a sub-diffusive spreading. A more refined statistics is necessary in order to get the quantitative information about the dependence of the asymptotic localization length on the relaxation time.

4 Summary and conclusions

In summary, we studied the dynamics of an electronic wave packet in a linear random chain with non-adiabatic electron-phonon interaction. By using the discrete nonlinear Schrödinger equation we investigated the competition of diagonal disorder and electron-phonon interaction in the limit of non-adiabatic coupling. In conclusion, we have qualitatively demonstrated that the sub-diffusive spreading of the second moment of the wave packet probability distribution does not take place if a finite nonlinear response time is considered. This effect appears for any finite response time with no indication of a threshold in the response time. It is important to keep in mind that, although this work particularly addressed the nonlinearity arisen from an underlying electron-phonon interaction, the results showed here are valid for any nonlinear system with a finite response time. Therefore, one expects the general aspects of wave propagation in disordered nonlinear systems to be substantially modified when a finite response time is included to push the analysis beyond the adiabatic regime. Let us stress that the adiabatic limit of our model has been widely explored in connection with Bose-Einstein condensates, optical and transport properties of biological systems. Therefore, our results points out to a not intuitive phenomenology related to the slow response of the nonlinearity that can drastically modify the transport properties of low-dimensional random systems. We hope that the present work will stimulate further studies along this line.

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References

1. E. Abrahams, P.W. Anderson, D.C. Licciardello, T.V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979)
2. F. Khoeini, A.A. Shokri, F. Khoeini, Eur. Phys. J. B **75**, 505 (2010)
3. A.A. Shokri, F. Khoeini, Eur. Phys. J. B **78**, 59 (2010)
4. D.S. Wiersma, P. Bartolini, A. Lagendijk, R. Righini, Nature **390**, 671 (1997)
5. J. Billy et al., Nature **453**, 891 (2008)
6. G. Roati et al., Nature **453**, 895 (2008)
7. J.E. Lye et al., Phys. Rev. Lett. **95**, 070401 (2005)
8. D. Clément, et al., Phys. Rev. Lett. **95**, 170409 (2005)
9. C. Fort, et al., Phys. Rev. Lett. **95**, 170410 (2005)
10. C. Miniatura, R.C. Kuhn, D. Delande, C.A. Mller, Eur. Phys. J. B **68**, 353 (2009)
11. F. Dalfovo, S. Giorgini, L.P. Pitaevskii, S. Stringari, Rev. Mod. Phys. **71**, 463 (1999)
12. C. Ryu, M.F. Andersen, A. Vaziri, M.B. d'Arcy, J.M. Gross-man, K. Helmerson, W.D. Phillips, Phys. Rev. Lett. **96**, 160403 (2006)
13. G. Behinaein, V. Ramareddy, P. Ahmadi, G.S. Summy, Phys. Rev. Lett. **97**, 244101 (2006)
14. J.F. Kanen, S. Maneshi, M. Partlow, M. Spanner, A.M. Steinberg, Phys. Rev. Lett. **98**, 083004 (2006)
15. M. Johansson, M. Hörnquist, R. Riklund, Phys. Rev. B **52**, 231 (1995)
16. P.K. Datta, K. Kundu, Phys. Rev. B **53**, 14929 (1996)
17. Z. Pan, S. Xiong, C. Gong, Phys. Rev. E **56**, 4744 (1997)
18. W.S. Dias, M.L. Lyra, F.A.B.F. de Moura, Phys. Rev. B **82**, 233102 (2010)
19. A.S. Pikovsky, D.L. Shepelyansky, Phys. Rev. Lett. **100**, 094101 (2008)
20. I. García-Mata, D.L. Shepelyansky, Phys. Rev. E **79**, 026205 (2009)
21. A. Iomin, Phys. Rev. E **81**, 017601 (2010)
22. S. Tietsche, A. Pikovsky, Europhys. Lett. **84**, 10006 (2008)
23. D.L. Shepelyansky, I. García-Mata, Eur. Phys. J. B **71**, 121 (2009)
24. Y. Lahini, A. Avidal, F. Pozzi, M. Sorel, R. Morandotti, D.N. Christodoulides, Y. Silberberg, Phys. Rev. Lett. **100**, 013906 (2008)
25. S.E. Skipetrov, R. Maynard, Phys. Rev. Lett. **85**, 736 (2000)
26. T. Schwartz, G. Bartal, S. Fishman, M. Sergev, Nature **446**, 53 (2007)
27. D. Abhishek, J.L. Lebowitz, Phys. Rev. Lett. **100**, 134301 (2008)
28. V.M. Kenkre, H.-L. Wu, Phys. Rev. B **39**, 6907 (1989)
29. P. Grigolini, H.-L. Wu, V.M. Kenkre, Phys. Rev. B **40**, 7045 (1989)
30. V.M. Kenkre, D.K. Campbell, Phys. Rev. B **34**, 4959 (1986)
31. F.A.B.F de Moura, I. Gléria, I.F. dos Santos, M.L. Lyra, Phys. Rev. Lett. **103**, 096401 (2009)
32. F.A.B.F. de Moura, E.J.G.G. Vidal, I. Gléria, M.L. Lyra, Phys. Lett. A **374**, 4152 (2010)