Transport of localized and extended excitations in a nonlinear Anderson model

M. I. Molina*
Facultad de Ciencias, Departamento de Física, Universidad de Chile, Casilla 653, Las Palmeras 3425, Santiago, Chile

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We study the propagation of electrons (or excitations) through a one-dimensional tight-binding chain in the simultaneous presence of nonlinearity and diagonal disorder. The evolution of the system is given by a disordered version of the discrete nonlinear Schrödinger equation. For an initially localized excitation we examine its mean square displacement $\langle n^2(t)\rangle$ for relatively long times $Vt\sim 10^4$, for different degrees of nonlinearity. We found that the presence of nonlinearity produces a subdiffusive propagation $\langle n^2(t)\rangle \sim t^{\alpha}$, with $\alpha\sim 0.27$ and depending weakly on nonlinearity strength. This nonlinearity effect seems to persist for a long time before the system converges to the usual Anderson model. We also compute the transmission of plane waves through the system. We found an average transmissivity that decays exponentially with system size $\langle T\rangle \sim \exp(-\beta L)$, where β increases with nonlinearity. We conclude that the presence of nonlinearity favors (inhibits) the propagation of localized (extended) excitations. [S0163-1829(98)06340-1]

In condensed matter the presence of nonlinearity can lead to the formation of localized mobile excitations (such as polarons), while the presence of disorder produces localized modes whose mobility is inhibited, most notably in low-dimensional systems (Anderson localization). Thus, it is interesting to consider the combined effect of the simultaneous presence of nonlinearity and disorder on localization and transport properties of a typical low-dimensional system.[1] With that idea in mind, we consider in this work the propagation of a generic quasiparticle (electron or exciton) in a one-dimensional chain in the tight-binding formalism. Due to a strong interaction between the quasi-particle and the vibrational degrees of freedom of the chain, and assuming that the vibrational time scale is much shorter that the hopping time scale, the effective electronic evolution equation is given by the discrete nonlinear Schrödinger (DNLS) equation:

$$i\,\frac{dC_n}{dt}=(\epsilon_n-\chi_n|C_n|^2)C_n+V(C_{n+1}+C_{n-1}), \qquad (1)$$

where $C_n(t)$ is the probability amplitude of finding the excitation on site n at time t, ϵ_n represents the site energies of a one-dimensional crystal, V is the nearest-neighbor hopping term, and χ_n is the nonlinearity parameter, proportional to the square of the (strong) electron-phonon coupling on site n. The special case $\chi_n=0$ and ϵ_n random, describes a one-dimensional Anderson model characterized by having all of its eigenstates localized and a completely inhibited electronic transport.[2] In a previous work[3] we considered the special case of Eq. (1) where the disorder resides entirely in the nonlinearity parameter: $\epsilon_n=\text{const}$ and $\chi_n=\chi$ or zero with 50% probability, that is, a nonlinear random binary alloy. The excitation was initially placed on a single impurity site and both probability profile and mean square displacement were studied for relatively long times. We found that a threshold of nonlinearity exists, $(\chi/V)_{\text{crit}}\sim 3.2$, below which the excitation propagates throughout the chain *ballistically* (i.e., like a free particle). Above threshold, there is partial localization (self-trapping) around the initial site, while the untrapped portion escapes to infinity also in a ballistic manner. The transmission of plane waves across the system showed a powerlike decay as a function of system size. Since the DNLS equation is obtained from the coupled system for the quasiparticle and vibrational degrees of freedom in the limit of a negligible oscillator inertia (antiadiabatic limit) we also examined the effect of a finite oscillator inertia on the self-trapping properties exhibited by the DNLS equation. We found that such inertia (treated in a semiclassical way) does not alter the existence of a nonlinearity threshold for self-trapping or the ballistic character of the propagation.[4] The above properties differ markedly from the well-known "Anderson localization" phenomenon, where the presence of a finite concentration of (linear) uncorrelated disorder completely inhibits the quasiparticle propagation, giving rise to a saturation of its mean-square displacement and an exponential decrease of the transmissivity of plane waves with system size.[2]

In the present work we study the rather complementary case, taking in Eq. (1) $\chi_n=\text{const}\equiv\chi$ and ϵ_n randomly distributed in a finite interval. The model to consider can then be taken as an Anderson model with a nonlinear background.

Localized excitation. For a fixed value of χ and a given random $\{\epsilon_n\}$ configuration, with $-1<\epsilon_n<1$, we compute the time evolution of the quasiparticle, which is initially placed completely on a single site ("site zero"), and examine its mean square displacement in time:

$$u(t)=\sum_{m=-\infty}^{\infty} m^2|C_m(t)|^2 \qquad (2)$$

followed by an average over a number of disordered site energy realizations, obtaining $\langle u(t)\rangle$. The system of equations (1) is solved numerically by means of a fourth-order Runge-Kutta algorithm. Numerical precision is checked by monitoring the conservation of probability (norm) $\Sigma_n|C_n(t)|^2=1$. In order to avoid undesired boundary effects, a self-expanding lattice was used.[3] We computed $\langle u(t)\rangle$ up

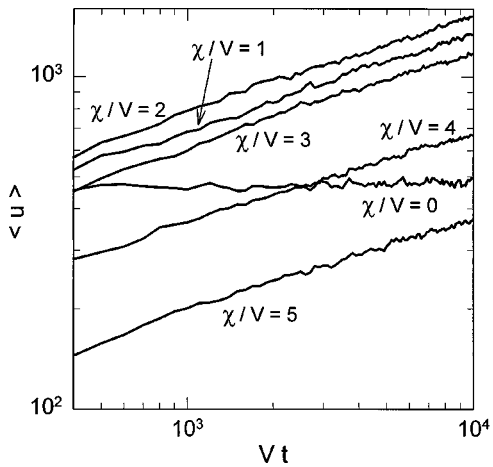

FIG. 1. Disorder-averaged (100 realizations) mean square displacement of an initially localized excitation, for different values of the nonlinearity parameter $(-1<\epsilon_n<1)$.

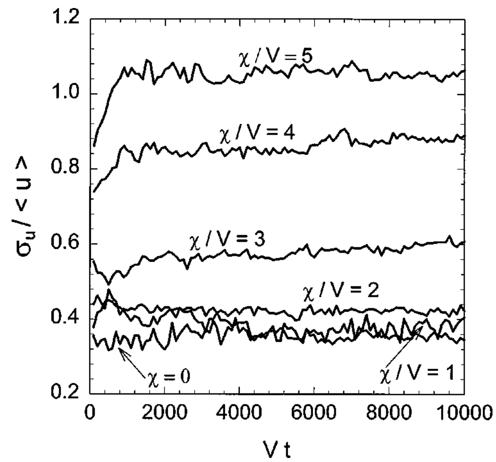

FIG. 2. Fluctuations $\sigma_u=\sqrt{\langle u^2\rangle-\langle u\rangle^2}$ in the mean square displacement of an initially localized excitation as a function of time, for different nonlinearity parameter values $(-1<\epsilon_n<1)$.

to times of the order of $Vt_{\max}=10^4$, averaging over 100 disorder configurations of the chain, going from $\chi=0$ up to $\chi=5V$. Results are shown in Fig. 1. The case $\chi=0$ shows the typical saturation in $\langle u(t)\rangle$ evidencing a complete quasiparticle localization. However, when $\chi\neq 0$, Anderson localization is destroyed and the quasiparticle propagates in a subdiffusive way, i.e., for long times $\langle u(t)\rangle\sim t^{\alpha}$ with $\alpha<1$. A minimum-squares fit finds α quickly reaching and staying close to 0.27, for $\chi\geqslant 1$ (see Table I). At this point it is interesting to point out that all the subdiffusive exponents are substantially smaller than the one conjectured by Shepeliansky ($\alpha=2/5$), based on a somewhat unclear analogy with dynamical localization in the kicked rotator model.[5] An examination of the fluctuations σ_u in $u(t)$ revealed that these grow at the same rate as the mean square displacement (Fig. 2). This behavior has also been observed in models described by long-range random interactions.[6] A sample-to-sample examination of the time-averaged probability at the initial site revealed the presence of a nonlinear trapping regime superimposed on a background of Anderson localization. The onset of this nonlinear trapping is realization dependent and determined mainly by the disorder environment around the initial site. In some cases, this disorder may hold the excitation longer in the vicinity of the initial site, allowing nonlinearity to self-trap more easily; or it may increase the local hopping from the initial site, in which case a stronger nonlinearity is needed to self-trap. Figure 3 compares a realization- and time-averaged probability at the initial site with the case of no disorder. The beginning of nonlinear trapping starts around $\chi=2V$, on average. Clearly, the presence of disorder smears considerably the onset of nonlinear trapping.

TABLE I. Subdiffusive exponent for the long time disorder-averaged (100 realizations) propagation of an initially localized excitation, for several different values of the nonlinearity parameter $(-1<\epsilon_n<1)$.

χ/V	α
0	0.02
0.2	0.08
1	0.282
2	0.287
3	0.262
4	0.265
5	0.266

What happens in the limit $t\to\infty$? Given that $|C_n|^2$ must necessarily decrease during propagation due to normalization (barring coherent motion, not observed in our case), the effect of nonlinearity decreases in time (and space) and, from Eq. (1), we expect that after a sufficiently long time, the model should reduce to the Anderson model. Therefore, the observed subdiffusive propagation should eventually *saturate*. We followed $u(t)$ for particular disorder realizations, up to times of 3×10^4 V without observing a discernible saturation.

From Fig. 1 we also observe that, for a given time, $\langle u(t)\rangle$ increases with nonlinearity up to $\chi/V\sim 2$. Thereafter, its amplitude decreases with increasing nonlinearity. This can be

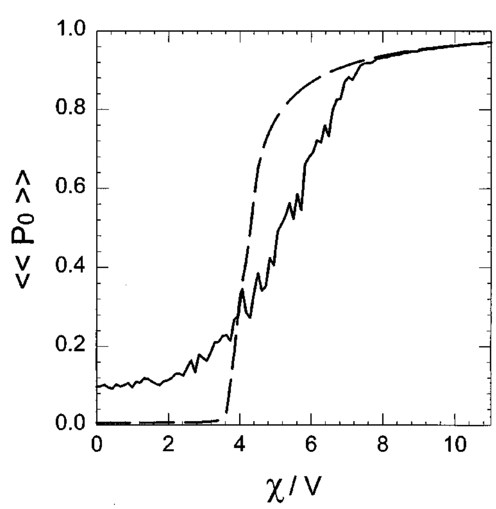

FIG. 3. Disorder- and time-averaged probability at the initial site $\langle\langle P_0\rangle\rangle=(1/t_{\max})\int_0^{t_{\max}}\langle P_0(t)\rangle\,dt$, of an initially localized excitation, as a function of nonlinearity (full line) $[-1<\epsilon_n<1$, $t_{\max}\sim O(10^2)$, 100 realizations]. The case of no disorder is also shown for comparison (dashed line).

understood as the effect of nonlinear self-trapping, which begins around $\chi/V=2$ on average, according to Fig. 3, where a finite fraction of the excitation begins to localize around a narrow vicinity of the initial site. Since the fraction of the excitation that can propagate is now effectively smaller, this renormalizes $\langle u(t)\rangle$ to smaller values as χ is increased.

Extended excitation. We now consider a segment of our disordered and nonlinear material, embedded in a linear, periodic chain between sites $n=0$ and $n=L$. Let us look for stationary solutions of Eq. (1) of the form $C_n(t)=\phi_n\exp(-iEt)$. We obtain

$$E\phi_n=(\epsilon_n-\chi|\phi_n|^2)\phi_n+V(\phi_{n+1}+\phi_{n-1}). \tag{3}$$

In particular, we consider the propagation of plane waves across the segment. We put

$$\phi_n=\begin{cases}R_0e^{ikn}+R_1e^{-ikn}, & n\leqslant 0\\ R_2e^{ikn}, & n\geqslant L,\end{cases} \tag{4}$$

which implies $E=2V\cos(k)$. For a given segment of length L its transmissivity is estimated as follows: given a disorder configuration and a wave vector k, we put $R_2=1$ (Ref. 7) at $n=L$ and iterate backwards using Eq. (3) until we reach the beginning of the segment, where R_0 is computed. The transmissivity is then $T=|R_2|^2/|R_0|^2$. This method for obtaining T, using a ''fixed output'' circumvents eventual problems with multiestability.[3,8] In Figs. 4(a)–4(c) we show transmitting (dark) and nontransmitting regimes (clear) for a segment of length $L=50$ and a given disorder realization with two different disorder widths: $0<\epsilon_n<0.3$ [Fig. 4(a)] and $0<\epsilon_n<0.6$ [Fig. 4(b)]. Each diagram was obtained by assigning arbitrarily a passing (nonpassing) character to a given wave vector k, whose T was above (below) a preset cutoff. The diagrams feature the presence of several branches (tongues) responsible for multiestability and a highly irregular, fractal-like shape. As the width of the disorder is increased, the transmitting region ''evaporates'' somewhat, decreasing its total area but creating new tongues and more irregular features. In Fig. 4(c) we show an enlargement of the region indicated in Fig. 4(b), depicting the presence of even smaller tongue structures. These irregular features are similar to the ones obtained for a nonlinear chain in the absence of disorder.[8]

For a given segment of length L we computed an average transmissivity $\langle T\rangle$ by averaging over all wave vectors $0\leqslant k\leqslant\pi$ and over many disorder configurations (a thousand, typically). The procedure outlined above was carried out with segments of length $L=20$ up to $L=2000$, examining in each case the decay rate of $\langle T\rangle$ as a function of L, for several different values of the nonlinearity parameter χ. The case $\chi=0$ is well known and leads to an exponential decay of the transmissivity with system size. For $\chi>0$ we found that this behavior *persists* at small $L(L<200)$ with decay rates *larger* than in the case of absence of nonlinearity. More exactly, $\langle T\rangle\sim\exp[-\beta(\chi)L]$ with β an increasing function of χ. This is vividly illustrated in Fig. 5(a). For large L values, the transmissivity seems to converge slowly to a power-law behavior [Fig. 5(b)]. The latter feature has also been observed in a related model, the *continuous* nonlinear random slab,[9]

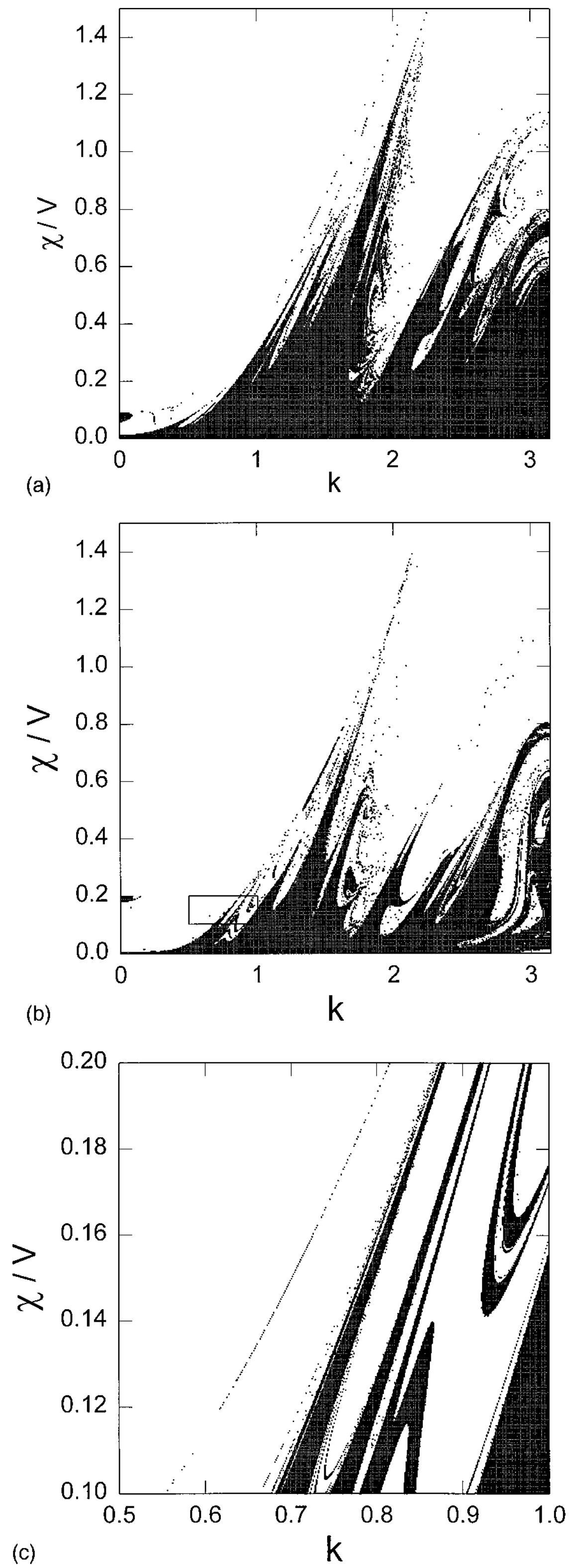

FIG. 4. Transmitting (dark) and nontransmitting (clear) regimes for a plane wave across a nonlinear ($\chi/V=1$) segment ($L=50$) with $0<\epsilon_n<0.3$ (a) and $0<\epsilon_n<0.6$ (b). In (c), an enlargement of the region indicated in (b) is shown.

where by means of the elegant invariant embedding method a power-law decay of transmissivity at large slab sizes was obtained.[9]

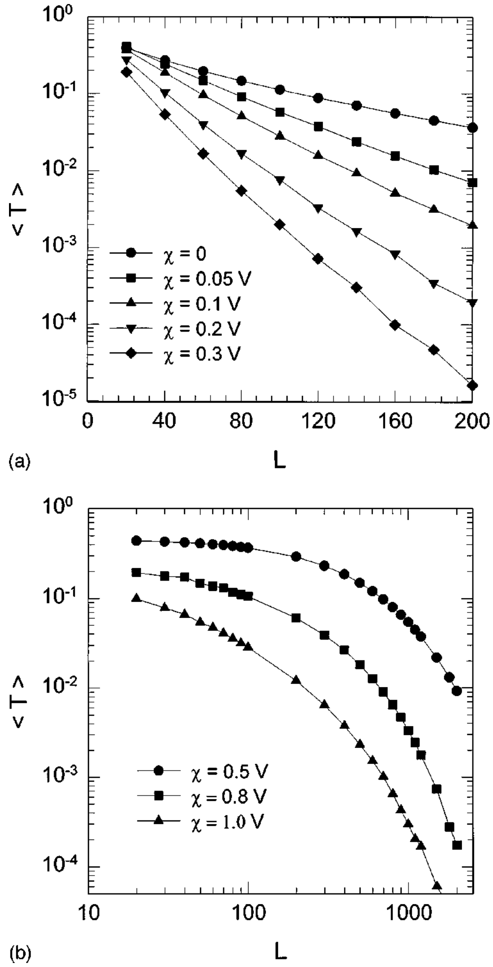

FIG. 5. Disorder- and wave vector-averaged transmissivity of plane waves across a disordered, nonlinear segment, as a function of segment size (number of realizations used: 100). (a) $0<\epsilon_n<1$. (b) Same as in (a), but for $0<\epsilon_n<0.1$ and larger χ and L values. Note that the horizontal scale is now logarithmic.

Discussion. The effect of nonlinearity in a discrete Anderson system is qualitatively different for the localized and extended excitations. In the first case, the presence of nonlinearity delays the onset of localization by generating a subdiffusive propagation for ''intermediate'' times of (at least) $Vt\sim 10^4$, much greater than the one required to generate localization in the absence of nonlinearity. On the contrary, in the second case, the effect of nonlinearity seems to reinforce that of disorder, giving rise to an exponential decrease in transmissivity even stronger than in the pure Anderson case, at least for not very large segments. This qualitative difference is due to the widely different nature of the excitation: In the localized excitation case, the propagation is aided by two factors: an initial, localized (''soliton-like'') state, whose mobility tends to be favored by nonlinearity, and the loss of incoherent random scattering from the random site energies, due to the loss of site superposition. This nonlinearity effect will ultimately disappear due to the spreading of the initial pulse, since the DNLS equation (1) does not really support discrete solitons,[10] and the system will ultimately revert back to an Anderson-like system. The situation for the extended excitation case is different, and can be understood qualitatively by starting with $\chi=0$ and increasing χ in a perturbative manner. For χ strictly zero, the probability profile inside the slab, possesses on average, an exponential envelope $|\phi_n|^2\sim\exp[\alpha(L-n)]$, for $0<n<L$. If we now increase χ from zero, we have, according to Eq. (3) an additional site energy term $\sim-\chi\,\exp[2\alpha(L-n)]$, which quickly supersedes the random site energies ϵ_n, and the transmission problem becomes one of a plane wave going through very high, correlated barriers, the hight of which increases very rapidly with the length of the slab. To aid in visualization, let us replace these exponential barriers with an effective constant-height barrier $E_{\rm eff}$. As is well known, in this case, only plane waves with wave vectors greater than $\arccos[1-(E_{\rm eff}/2V)]$ can propagate through a (long) slab. In our case, $E_{\rm eff}$ will be of the form $-\chi\,\exp(\gamma L)$, implying that, as soon as $\chi\neq 0$, there will be a strong inhibition of transmittance across the slab both as a function of χ and (more strongly) as a function of L. Contrary to the case of the localized excitation, the nonlinear effect does not ''wear out'' in space, since the portion of the wave function inside the slab is unnormalized.

We conclude from the present study that the presence of nonlinearity in a low-dimensional, discrete Anderson system, favors (inhibits) the propagation of initially localized (extended) excitations.

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*Electronic address: mmolina@abello.dic.uchile.cl

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