Dynamics of one electron in a nonlinear disordered chain

2012 J. Phys.: Condens. Matter 24 245401

(http://iopscience.iop.org/0953-8984/24/24/245401)

IOP Publishing Journal of Physics: Condensed Matter
J. Phys.: Condens. Matter **24** (2012) 245401 (5pp) doi:10.1088/0953-8984/24/24/245401

Dynamics of one electron in a nonlinear disordered chain

F A B F de Moura[1], R A Caetano[1] and B Santos[2]

[1] Instituto de Física, Universidade Federal de Alagoas, Maceió AL 57072-970, Brazil
[2] Observatório Nacional, 20921-400 Rio de Janeiro-RJ, Brazil

E-mail: fidelis@fis.ufal.br (F A B F de Moura)

Received 13 March 2012, in final form 12 April 2012
Published 17 May 2012
Online at stacks.iop.org/JPhysCM/24/245401

Abstract
In this paper we report new numerical results on the disordered Schrödinger equation with nonlinear hopping. By using a classical harmonic Hamiltonian and the Su–Schrieffer–Heeger approximation we write an effective Schrödinger equation. This model with off-diagonal nonlinearity allows us to study the interaction of one electron and acoustical phonons. We solve the effective Schrödinger equation with nonlinear hopping for an initially localized wavepacket by using a predictor–corrector Adams–Bashforth–Moulton method. Our results indicate that the nonlinear off-diagonal term can promote a long-time subdiffusive regime similar to that observed in models with diagonal nonlinearity.

The strongly established relationship between the extension of the wavefunction and the electrical nature of the system makes the study of the electronic character of the wavefunction a recurrent issue in condensed matter physics. Many factors play a role in the degree of localization of the wavefunction: however, since the seminal paper by Abrahams *et al* it is known that the presence of disorder is a central factor governing the extension of the wavefunction [1]. The authors showed that all states in a disordered system with a dimension less than two are localized in a fraction of the system, irrespective of the strength of the disorder. However, it has also been demonstrated that, in the presence of certain ingredients, delocalized states can appear. For example, delocalized states are observed when specific correlations are imposed on the statistic of the disorder [2, 3]. Delocalized zero-energy states are also found in quasi-one-dimensional systems with a random magnetic field [4]. The magnetic field also plays an interesting role in the localization properties in fractal space. It was demonstrated in a Sierpinski gasket that an incommensurate magnetic field can couple original highly degenerated localized states and make them delocalized [5, 6]. It is worth mentioning that, although the Anderson localization has been developed in the electronic context, such a prediction is still valid for every field described by a wave equation. For instance, Anderson localization of electromagnetic fields [7], water waves [8] and Bose–Einstein condensates (BEC) [9] have been reported in the literature. One interesting issue concerning the latter is that its dynamics is well described by the Gross–Pitaevskii equation [10] and the nonlinearity present in this equation reveals exciting new physical properties [11–13]. In the electronic context, nonlinearity in the Schrödinger equation can also be present. It was shown that the electron–phonon interaction is well described by a nonlinear Schrödinger equation [13, 14]. One of the most interesting phenomena induced by nonlinearity is self-trapping which occurs when the strength of the nonlinearity exceeds a critical value of the order of the bandwidth [13–15]. In this regime, an initially localized wavepacket does not spread over the system, remaining localized in a fraction of the system. The interplay between nonlinearity and disorder has been recently investigated and the nonlinear aspects seem to be dominant over the disorder [16–19]. In particular, there was observed a counter-intuitive subdiffusive spreading of an initially localized wavepacket, without any indication of saturation for long time runs [16]. From the experimental point of view, the competition between disorder and nonlinearity was investigated in coupled waveguides patterned on an AlGaAs substrate. The authors report that the presence of nonlinearity enhances the localization of linear modes. However, on the other hand, it induces the delocalization of nonlinear modes [20]. It must be stressed here that the study of the nonlinear Schrödinger equation is important in many branches of physics. For instance, the propagation of electromagnetic waves in nonlinear disordered media has been investigated [21, 22]. The influence of the anharmonic terms of the phonon–phonon interaction, which leads to nonlinearity, was also explored [23]. Usually,

the electron–phonon interaction included in the nonlinear Schrödinger equation commonly found in the literature describes the coupling between the lattice vibration and the diagonal electronic matrix elements of the electron Hamiltonian, namely diagonal linearity. In fact, it was shown that the lattice vibration can also couple with the off-diagonal electronic matrix elements [24].

Pan *et al* investigated the electronic time evolution in a disordered off-diagonal nonlinear medium [26]. The authors observe the second momentum of the electronic probability and the participation number for different nonlinearity strengths. They claim that the presence of off-diagonal nonlinearity destroys the delocalization found if only diagonal nonlinearity was present. In this work, we revisit this problem and numerically show that the presence of off-diagonal nonlinearity does not inhibit the delocalization in a disordered linear chain. We calculate the second momentum of probability and no saturation was found for times up to 10^7. We also show that not all states display the subdiffusive spreading regime. Only the components with energy close to the center of the band spread. On the other hand, states with energy at the band edge remain localized. This energy dependence was studied in the diagonal nonlinearity context by Mulansky *et al* [27]. The authors have demonstrated rigorously, in terms of the Gibbs distribution, that states with energy at the band edge cannot spread because there is no delocalized states which conserve the norm and the energy at the band edge. On the other hand, the norm and energy conservation do not prevent the appearance of delocalized states at the center of the band. We numerically show that this statement is still valid for off-diagonal nonlinearity.

1. Model and formalism

We consider an electron moving in a one-dimensional (1d) chain taking account of the coupling with atomic displacement (acoustical phonons). We write the Hamiltonian within the Su–Schrieffer–Heeger (SSH) approximation [24]. This model was originally developed in order to understand the electrical properties of linear polymers. Some assumptions are considered in this model. Firstly, interchain electron hybridization is neglected. The electron is treated in the adiabatic approximation since the gap between the bounding and antibounding states is large for polymers. This model also considers the small vibration regime, allowing us to expand the bounding energy to second order about the equilibrium atom positions. Furthermore, in the small vibration regime, the hopping terms can be treated in a first-order expansion about the equilibrium system [25]. Under those considerations, the Hamiltonian can be written as [24, 26, 29]

$$H = \sum_n \{(\dot{u}_n)^2/2 + (K/2)(u_n - u_{n-1})^2\} + \sum_n \epsilon_n c_n^\dagger c_n + \sum_n \{[V_0 + \tau(u_n - u_{n-1})](c_{n+1}^\dagger c_n + c_{n-1}^\dagger c_n)\} \quad (1)$$

where u_n is the atomic displacement, V_0 is the intrinsic hopping integral, ϵ_n is the on-site energy of the nth site, τ is the electron–phonon coupling constant, and $c_n^\dagger$ and c_n are the creation and annihilation operators for the electron at site n. Performing a variational calculation within an adiabatic approximation, it can be found that the displacement of each atom is proportional to the local electron density. By considering the wavefunction in the Wannier representation $|\Phi(t)\rangle = \sum_n \phi_n(t)|n\rangle$, the effective Schrödinger equation with a nonlinear hopping term is given by

$$i\hbar \frac{d\phi_n}{dt} = \epsilon_n \phi_n + [V + \chi(|\phi_n|^2 + |\phi_{n+1}|^2)]\phi_{n+1} + [V + \chi(|\phi_n|^2 + |\phi_{n-1}|^2)]\phi_{n-1} \quad (2)$$

where χ is the parameter describing the effective electron–phonon coupling. We solve the set of nonlinear coupled differential equations using a predictor–corrector Adams–Bashforth–Moulton formalism initialized by the Dormand–Prince Runge–Kutta method of order eight with time step $\Delta t = 0.01$. Our calculations for long times were done by using the tenth-order Adams–Bashforth formalism as the predictor formula and the ninth-order Adams–Moulton procedure as the corrector. The time step used here is sufficient to keep the wavefunction normalization for a long time ($|1 - \sum_n |\phi_n(t)|^2| < 10^{-10}$). In order to have an additional confirmation of our results, we have also used the standard Dormand–Prince Runge–Kutta method with $\Delta t = 0.01$ for entire integrations (not shown here). We have found exactly the same results to within the numerical tolerance. However, as is well known in the literature, the computational time required in the Runge–Kutta formalism is longer than the time required by the predictor–corrector algorithm. Aiming to characterize the dynamic behavior of an initially localized wavepacket, i.e. $\{\phi_n(t = 0) = \delta_{n,0}\}$, we computed typical quantities that can give information on its spatial extension, namely the participation function and wavepacket mean-square displacement which are defined as [15, 29]

$$\xi(t) = 1 \Big/ \sum_n |\phi_n(t)|^4 \quad (3)$$

and

$$\sigma(t) = \sqrt{\sum_n [(n - \langle n(t)\rangle)^2]|\phi_n(t)|^2}, \quad (4)$$

$\langle n(t)\rangle = \sum_n n|\phi_n(t)|^2$. In the long-time regime, the scaling behavior of the last quantity can also be used to distinguish between localized and delocalized wavepackets. Note that $\sigma(t)$ varies from 0, for a wavefunction 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, we perform calculations with $t_{\max} \approx 10^7$.

2. Results and discussion

The main results were obtained following the time evolution of a wavepacket initially localized at the center of a self-expanding chain. The self-expanding chain was used to minimize the border effects; whenever the probability

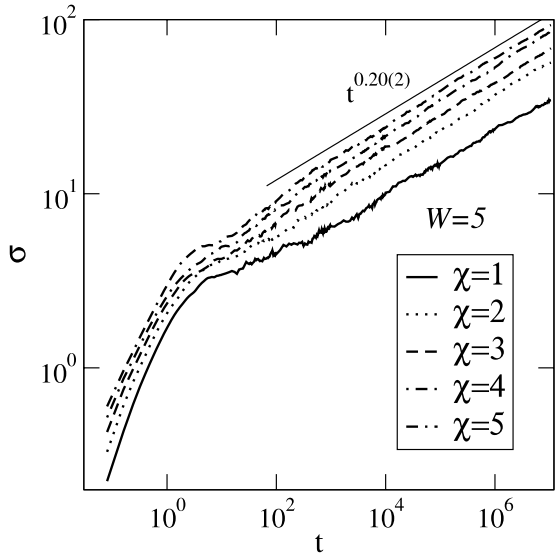

Figure 1. Mean-square displacement $\sigma(t)$ versus time for several values of the off-diagonal electron–phonon coupling constant χ. Our numerical results indicate that off-diagonal nonlinearity induce the subdiffusive spreading of wavepacket $\sigma \propto t^{0.20(2)}$.

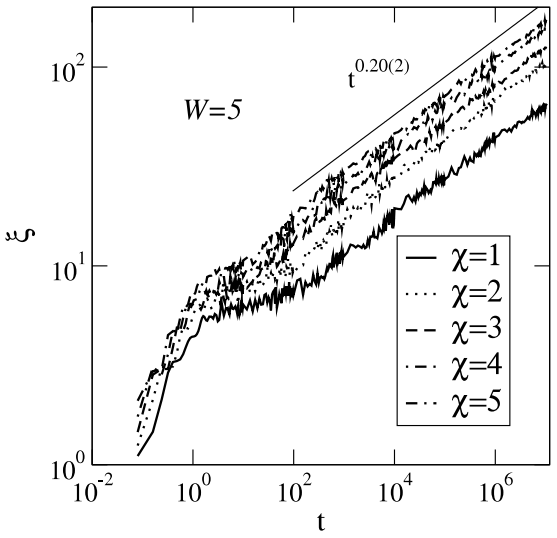

Figure 2. Plot of the participation number ξ versus time. The results were obtained following the time evolution of a wavepacket initially fully localized at the center of a self-expanding nonlinear chain. The width of diagonal disorder used here was $W = 5$. In good agreement with mean-square displacement calculation, we obtained again a subdiffusive regime $\xi \propto t^{0.20(2)}$.

of finding the particle at the ends of the chain exceeded 10^{-30}, ten new sites were added to each end. The numerical convergence and method stability are checked at each 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 order to prevent the effects of a specific disorder configuration, we take the average over 20 disorder configurations. Figure 1 shows the mean-square displacement $\sigma(t)$ for several values of the off-diagonal electron–phonon coupling constant χ. The width of the diagonal disorder used was $W = 5$. In the absence of nonlinearity ($\chi = 0$), the well-defined Anderson localization regime takes place and the wavepacket does not show any spreading [30]. However, when the nonlinear hopping is switched on, we observe a subdiffusive regime, $\sigma \propto t^{0.20(2)}$. Moreover, in figure 2 we plot calculations of the participation number ξ versus time for the same chains used in figure 1. This figure ratifies figure 1 since the subdiffusive regime obeys the same power law $\xi \propto t^{0.20(2)}$. It should be stressed that the values of the exponent obtained here are of the same order of magnitude reported in [16] where only diagonal nonlinearity was considered. However, this result is in contrast to the calculation of [26], where a localized regime was numerically found. We believe that the discrepancy between our results and [26] is due to the short time analysis performed by the authors.

It is worth analyzing an anomaly present in this model. For $\chi = -1$, the dynamics of an initially delta localized wavepacket shows a huge localization behavior. In fact, it is a consequence of the initial wavepacket used. When an initial wavepacket such as $\{\phi_n(t = 0) = \delta_{n,0}\}$ is considered, for $\chi = -1$, the effective hopping terms between the initial site 0 and the nearest-neighbor sites are zero ($t_{0,1}(t = 0) = t_{-1,0}(t = 0) = 0$) and therefore self-trapping takes place. In order to overcome this anomalous behavior presented by this model, we perform the time evolution of an initial Gaussian wavepacket defined by

$$\phi_n(t = 0) = A(\Sigma) \exp[-(n - n_0)^2/4\Sigma^2]. \quad (5)$$

Here Σ is the variance of the initial wavepacket and $A(\Sigma)$ is the normalization constant. In figures 3(a)–(b) we plot the mean-square displacement, σ, and the participation number, ξ, versus time for $\chi = -1$ and $\Sigma = 1$. We observe a subdiffusive spreading regime similar to those found in figures 1 and 2. The solid line in figure 3(b) represents the participation number of an initially fully localized wavepacket ($\Sigma = 0$) in this chain with $\chi = -1$. In figure 4 we compute respectively the mean-square displacement (left panel) and participation number (right panel) for $\chi < -1$ and $W = 5$. The numerical results report that the wavepacket dynamic presents the same subdiffusive regime that was observed for $\chi > 0$. We also analyze the influence of the degree of disorder, W, on the dynamic properties of the wavepacket. In figure 5 we plot the mean-square displacement and the participation number for nonlinear chains with off-diagonal nonlinearity $\chi = 3$ varying the width of diagonal disorder ($W = 6$–9). One can observe that the subdiffusive regime is robust concerning the disorder magnitude. In fact, this behavior is similar to that found in [16] where only diagonal nonlinearity was considered.

Before concluding this paper, we call attention to the fact that not all states are delocalized. A fraction of the states remain localized even with the presence of nonlinearity. As discussed in [27], the presence of nonlinearity promotes the emergence of thermalized states, which present the subdiffusive spreading behavior. The authors show that only states with energy close to the center of the band can be thermalized and states at the band edge remain localized. In order to verify if this property is held for off-diagonal nonlinearity, we perform the time evolution of states with energy at the center of the band and one state with energy

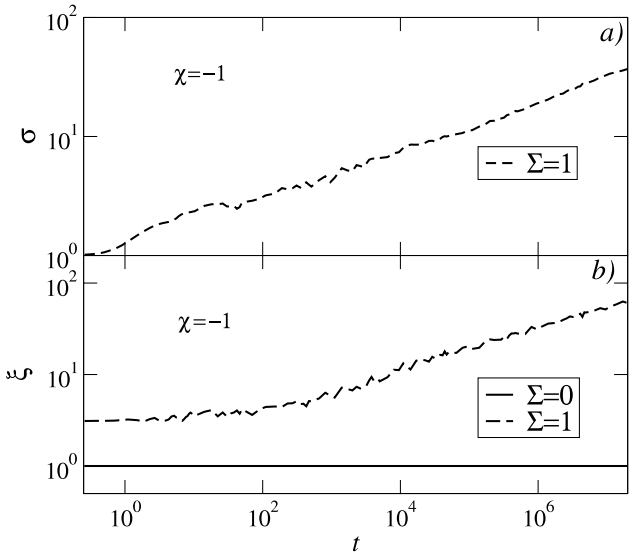

Figure 3. For chains with off-diagonal nonlinearity $\chi = -1$ we study the time evolution of an initially Gaussian wavepacket with variance Σ. We compute the mean-square displacement σ (a) and the participation number ξ (b) versus time for $\chi = -1$ and $\Sigma = 1$. We observe a subdiffusive regime similar to that found in figures 1 and 2. For $\Sigma = 0$ (solid line in figure 3(b)) the hopping of the initial site with its nearest-neighbor sites is zero ($t_{0,1}(t = 0) = t_{-1,0}(t = 0) = 0$). therefore we obtain $\xi = 1$ which represents a localized behavior.

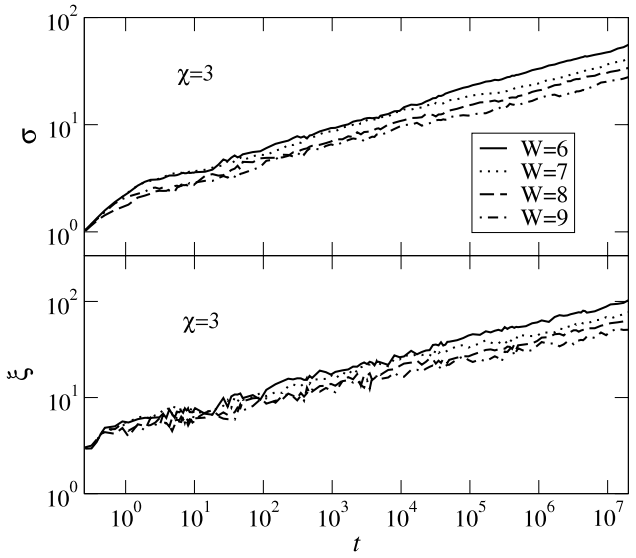

Figure 5. (a) The mean-square displacement and (b) the participation number for a nonlinear chain with off-diagonal nonlinearity $\chi = 3$ and distinct widths of diagonal disorder ($W = 6$–9). The subdiffusive regime remains stable.

at the band edge. The initial states are selected by exact diagonalization of the Hamiltonian of a chain with 100 sites, in the absence of nonlinearity and taking the states with the selected energy. In figure 6 we show $\sigma(t)$ (upper panel) and $\xi(t)$ (lower panel) for states with energy equal to 0.002 (continuous line), 0.04 (dotted line) and 3.75 (dashed line). One can see that states with energy close to the center of the band display the subdiffusive spreading and the state with energy close to the band edge remains localized.

3. Summary and conclusion

In this work we include the coupling between lattice vibration and off-diagonal electronic matrix elements. Within the clas-

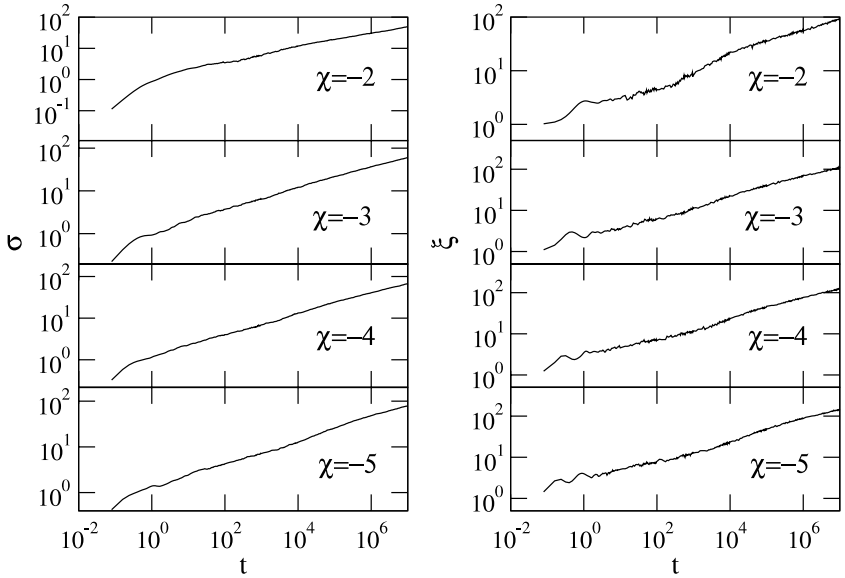

Figure 4. Left panel: the mean-square displacement versus time. The results were obtained following the time evolution of a wavepacket initially fully localized at the center of a self-expanding nonlinear chain with $\chi = -2, -3, -4, -5$ and $W = 5$. Right panel: calculations of the participation number for the same cases of the left panel. The numerical results indicate the same subdiffusive regime that was observed for $\chi > 0$.

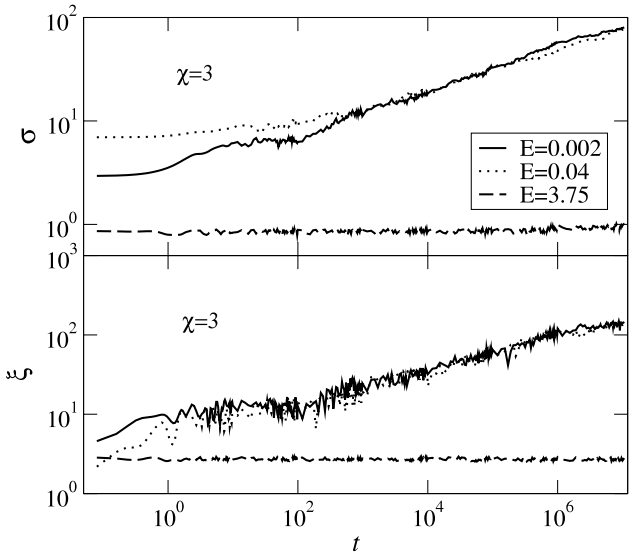

Figure 6. Upper panel—the mean-square displacement, $\sigma(t)$, versus time for three different initial states and nonlinearity, $\xi = 3$. The initial states are eigenstates of the linear Hamiltonian with energies 0.002 (continuous line), 0.04 (dotted line) and 3.75 (dashed line). The first two initial states are close to the center of the band while the last one is at the border edge. Lower panel—the participation ratio, $\xi(t)$, versus time for the same initial states of the upper panel. One can notice that the subdiffusive regime takes place only for the initial states at the center of the band.

sical harmonic Hamiltonian and the Su–Schrieffer–Heeger approximation, a disordered Schrödinger equation is written with the presence of off-diagonal nonlinearity. We solve the effective Schrödinger equation with nonlinear hopping for an initially localized wavepacket using a predictor–corrector tenth-order Adams–Bashforth–Moulton [28] method initialized by the Dormand–Prince Runge–Kutta method of order eight. Our main result indicates that the nonlinear off-diagonal term can promote a long-time subdiffusive regime, similar to those observed in the models with diagonal nonlinearity, however, contrary to the behavior reported in [26]. We also show that not all states display the subdiffusive regime. There is a fraction of the states, with energy at the border edge, that remains localized. The inclusion of the off-diagonal nonlinearity is crucial in order to give a detailed description of the electronic properties of disordered systems and can be experimentally tested in BEC systems [31, 11] and disordered photonic lattices [32].

Acknowledgments

This work was partially supported by CNPq, CAPES, FINEP (Federal Brazilian agencies) and INCT-Nano(Bio)Simes, as well as FAPEAL (Alagoas State agency).

References

[1] Abrahams E, Anderson P W, Licciardello D C and Ramakrishnan T V 1979 *Phys. Rev. Lett.* **42** 673
[2] Phillips P and Wu H-L 1991 *Science* **252** 1805
[3] Dunlap D H, Wu H-L and Phillips P W 1990 *Phys. Rev. Lett.* **65** 1
[4] Chan W L, Wang X R and Xie X C 1996 *Phys. Rev.* B **54** 11213
[5] Wang X R 1995 *Phys. Rev.* B **51** 9310
[6] Wang X R 1996 *Phys. Rev.* B **53** 12035
[7] Wiersma D S, Bartolini P, Lagendijk Ad and Righini R 1997 *Nature* **390** 671
[8] Billy J *et al* 2008 *Nature* **453** 891
[9] Roati G *et al* 2008 *Nature* **453** 895
[10] Dalfovo F, Giorgini S, Pitaevskii L P and Stringari S 1999 *Rev. Mod. Phys.* **71** 463
[11] Ryu C, Andersen M F, Vaziri A, d'Arcy M B, Gross-man J M, Helmerson K and Phillips W D 2006 *Phys. Rev. Lett.* **96** 160403
[12] Behinaein G, Ramareddy V, Ahmadi P and Summy G S 2006 *Phys. Rev. Lett.* **97** 244101
[13] Johansson M, Hörnquist M and Riklund R 1995 *Phys. Rev.* B **52** 231
[14] Datta P K and Kundu K 1996 *Phys. Rev.* B **53** 14929
[15] de Moura F A B F, Gléria I, dos Santos I F and Lyra M L 2009 *Phys. Rev. Lett.* **103** 096401
[16] Pikovsky A S and Shepelyansky D L 2008 *Phys. Rev. Lett.* **100** 094101
[17] Gracía-Mata I and Shepelyansky D L 2009 *Phys. Rev.* E **79** 026205
[18] Iomin A 2010 *Phys. Rev.* E **81** 017601
[19] Tietsche S and Pikovsky A 2008 *Europhys. Lett.* **84** 10006
[20] Lahini Y, Avidal A, Pozzi F, Sorel M, Morandotti R, Christodoulides D N and Silberberg Y 2008 *Phys. Rev. Lett.* **100** 013906
[21] Skipetrov S E and Maynard R 2000 *Phys. Rev. Lett.* **85** 736
[22] Schwartz T, Bartal G, Fishman S and Sergev M 2007 *Nature* **446** 53
[23] Abhishek D and Lebowitz J L 2008 *Phys. Rev. Lett.* **100** 134301
[24] Su W P, Schrieffer J R and Heeger A J 1979 *Phys. Rev. Lett.* **42** 1698
Su W P, Schrieffer J R and Heeger A J 1980 *Phys. Rev.* B **22** 2099
Heeger A J, Kivelson S, Schrieffer J R and Su W-P 1988 *Rev. Mod. Phys.* **60** 781
[25] Salem L 1966 *The Molecular Orbital Theory of Conjugated Systems* (New York: Benjamin)
[26] Pan Z, Xiong S and Gong C 1997 *Phys. Rev.* B **56** 4744
[27] Mulansky M, Ahnert K, Pikovsky A S and Shepelyansky D L 2009 *Phys. Rev.* E **80** 056212
[28] Hairer E, Nørsett S P and Wanner G 2010 *Solving Ordinary Dierential Equations I: Nonstiff Problems* (*Springer Series in Computational Mathematics*) (Berlin: Springr)
Press W H, Flannery B P, Teukolsky S A and Wetterling W T 2007 *Numerical Recipes: The Art of Scientific Computing* 3rd edn (New York: Cambridge University Press)
[29] Dias W S, Lyra M L and de Moura F A B F 2012 *Eur. Phys. J.* B **85** 7
[30] de Moura F A B F, Fulco U L, Lyra M L, Domínguez-Adame F and Albuquerque E L 2011 *Physica* A **390** 535
[31] Lye J E *et al* 2005 *Phys. Rev. Lett.* **95** 070401
[32] Schwartz T, Bartal G, Fishman S and Segev M 2007 *Nature* **446** 52