Wave-Packet Dynamics in Chains with Delayed Electronic Nonlinear Response

F. A. B. F. de Moura, Iram Gléria, I. F. dos Santos, and M. L. Lyra

Instituto de Física, Universidade Federal de Alagoas, Maceió AL 57072-970, Brazil

We study the dynamics of one electron wave packet in a chain with a nonadiabatic electron-phonon interaction. The electron-phonon coupling is taken into account in the time-dependent Schrödinger equation by a delayed cubic nonlinearity. In the limit of an adiabatic coupling, the self-trapping phenomenon occurs when the nonlinearity parameter exceeds a critical value of the order of the bandwidth. We show that a weaker nonlinearity is required to produce self-trapping in the regime of short delay times. However, this trend is reversed for slow nonlinear responses, resulting in a reentrant phase diagram. In slowly responding media, self-trapping only takes place for very strong nonlinearities.

　　　　　　PACS numbers: 71.30.+h, 05.60.Gg, 71.38.Ht, 73.20.Jc

The study of the physical mechanisms involved in transport phenomena taking place in nonlinear systems is a fundamental issue in solid state physics. Concerning the electronic transport, nonlinearity arises from the interaction between electrons and lattice vibrations [1–7]. In this context, the discrete nonlinear Schrödinger equation (DNLSE) effectively describes the influence of lattice vibrations on the electron dynamics. The most important property associated with the DNLSE is the self-trapping which occurs when the nonlinearity parameter exceeds a critical value of the order of the bandwidth [1–3]. In this regime, an initially localized electronic wave packet does not spread continuously over the lattice. Therefore, the probability of finding the electron at its initial site remains finite in the long-time limit.

In low-dimensional systems, the effect of nonlinearity seems to be dominant over the role played by disorder [8–11]. Recently, the spreading of an initially localized wave packet in two nonlinear chains with disorder was studied [8]. Considering a discrete nonlinear Schrödinger and quartic Klein-Gordon equations with disorder, it was proved that the second moment and the participation number of the wave packet do not diverge simultaneously [8]. The spreading of an initially localized wave packet in a one-dimensional discrete nonlinear Schrödinger lattice with disorder was also recently studied [9]. It was observed that the Anderson localization is destroyed and a subdiffusive dynamics takes place above a certain critical nonlinearity strength. [9] Moreover, analytical and numerical calculations for a reduced Fermi-Pasta-Ulam chain demonstrated that energy localization does not require more than one conserved quantity [10].

From the experimental point of view, the interplay between disorder and nonlinearity was investigated in Ref. [11]. The evolution of linear and nonlinear waves in coupled optical waveguides patterned on an AlGaAs substrate was directly measured. Nonlinear perturbations enhance localization of linear waves while they induce delocalization of the nonlinear ones [11]. In the presence of disorder, a transition from ballistic wave-packet expansion to exponential localization was observed. Within a more general scope, the study of wave propagation in nonlinear systems is a very interesting problem with several applications in many branches of physics. For example, by using a model with diagonal and off-diagonal electron-phonon-like terms, the role played by the degree of integrability and the resulting extreme event statistic were recently studied [12]. The main motivation was to explain the sudden appearance of sea waves of extremely large amplitude in relatively calm seas.

Usually, the nonlinearity produced by the electron-phonon interaction is assumed to be instantaneous. However, this effective nonlinearity is limited by the finite response time of the medium, and corrections are expected in the nonadiabatic regime. Actually, the relaxation of the nonlinearity is known to have a deep influence on the electronic wave-packet dynamics [13–16]. Using nonadiabatic nonlinear models, Kenkre and co-workers [13,14] considered the problem of a two-level system driven by a relaxation process of the nonlinearity. It was shown that there is a stationary self-trapping regime and a coexistence of static and dynamical transitions for certain degrees of nonlinearity and relaxation time [13]. These features contrast with the persistent oscillatory dynamics displayed by the adiabatic nonlinear dimer model in both delocalized and self-trapped regimes [15]. Moreover, it was shown that localized stationary states of a dimer model are destroyed above a critical temperature [14].

In this Letter, we address the question regarding the influence of noninstantaneous nonlinearity on the long-distance electronic transport in linear chains. This physical scenario is particularly suited to the study of electronic transport in macromolecules, such as DNA, on which the electron-phonon coupling is expected to play a relevant role [17]. Here, we will effectively take into account the nonadiabatic nature of the electron-phonon interaction by introducing a delayed third-order nonlinearity in the one-electron time-dependent Schrödinger equation. Delayed

differential equations usually describe physical systems presenting a finite response time [18]. Within a tight-binding approach, the time evolution of the coefficients of the wave vector expanded in the localized orbitals basis $[|\Psi(t)\rangle = \sum_j c_j(t)|j\rangle]$ takes the form

$$i\dot{c}_j(t) = V[c_{j+1}(t) + c_{j-1}(t)] - \chi|c_j(t-\tau)|^2 c_j(t), \quad (1)$$

where we used units of $\hbar = 1$ and considered the on-site potentials $\epsilon_j = 0$. V is the hopping integral between nearest-neighbor sites, and χ is a nonlinear parameter which is proportional to the local electron-phonon coupling [16]. The nonadiabatic nature of the electron-phonon interaction is represented by a delayed contribution to the on-site potential proportional to $|c_j(t-\tau)|^2$ where τ is the typical response time. To analyze the wave-packet propagation, we solve Eq. (1) using the fourth-order Runge-Kutta method to obtain the temporal evolution of an initially localized wave packet $[|\Psi(t=0)\rangle = \sum_j c_j(0)|j\rangle$ with $c_j(0) = \delta_{j,j_0}]$. We follow the time evolution of the amplitude of the wave function at the initial site, calculating the so-called return probability [19],

$$R_0(t) \equiv |c_{j_0}(t)|^2. \quad (2)$$

Usually, the electron escapes from its initial position when the amplitude $c_{j_0}(t)$ vanishes as t evolves. Conversely, the amplitude remains finite for a self-trapped wave packet. In order to have a better description of the wave-packet dynamics, we also compute the time-dependent participation function defined as

$$P(t) = 1 \bigg/ \sum_j |c_j(t)|^4. \quad (3)$$

The participation function $P(t)$ gives an estimate of the number of sites over which the wave packet is spread at time t. In the long-time regime, its scaling behavior can also be used to distinguish between localized and delocalized wave packets [19]. In particular, the asymptotic participation number becomes size-independent for localized wave packets. On the other hand, it scales linearly with the chain size in the delocalized regime.

In our numerical simulations, we set the parameter V as the energy unit. Further, we considered the open boundary condition with the wave packet initially located at the chain center. However, the main following analysis regarding the self-trapped–delocalized transition and phase diagram holds for the periodic boundary condition as well. We assume $c_j(t < 0) = 0$ for any site j. This condition corresponds to the situation on which the electron is injected in the system at time $t = 0$, with the electronic density being null for negative times. In Fig. 1(a), we report the time evolution of the return probability on a chain with $N = 2 \times 10^3$ sites for the case of instantaneous nonlinearity ($\tau = 0$) for distinct strengths of the nonlinear parameter χ. The plots show the usual behavior exhibited by the
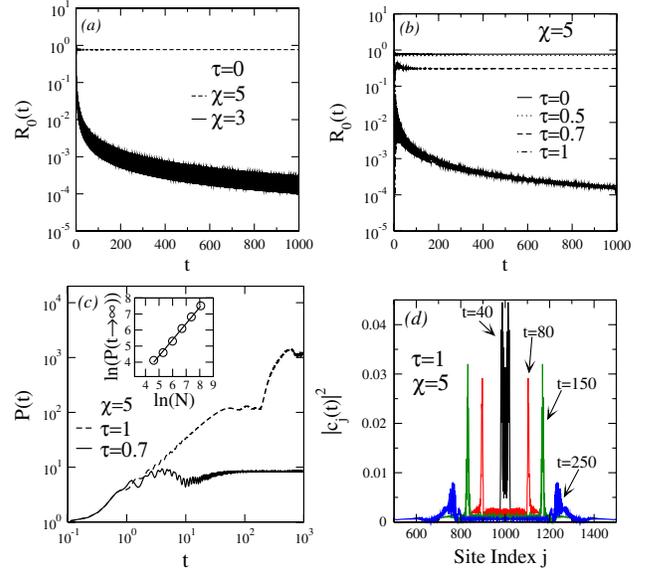

FIG. 1 (color online). (a) Return probability $R_0(t)$ for $\chi = 3$ and $\chi = 5$ in a chain with $N = 2 \times 10^3$ sites with an instantaneous nonlinearity. $R_0(t)$ asymptotes a constant value for $\chi > 3.5$, corresponding to a self-trapped wave packet. It continuously decays for $\chi < 3.5$ as the wave packet becomes delocalized. (b) $R_0(t)$ for $\chi = 5$ with different values of τ. Even for such strong nonlinearity, $R_0(t \to \infty)$ becomes of the order of $1/N$ for $\tau = 1$. This breakdown of self-trapping is a delay-induced transition. (c) The participation number $P(t)$ for $\tau = 0.7$ and $\tau = 1$ for $\chi = 5$. A long delay time allows for the spread of an initially localized wave packet. The inset shows the linear finite-size scaling of the asymptotic participation number for $\tau = 1$, typical of delocalized states. (d) Snapshots of the wave packet in the initial transient regime ($t = 10$), within the plateau ($t = 80, 150$) on which the width of the wave packet around the peaks is roughly constant in time, and after the plateau ($t = 250$) showing the smearing out of the wave front.

DNLSE with adiabatic electron-phonon interaction [3]. For strong nonlinearities $\chi > 3.5$, the return probability $R_0(t)$ approaches a constant value in the a long-time limit, thus indicating that the wave packet is localized [1,2]. This behavior is the so-called self-trapping, on which the electron remains localized around its initial position due to its coupling with the lattice vibrations. The critical nonlinearity is of the order of the energy bandwidth because χ accounts for the effective on-site potential felt by the initially localized electron. If χ is much larger than the energy bandwidth, this state cannot be efficiently mixed with the other energy states. For $\chi < 3.5$, the asymptotic return probability is vanishingly small (of the order of $1/N$), which characterizes the regime of extended states. In Fig. 1(b), we focus on the effect of the nonlinearity delay time τ on the self-trapping transition. We consider an electron-phonon coupling sufficiently strong to induce self-trapping in the adiabatic limit. We observe that the gradual increase in the delay time leads to a decrease of the return probability. This delocalization process, correspond-

ing to a breakdown of self-trapping, is a delay-induced
transition. In Fig. 1(c), we show data for the time-
dependent participation number $P(t)$ in this strong non-
linear regime ($\chi = 5$). The self-trapping phenomenon is
indeed destroyed when the delay time is increased, with the
asymptotic participation number becoming of the order of
the chain size. It is interesting to notice that the participa-
tion number exhibits an intermediate plateau in the delo-
calized regime. The time evolution of $P(t)$ in this regime
reflects a solitonlike wave-packet dynamics [see Fig. 1(d)].
During the initial stage, the wave packet splits from its
single peak structure to a structure with two peaks that
move in opposite direction [20]. The participation number
grows almost linearly during this initial process. After the
wave-packet splitting, the wave fronts display a solitonlike
behavior, with the width around the peaks being roughly
time-independent [1]. In this regime, the participation
number becomes time-independent because the main con-
tribution for it comes from the region around the wave-
packet peaks. Further, there is a dynamical transition to a
regime on which the wave-front peaks lose their solitonlike
behavior. The width of the wave front starts to increase in
time and, consequently, the participation number restarts to
grow. It is interesting to stress that a dynamical transition
has also been found in nonlinear dimers with nonadiabatic
nonlinearity [13]. Finally, the participation number
achieves its final saturation when the wave fronts reach
the chain boundaries. The linear finite-size scaling, shown
in the inset of Fig. 1(c), clearly characterizes the delocal-
ized nature of the asymptotic wave packet in this regime.

Data for the long-time return probability $R_0(t \to \infty)$
versus the delay time τ are shown in Fig. 2 for nonlinearity
strengths ranging from $\chi = 2.5$ up to 8. The reported
values are averages in the statistically stationary regime
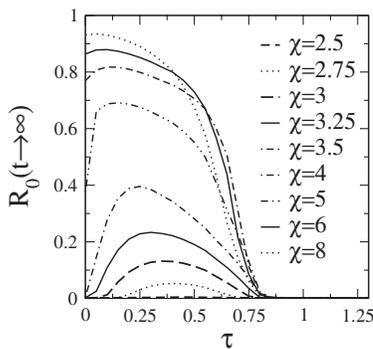of the return probability. These values are finite and inde-

pendent of the chain size when self-trapping takes place.
On the other hand, the asymptotic return probability van-
ishes as $1/N$ in the delocalized regime. For $\chi < 2.5$, the
asymptotic return probability approaches zero irrespective
of the delay time. In contrast with the delocalization tran-
sition induced by large delay times, a short delay can
promote self-trapping [$R_0(t \to \infty) > 0$] for nonlinearities
slightly below the adiabatic critical one $2.5 < \chi < 3.5$. The
physical reason for the decreasing of the critical nonlinear
strength in the regime of fast nonlinear responses is that the
nonlinearity comes from the electron coupling with the
electronic density at a previous time. With the electron still
relatively localized around its initial position in the begin-
ning of the wave-packet time-evolution, the retarded elec-
tronic density at the initial site is larger than the
instantaneous one. Therefore, a smaller nonlinear strength
is required to promote the self-trapping in comparison with
the instantaneous case. Therefore, our results indicate that
the self-trapping regime has a reentrant character taking
place in a finite range of short delay times. In Fig. 3 we plot
some numerical results for $R_0(t \to \infty)$ versus the strength
of the electron-phonon coupling χ. Here, we considered
delay times ranging from $\tau = 0$ up to 0.8. These results
give further support to the above described picture: (i) for
large delays the self-trapping phenomenon disappears (see
results for $\tau = 0.8$) in the range of nonlinearity strengths
shown, and (ii) for small but finite delays, self-trapping
starts below the critical nonlinearity of the adiabatic limit.
It is interesting to notice that the return probability reaches
a maximum at a finite nonlinear coupling in the regime of
short delay times. This nonmonotonic behavior also con-
trasts with the continuous increase of the return probability
for the case of an instantaneous nonlinearity. Finally, we
plot the phase diagram in the "χ-vs-τ" plane in Fig. 4. The
reentrant character of the transition is reflected by the
nonmonotonic dependence of χ_c as the delay time is
increased. The extended states were characterized using
the criterion $R_0(t \to \infty) \approx 1/N$ and $P(t \to \infty) \propto N$. The
slight decrease of the critical nonlinear strength for short

FIG. 2. $R_0(t \to \infty)$ versus the delay time τ with $\chi = 2.5$ up to
8. A breakdown of the self-trapping phenomenon takes place for
large delay times. For intermediate electron-phonon interactions
$2.5 < \chi < 3.5$, we observe that a short delay can induce self-
trapping [$R_0(t \to \infty) > 0$] which is absent in the limit of instan-
taneous nonlinearity. In this range of nonlinear couplings, a
sequence of delocalized $\to$ self-trapped $\to$ delocalized regimes
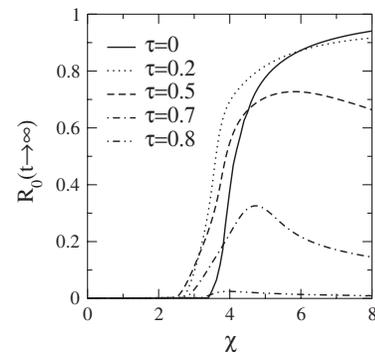is depicted as the delay time is increased.

FIG. 3. $R_0(t \to \infty)$ versus the strength of the electron-phonon
coupling χ for $\tau = 0$ up to 0.8. A delayed nonlinearity can
induce self-trapping even for nonlinear couplings below the
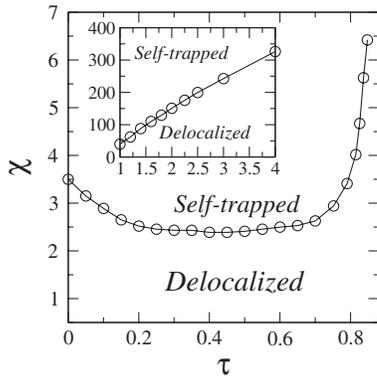critical value in the adiabatic limit $\chi = 3.5$.

FIG. 4.   Phase diagram in the "χ-vs-τ" parameter space show-
ing the delocalized–self-trapped transition induced by a time
delayed electron-phonon interaction. The regime of delocalized
wave packets was characterized using the criterion $R_0(t \to \infty) \approx$
$1/N$ and $P(t \to \infty) \propto N$. The critical nonlinearity has a non-
monotonic behavior in the regime of short response times. In the
inset, we show the critical line in the regime of longer response
times at which much stronger nonlinearities are required to
promote self-trapping.

delay times is replaced by a fast increase at longer delays,
as shown in the inset of Fig. [4]. Actually, the wave packet
spreads substantially before the nonlinearity takes action in
slowly responding media. As a consequence, a strong
nonlinearity is required to stop the subsequent wave-packet
spread.

In summary, we considered the problem of one electron
moving on a chain under the influence of a delayed third-
order nonlinearity which effectively incorporates the effect
a nonadiabatic electron-phonon interaction. In the case of
an instantaneous nonlinear response, this system presents a
delocalized–self-trapped transition at a critical nonlinear
strength $\chi \simeq 3.5$ [1,3]. We found that for the case of long
delay times, self-trapping takes place only for much
stronger nonlinearities. As a consequence, the electronic
transport retains its metallic character in slowly responding
media for a wide range of nonlinear strengths. On the other
hand, we report a reentrant behavior of the self-trapping
transition point in the regime of fast nonlinear responses
with self-trapping occurring even below the critical non-
linear strength of instantaneously responding media. In a
finite range of nonlinearities below the adiabatic critical
value, a short delay time can promote the stabilization of
self-trapping. A second transition takes place at a longer
delay time above which the wave packet becomes again
delocalized.

It is important to stress that the presently reported delay-
induced self-trapping–delocalization transition is of a na-
ture distinct from the one taking place in dimerlike struc-
tures [13]. While in the latter the delay promotes the decay
of the oscillations in the population levels and a transition
from two distinct oscillatory dynamical regimes, the pres-
ently reported transition deals with the long-distance elec-

tron transport. The phenomenon reported here shall be
inherent to dynamical systems described by delayed non-
linear differential equations. Therefore the influence of the
nonlinear response time on the electronic wave-packet
dynamics is expected to have a similar counterpart in
general (acoustic, electromagnetic) wave transport in non-
linear media. It would be interesting to have further studies
in this direction.

[1] M. Johansson, M. Hörnquist, and R. Riklund, Phys. Rev. B
52, 231 (1995).
[2] P. K. Datta and K. Kundu, Phys. Rev. B **53**, 14929 (1996).
[3] Z. Pan, S. Xiong, and C. Gong, Phys. Rev. E **56**, 4744
(1997).
[4] M. V. Ivanchenko, Phys. Rev. Lett. **102**, 175507 (2009).
[5] S. Flach, D. O. Krimer, and Ch. Skokos, Phys. Rev. Lett.
102, 024101 (2009).
[6] Ch. Skokos, D. O. Krimer, S. Komineas, and S. Flach,
Phys. Rev. E **79**, 056211 (2009).
[7] G. Sangiovanni, M. Capone, C. Castellani, and M. Grilli,
Phys. Rev. Lett. **94**, 026401 (2005).
[8] G. Kopidakis, S. Komineas, S. Flach, and S. Aubry, Phys.
Rev. Lett. **100**, 084103 (2008).
[9] A. S. Pikovsky and D. L. Shepelyansky, Phys. Rev. Lett.
100, 094101 (2008).
[10] D. Hajnal and R. Schilling, Phys. Rev. Lett. **101**, 124101
(2008).
[11] Y. Lahini, A. Avidan, F. Pozzi, M. Sorel, R. Morandotti,
D. N. Christodoulides, and Y. Silberberg, Phys. Rev. Lett.
100, 013906 (2008).
[12] A. Maluckov, Lj. Hadzievski, N. Lazarides, and G. P.
Tsironis, Phys. Rev. E **79**, 025601(R) (2009).
[13] V. M. Kenkre and H.-L. Wu, Phys. Rev. B **39**, 6907 (1989).
[14] P. Grigolini, H.-L. Wu, and V. M. Kenkre, Phys. Rev. B **40**,
7045 (1989).
[15] V. M. Kenkre and D. K. Campbell, Phys. Rev. B **34**, 4959
(1986).
[16] D. Chen, M. I. Molina, and G. P. Tsironis, J. Phys.
Condens. Matter **5**, 8689 (1993).
[17] Mikrajuddin, K. Okuyama, and F. G. Shi, Phys. Rev. B **61**,
8224 (2000); W. Zhang, A. O. Govorov, and S. E. Ulloa,
Phys. Rev. B **66**, 060303 (2002); M. Taniguchi and T.
Kawai, Phys. Rev. E **72**, 061909 (2005); E. Macia, Phys.
Rev. B **76**, 245123 (2007).
[18] M. Berezowski, Chaos Solitons Fractals **12**, 83 (2001);
J. M. Buldú, J. García-Ojalvo, and M. C. Torrent, Phys.
Rev. E **69**, 046207 (2004); R. Vicente, S. Tang, J. Mulet,
C. R. Mirasso, and J.-M. Liu, Phys. Rev. E **73**, 047201
(2006); F. Ishida and Y. E. Sawada, Phys. Rev. E **75**,
012901 (2007).
[19] H. N. Nazareno and P. E. de Brito, Phys. Rev. B **60**, 4629
(1999).
[20] D. E. Katsanos, S. N. Evangelou, and S. J. Xiong, Phys.
Rev. B **51**, 895 (1995).